ADAPTIVE SPECIES

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Acknowledgements

Numerous people contributed directly or indirectly to this thesis. Primarily, I am grateful to all my colleagues of the 5th floor, who welcomed the alien 'Robot-Guy' with open arms and helped me constantly to become an 'Evolution-Guy' in the end. First and foremost I want to thank my advisor, Nico Michiels, for all his support. It has been an honour to be his Ph.D. student. Furthermore, I am especially grateful to Thomas D'Souza and Katja Heubel. I would like to thank Thomas for arousing my interest in the topic of multi-level selection as my initial co-supervisor. To Katja, who became an unofficial co-supervisor at a later stage, I am thankful to her for constantly having been keen to discuss theory and supporting me immensely. A big thank-you goes also to Hanna Kokko from the University of Zürich, who has been so generous to discuss and examine the final version of my thesis.

Furthermore, I am grateful for all my friends outside the lab and for my family. They enriched my non-academic life so enormously, that academic stress became more than bearable. I am especially grateful to Sarah May. While I was writing up my thesis, she was writing her own in cultural studies. I was lucky she invited me to team up with her at the University library. We managed to enter a motivational symbiosis which became invaluable to me. And a lot of fun.

Contents

Introduction

This thesis is an attempt to theoretically investigate the mechanistic pathways of natural selection on the origination and maintenance of a biologically structured world. It therefore connects to one of the most challenging issues in evolutionary biology, which is the synthesis of population-level dynamics (microevolution) with large-scale speciation patterns (macroevolution). While historically biologists mainly tried to examine the upward causation, here I am also interested in the accompanying, downwards directed feedback loop: the influence of macroevolution on organismic traits. This feedback loop is especially interesting if the traits that are affected by its effect, are simultaneously those that caused the loop to start in the beginning: traits that are associated with variations in speciation and extinction rates. Therefore, this thesis revolves around a series of biological questions: What is the nature of species; do they really exist? If they do, can species constitute a unit of selection? Does selection among species affect speciation or extinction rates? Which traits play a major role in causing this variation?

In **chapter 1**, 'On the Origin of Species with Species Selection', I shall argue that an integration of species selection into adaptive speciation theory can help to resolve the reported discrepancy between microevolutionary predictions of trait evolution and macroevolutionary observations from the fossil record. The discussion requires a thorough introduction into the abstract principles of natural selection and into the 'levels-of-selection' question of evolutionary

biology. Further, an overview of the theoretical concepts of speciation in general and adaptive speciation in particular is needed. These will provide the procedural descriptions of the expected feedback from selection on species properties that show correlations to variations in species diversification and extinction rates. I shall conclude with a detailed reflection on the assumed causal relations between identified species traits and proposed mechanisms that drive speciation.

In **chapter 2**, 'Modelling Speciation at Multiple Levels', I formulate the building blocks needed to create a model that combines different approaches to adaptive speciation and species selection processes enabling me to address the questions raised in chapter 1. This chapter first examines the tools traditionally used to model speciation and multi-level selection dynamics and identifies their pros and cons in this context. Both theories have produced successful models that have changed our view on challenging topics such as sympatric speciation or the evolution of altruism. The chapter describes why I think that Agent-Based Modelling (ABM), extended with an explicit representation of multiple levels, promises novel insights on the effects of emergent properties. Finally, I shall develop a prove-of-concept implementation that introduces a hierarchical agent structure with agents which represent ecological cluster of diversifying organisms.

Chapter 3, 'Species Coexistence Promotes Sex with Assortative Mating', combines the theoretical considerations of chapter 1 and chapter 2 on a specific trait that stands out both in its evolutionary consequences and its resistance to generalizing descriptions: sexual reproduction. I shall present a simulation model that explores the evolutionary influence of this trait on interspecific competition and extinction. My results show that assortative mating might play a key role in the answer to the long standing question on the origin and maintenance of sex, as a mechanism that facilitates species coexistence and species diversity.

Chapter 1

On the Origin of Species with Species Selection

INTRODUCTION

One of the big hopes with the development of the Modern Synthesis of evolution was the explanation of macroevolutionary patterns with microevolutionary processes. More than 60 years later, however, we must admit that this goal is more challenging than expected (Mallet 1995). Local biotic interactions failed to demonstrate their prominent role in the generation of large scale temporal and spatial patterns. Examples are the massive diversity difference between temperate zones and the tropics (Mittelbach et al. 2007) or the inconsistencies of the fossil record with macroevolutionary expectations from low-level community processes (Ricklefs 2004; Rabosky 2013). Some biologists even argue that a complete understanding of macroevolution is impossible to achieve within the limits of microevolution (Jablonski 2008a) — and that Darwin was the first to realize this (Reznick and Ricklefs 2009).

The desire for a unifying model resulted in calls for a better integration of the two often independently acting research fields of

evolutionary ecology and palaeontology (Jablonski 2008a; Rabosky 2010). These received a warm welcome (Fritz et al. 2013). Biologists started to reconsider the feedback from speciation and extinction rates on population dynamics with positive results, something which had long been predicted (Ricklefs 1987; Rosenzweig 1995). Multiple studies reveal long-term benefits of short-term detrimental traits (Goldberg et al. 2010; Raffaele and Kamoun 2012; Wright, Kalisz and Slotte 2013), partially due to new statistical methods that enabled to link character evolution with phylogenetic data (Maddison, Midford and Otto 2007; Magnuson-Ford and Otto 2012; Ng and Smith 2014). Furthermore, new models suggest that extinction rates as well as speciation rates are dependent on species-level properties, such as the degree of interspecific competition (Etienne et al. 2012; Rabosky 2013) or species age (Hagen et al. 2015).

These views lead to the conclusion, that selection on aggregate and emergent species-level traits that increase a species net-diversification rate could indeed overwrite organismic selection — a phenomenon termed *species selection*. While the idea of selection at the species-level has a long history (Eldredge and Gould 1972; Stanley 1975), it resulted in a renewed interest to identify those species traits that directly influence speciation and extinction rates and are foci of selection (Jablonski 2008b; Rabosky and McCune 2010). Largely unexplored, however, is how these traits can be incorporated into adaptive speciation theory.

In the following I would like to illustrate that the integration of adaptive processes above the traditional microevolutionary focus (the organismic level) provides conceptual key elements towards a harmonization between ecology, evolution and palaeontology. After introducing hierarchical constructs in evolutionary theory, I shall lay out an extension to adaptive speciation theory with a 'multi-level speciation' perspective.

1.1 HIERARCHICAL PERSPECTIVES OF EVOLUTION

Natural selection is the most fundamental process in evolution. Yet, it is a simple concept. Reproducing individuals with differential reproductive success linked to inheritable variation in traits, 'embody the principle of evolution by natural selection' (Lewontin 1970). With this principle Darwin (1859) provided the ultimate explanation for the origin of the diversity of life we observe in nature. Although the described process can be applied to any unit that fulfils these criteria, the units Darwin had in mind were individuals living in interbreeding populations.

A decade later, however, Darwin (1871) showed that his principles can be transferred to higher units as well. By that time, he was puzzled about the evolution of altruism, a costly behaviour without a directly outweighing benefit. He argued that such an adaptation might be the result of selection at a group- or colony-level, if groups of altruists show a fitness benefit relative to other groups. Despite this interesting insight, it took more than century for people staring to discuss its biological relevance (Wynne-Edwards 1962; Maynard Smith 1964).

At the heart of Darwin's observation lies the fact, that all living things on earth are organized in hierarchical levels. Multicellular organisms for example, the traditional focus of evolutionary biology, are just one level of many. Furthermore, these organisms consist of cells, units at a lower level and also form groups of genetic similarity at a higher level: species. These three factors, the *abstract nature* of evolution, observable *adaptations* that show a benefit for the group at a cost for the individual and the *hierarchical organization* of the biological world constitute the basis of what is known as multi-level selection theory.

Although simple in its essence, multi-level selection gets more complicated if we zoom into its incarnations, which is why I shall introduce them in more detail in the next section. For now it is

sufficient to know that there are two ways selection can be extended to a hierarchical setting. The one I focus on here is species selection, a theory which considers species as entities with their own independent fitness, defined as the net diversification rate (Jablonski 2008a). Although broadly accepted as a plausible macroevolutionary extension to natural selection theory, species selection lacks a thorough integration into speciation theory. While many traits have been identified, that are associated with diversification and extinction differences, the general mechanisms which cause them, are not thoroughly analysed. In the following I shall try to fill this gap.

1.2 TWO TYPES OF MULTI-LEVEL SELECTION

Since concepts require unambiguous terminology, a few terms must be introduced first. As written above, 'hierarchy', the nesting of units inside other units, is one of the central ideas in multi-level selection theory. In the following conceptual layout I shall refer to the abstract lower-level unit as 'particles' and to the abstract higher-level units as 'collectives' in analogy to Okasha (2006) (who reused them from Hamilton (1975) and Kerr and Godfrey-Smith (2002)). I also use them in a strictly relative sense, so that actual manifestations of these two abstractions, e.g. 'gene', 'organism' or 'species', might represent particles at one level and collectives at another.[1]

The reason for preferring 'particle' and 'collective' over the more commonly used terms 'individual' and 'group', is that the latter come with an additional meaning which is better to avoid. While 'individual selectionists' use 'individual' traditionally in the generic 'particle' sense (Hull 1978, 1980), most biologists usually treat it as a synonym for 'individual organism' (Pepper and Herron 2008). Furthermore, 'individual' adds a notion of individuality to the particles, whose criteria are difficult to generalize across the levels (Gould and

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[1] Here I use 'organism' broadly as 'single member of a species'.

Lloyd 1999).[2] The usage of 'groups' shifts the context too close to 'group selection', which is only a small and controversial part of the bigger story as we shall see below.

Another important issue to clarify, is the inherent ambiguity in the concept of multi-level selection (Arnold and Fristrup 1982; Sober 1984; Mayo and Gilinsky 1987; Damuth and Heisler 1988; Okasha 2006). It is caused by the two ways in which selection can be applied to a hierarchical organization. On the one hand, we can split selection into distinct selection pressures acting separately on the particle and collective level while still measuring fitness at the particle level only. The collective fitness is thereby a function (e.g. the average) of the fitness of its constituting particles. On the other hand, we can consider collectives independently evolving units with their own independent fitness definition; the fittest collective leaves the most offspring collectives. Hence, the first decision to make is whether we take collectives as an environmental property of particles or as particles themselves. The commonly used labels for these two distinct meanings were introduced by Damuth and Heisler (1988) who referred to the first approach as multi-level selection 1 (MLS1) and to the second as multi-level selection 2 (MLS2).

In the field of MLS1, two competing theories exist: inclusive fitness and group selection. Both of them try to explain adaptations at the particle-level from combined selection at the particle- and at the collective-level. They differ, however, in their underlying mechanisms. Inclusive fitness theory expresses the idea that the evolution of an altruistic behaviour can be favoured if the benefits are gained by genetically close relatives, especially those of common descent (half or full siblings). It was formulated by Hamilton (1964) who stated that cooperation is selected for if relatedness R is greater than the cost-to-benefit ratio and formalized it into the well known inequality $R > c/b$. With its focus on common descent, inclusive

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[2]For a detailed discourse on this topic I recommend the book *The Evolution of Individuality* by Buss (1987).

fitness theory is also known as kin selection theory. Although inheritance is indeed the most common way for generating similarities, kinship is not necessarily a prerequisite for relatedness as Hamilton (1975) noted later. The only requirement is a 'statistical tendency for the recipients of altruists to be altruists themselves' (Okasha 2006). Group selection, however, does not rely on relatedness to describe an adaptive process. In the 'trait-group' model presented by Wilson (1975), particles undergo a two-step life-cycle. During the first part, particles assort in groups in which they perform a costly interaction. Particles that reside in a group with a high number of altruists, however, benefit from the fitness-affecting interaction of their members. As a result, during the second step of a particle's life-cycle, at which it reproduces, the number of offspring it leaves correlates with the number of altruists in its group of origin.

The biological relevance of kin and group selection has been examined by scientists to some extent very productively — despite heated discussions (Okasha 2006; Leigh 2010; Eldakar and Wilson 2011; Frank 2013). The issues addressed by kin selection and group selection are traditionally behavioural phenomena in social animals such as cooperation, altruism and spite, but also unexpected population genetic observations such as selfish genetic elements or genomic imprinting. Therefore, the focus was mainly on population-level dynamics, rather than on macroevolutionary processes. Although some studies additionally recognized that kin- or group-selected adaptations might influence species richness and extinction risk (Billiard and Lenormand 2005) and that a positive feedback from these effects might be likely (Tsuji 2013), this topic is rarely addressed with MLS1. The reason is, that there seems no obvious link between a species' tendency to diversify and the fitness of its constituting organisms. It implies a second, distinct level of fitness, which is an indicator of MLS2.

1.3   SPECIES SELECTION

The primarily envisioned realization of the MLS2 concept is known as species selection and stems from the idea that species themselves represent not only collectives of organisms but also independently evolving particles due to interspecific competition. A species fitness is hereby defined as its net diversification rate (diversification rate divided by extinction rate). The more offspring species an ancestral species produces that survive to diversify in the future, the higher its fitness relative to a less-diversifying sister species. The idea gets interesting when the trait that explains the fitness differences between sister species is not affected by selection between the organisms within a species. Following this, species selection either opposes or assists organismic selection and might lead to genotypic compositions within a species that are different from what to expect with organismic selection as the sole force. These traits therefore have the potential to aid in understanding macroevolutionary patterns in nature that contradict expectations of what micro-evolution should produce.

The concept of species selection was primarily elaborated in the 1970s through the work of Eldredge and Gould (1972) and Stanley (1975). Their reasoning was that gradual microevolutionary processes are too slow to be accountable for major macroevolutionary events and suggested that selection at the species level could be made responsible instead. Furthermore, it was seen as a logical consequence of the theory of punctuated equilibrium (PE) and 'Wrigth's rule'. PE is an interpretation of fossil record observations, which suggest that species remain in 'stasis' for most of their lifetime and get interrupted by short events of rapid evolution leading to the formation of new species (Sepkoski 2012, provides a good overview on the topic). Wrigth's rule states that these speciation events result in random changes in the species traits (Gould and Eldredge 1977). The combination of these claims, however, challenged the dominant view of the neo-Darwinian synthesis. It therefore provoked serious

criticism (Charlesworth, Lande and Slatkin 1982) and resulted in limited support for the concept over the last decades; even Gould adjusted his opinion multiple times (Lieberman and Vrba 2005). Novel statistical approaches linking character evolution with phylogenetic trees (Maddison, Midford and Otto 2007), led to a returning interest in PE (Magnuson-Ford and Otto 2012). It furthermore resulted in attempts to reformulate the PE hypothesis, with the argument, that the theory might actually be 'tangle of ... unnecessarily conflated questions' about speciation (Pennell, Harmon and Uyeda 2014). Independent of the mixed view on PE, however, today it seems as if there is a broad agreement on the plausibility of species selection and its contribution to variations in species richness (Jablonski 2008b; Rabosky and McCune 2010; Goldberg et al. 2010; Simpson 2013), but disagreement over its empirical importance.

Broad sense species selection can be categorized into two different subclasses according to the type of the trait that is affected by it (Jablonski 2008b). Traits can either be an *aggregate* of a character at the organismic level, such as body size or the degree of ecological specialization, and influence speciation as a side effect. Vrba (1984) named this 'effect macroevolution'. Alternatively, the traits can identify an *emergent* property, such as population size, which cannot be described as an organismic feature. If an emergent trait is the trait under selection, species selection is refined as 'strict-sense' species selection (ibid.). Although this distinction is not important to classify 'broad-sense' species selection as a multi-level selection setting, Jablonski (2008b) points out that it is nevertheless necessary if we move from pattern to process. Then, the hierarchical level of the target of selection becomes a key consideration to understand causal relations. While selection for aggregate traits might coincident with an increase in organismic fitness and diversification as a side product, emergent traits cannot affect organismal fitness directly.

For this reason, a thorough analysis of species traits and species selection is essential to better understand the mechanisms that drive macroevolution. Primarily, a disentanglement of their influence on

speciation and extinction would be a huge step towards this goal. While for phylogenies of extant taxa, tools such as the binary-state speciation-extinction model (BiSSE) developed by Maddison, Midford and Otto (2007) are able to generate good estimates of such effects, the actual causal relations stay hidden. For most cases of species selection it is unknown whether differences in diversification or extinction rates generate the differences in fitness (Rabosky and McCune 2010). In the following I shall therefore try to interlink speciation with selection on species traits as processes rather than patterns. Assistance towards this goal comes from the recently increased interest on adaptive speciation, which generated novel theories about the underlying mechanisms.

1.4   SPECIES SELECTION AND THE NATURE OF SPECIES

As a starting point, I shall examine the primary prerequisite for selection among species, namely the assumption that species represent discrete entities. Although most biologists agree that nature is discontinuous, there is little agreement on which concept explains this observation best (Hull 1997). Wilkins (2010) counted 26 species concepts in 2010 — some of them competing, some combinations of others (cf. Coyne and Orr 2004). Although several attempts have been made to create a unifying species concept (Hausdorf 2011), still no universally applicable concept of what a species actually is exists (Clarke and Okasha 2013). Nevertheless, the plethora of concepts and the vast amount of research spent on it, indicate that a single species concept is a desirable goal. More and more biologists, however, see this as wishful thinking. Hey et al. (2003) argued, species are better seen as hypotheses than facts and that biologists have to accept the uncertainty which is inherent to whatever definition.

One reason that the 'species problem' has been such a long-standing issue, is that it primarily stems from a semantic ambiguity rather than from a theoretic misconception. As Hey et al. (ibid.,

p.599) pointed out, the term species is used with different meanings: it can refer to the name of a taxonomic rank, a particular taxon of that rank (e.g. the species taxon *Homo sapiens*) or an evolving group of organisms. This confusion stems from the fact that different biologists use species concepts for different purposes (Coyne and Orr 2004):

> '[It] 1. helps us classify them in a systematic manner; 2. corresponds to the discrete entities that we see in nature; 3. helps us to understand how discrete entities arise in nature; 4. represents the evolutionary history of organisms; and 5. applies to the largest possible number of organisms.'

The necessary question that follows is about the consequences of a vague species definition. Does the above imply, that everything that seems to depend on a universal species concept is predestined to fail? Definitely not. For now, accepting the fuzzy nature of species seems to be the most productive attitude. As Brookfield (2002) pointed out, at the heart of the species problem lies the fact that it cannot be resolved with normal scientific methods. According to him, people should simply choose their favourite and 'get on with the science'. Rather than trying to resolve the issue, I consider the 'fuzzy' view sufficient for the subsequent incorporation of species selection into the speciation process. The only requirement is to accept species as particles and not just as collectives, which connects to the 'individuality thesis' of Ghiselin (1974) and Hull (1978). For the question of how they originate, however, I shall use a pluralistic approach, as we shall see in the following.

As a last thought on the theory of species as a discrete unit, species selection can benefit from the idea to use species in a rank-free manner as proposed by Okasha (2011). According to the authors, the question whether something counts as a species, should be seen as purely relative. As a result, the definition of species depends on

the context, the organism in question, making absolute assignments obsolete. In this conception, 'species' has no explicit meaning in the ecological hierarchy and therefore does not require a common set of attributes. The same holds for the definition of 'organism' — a challenging question in itself (Buss 1987; Pepper and Herron 2008; Folse and Roughgarden 2010; Clarke 2011; Clarke and Okasha 2013).

The most important question for species selection is to which extend the non-random generation of child species and the evolution of prevention strategies against extinction can be adaptive. Therefore, the theory of species selection is primarily linked to the concept of speciation. From an evolutionary perspective, all speciation processes can be partitioned into two phases. In the first phase, the organisms split up into two populations up to a point when interactions (both competition and cooperation, e.g. mating) between organisms of different populations is lower than of organisms within the same. Depending on the situation, this might be the result of geographic processes or intra-specific competition. The resultant isolation is the prerequisite for the second phase, in which theses isolated populations can start to differentiate genetically. Speciation is completed when this genetic divergence results in stable coexistence on secondary contact.

Most evolutionary biologists therefore favour species concepts that include a description of isolation processes. The most advocated form to study speciation is to focus on the establishment of reproductive isolation, as first envisioned by Dobzhansky (1937) and Mayr (1942) in their Biological Species Concept (BSC). According to them, species can be defined as 'groups of interbreeding natural populations that are reproductively isolated from other such groups' (Coyne and Orr 2004). The reproductive isolation mechanisms in the BSC can be of several kinds. Indeed, there are so many that Kirkpatrick and Ravigné (2002) argued, that biologists have 'balkanized the subject of speciation' with a wealth of proposals to very specific scenarios. This shows, that the BSC has both a wide acceptance and

probably not fewer problems that other concepts.

Taking the reproductive isolation mechanisms as the primary force driving the origin of new species, the question can be refined to the adaptive potential of these mechanisms, i.e. to which extend it is driven by natural, sexual or — the major focus here — species selection. One of the classical speciation process classifications is the spatial context of the diverging populations. Biologists traditionally distinguish between allopatry, parapatry and sympatry, although this simplicity does not capture the true geographic complexity (Butlin, Galindo and Grahame 2008; Butlin et al. 2012). The most fundamental question, however, that stems from this approach, is about the necessity of geographical heterogeneity to prevent gene flow. If isolation requires geographic barriers, then any modification of speciation rates through selection is impossible to achieve. Therefore, species selection, which implies competition, can only be effective if species coexist in space (and time). Hence, the possibility of sympatric speciation is a prerequisite for the plausibility of species selection. Although still controversial, a number of recent studies indeed show that speciation in the presence of gene flow is both theoretically (Dieckmann and Doebeli 1999; Weissing, Edelaar and Van Doorn 2011) and empirically (Papadopulos et al. 2011; Hadid et al. 2013, 2014) feasible.

1.5   SPECIES ADAPTATIONS AND ADAPTIVE SPECIATION

The possible pathways leading to adaptive modifications of sympatric speciation are diverse, as illustrated in figure 1.1, which is a modified version of a diagram created by Weissing, Edelaar and Van Doorn (2011). With their 'schematic classification of speciation models', the authors reviewed how the three major classes — classical models, sexual models and ecological models — each offer their own set of requirements for effective speciation. Their aim, as is mine, is to build an integrative view of the link between micro- and macroevolution.

Their focus, however, was limited on the adaptivity of speciation by natural or sexual selection. What the authors did not integrate, is the effect of higher-level selection processes. Here, I shall try to extend the causality chain and describe the processes that may enable species selection to affect the speciation process itself.

In general, species selection was defined as a process that favours any trait that increases speciation rate or reduces extinction rate. Although these rates are ultimately expressing the divergence and death of organisms, the traits must not necessarily be organismic. In the following we shall see that species traits, aggregate or emergent, can play an important role too as they affect the context in which speciation happens.[3] While emergent traits are commonly accepted to influence speciation rates, attributing the same influence to aggregate traits was contested in the past (Vrba 1984). In a more recent publication, however, Rabosky and McCune (2010) argue that aggregate traits that show the same effect on diversification do exists, for example floral symmetry (Sargent 2004). A prerequisite for any species trait to be an effective component of species selection is the heritability of that trait. While relatively uncontroversial for most aggregate traits, its presence in emergent species traits constitutes a tough challenge to prove (Jablonski 2008b). While some indications exist for the heritability of geographic range size (Jablonski 1987; Waldron 2007), this is a largely unexplored topic with immense implications for the theory of species selection.

One possible path to increased speciation rates can result from aggregate species traits that have a positive effect on disruptive natural selection (arrow M1[b] in Fig. 1.1). Disruptive selection implies that common phenotypes have a lower fitness than rare phenotypes. One of the many outcomes of this frequency dependent selection is sympatric speciation (Coyne and Orr 2004; Dieckmann et al. 2004). Therefore, traits that are both subject to divergent selection

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[3]A comprehensive list of proposed aggregate and emergent species traits has been collected by Jablonski (2008b).
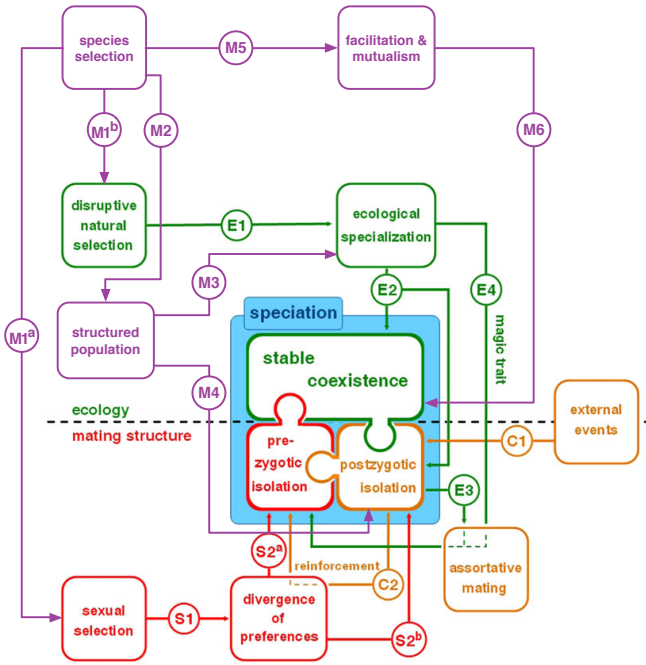
Figure 1.1 Schematic classification of speciation models, modified after Weissing, Edelaar and Van Doorn (2011). The figure summarizes the different pathways leading to the two requirements for (sexual) speciation: Reproductive isolation (pre- and postzygotic) and stable ecologic coexistence. This version shows how I envision species selection (purple) integrates into the three major classes of speciation models: classical models (orange), sexual models (red) and ecological models (green). Species selection is expected to increase frequencies of traits that support sexual selection (M1[a]) or natural selection (M1[b]) and therefore create new species as a side product. Further, species-traits which provide a context favourable for speciation events should be selected for as well. An increased population structure (M2) is associated with ecological specialization (M3) or postzygotic isolation (M4). Positive species interactions, in form of mutualism and facilitation, aid species coexistence (M5, M6).

and likely to cause the population to split into separate species — rather than causing other outcomes (Rueffler et al. 2006) — should be selected for at the species level. Ecological specialization is the prime example of such a trait, which facilitates diversification by increasing ecological opportunities and limiting gene flow (Schluter 2000; Rundle and Nosil 2005). Since adaptive speciation in sexual populations requires both ecologic diversification and a divergence of mating preferences (Weissing, Edelaar and Van Doorn 2011), further good candidate traits of such kind are 'magic traits'. These are defined as traits that are subject to local adaptation and simultaneously contribute to non-random mating, such as body size, beak morphology or colour-pattern (Servedio et al. 2011; Thibert-Plante and Gavrilets 2013).

For many of these aggregate traits it is however unclear to which extend their evolution can be attributed to species selection, as they might simultaneously increase organismic fitness. An example for an aggregate trait that is not associated with a direct fitness benefit at the organismic level is sexual reproduction (Okasha 2006). Nevertheless, sex is the prerequisite for all sexual isolation mechanisms (arrow M1[a] in Fig. 1.1), whether pre- or postzygotic, and therefore creates a beneficial context for 'by-product speciation' (Schluter 2001).

Environments favourable for speciation mechanisms are also influenced by emergent species traits. Especially population structure traits are associated with ecologic specialization and postzygotic isolation (arrow M2 in Fig. 1.1). Range fragmentation for example was found to be positively correlated to species richness in birds (Owens, Bennett and Harvey 1999). While the authors did not discuss the universality of their finding, we can speculate that a tendency to form metapopulations generally contributes to postzygotic isolation, as external events do in classic speciation models (arrows M4 and C1 in Fig. 1.1). Ecological specialization often correlates with spatial population properties such as geographic range, density and size (Futuyma and Moreno 1988; Brown 1995). While the causal relation is often viewed as originating from specialization, I

see no constraint to the reverse, that for example smaller geographic ranges can result in higher degrees of specialization (arrow M3 in Fig. 1.1).

Not only isolation mechanisms can be the product of species selection, stable coexistence of species is also likely to be assisted by this selective force. This can happen either through indirect assistance of ecological specialization as described above (cf. arrows M3 and E1 in Fig. 1.1), or through mechanisms that counteract interspecific competition. One such example are positive species interactions, known as mutualism and facilitation (arrows M5 and M6 in Fig. 1.1). Although a topic which was relatively ignored for a long time (Bruno, Stachowicz and Bertness 2003), positive species interactions recently received increased attention in the scientific community. Support for this idea comes especially from plant ecologists (Callaway 2007; Brooker et al. 2008), some of which also recognize its potential for driving higher-level selection processes (McIntire and Fajardo 2011). Although much of the current research is at an early stage (Bronstein 2009), some researchers argue that mutualistic species interactions do not only have the possibility to extend realized ecological niches but also decrease the likelihood of competitive exclusion (Bruno, Stachowicz and Bertness 2003).

1.6   DIVERSIFICATION IN SEXUALS AND ASEXUALS

In the previous sections we showed that one specific trait, sexual reproduction, plays a prominent role in speciation theory — especially in the BSC. A substantial part of the earth's biological diversity, however, consists of organisms that reproduce only asexually (Vrijenhoek 1998). Therefore, one challenge towards a more universal species concept is a definition of species independent of their reproductive mode. By using reproductive isolation as a fundamental characteristic of species, as the BSC does, every asexual organism would in fact constitute a species of its own, which is neither intuitive nor realistic. It has been theorized, that sexuality is not a prerequisite for

organisms to diversify into genetic and morphological entities (Barraclough, Birky and Burt 2003). Furthermore, models have been proposed to identify species in populations of asexual and clonal organisms (Birky et al. 2010), with successful application to bdelloid rotifers (Birky et al. 2005).

Given that speciation in asexual organisms is theoretically at least as likely as it is in sexuals, what are the implications of the reproductive mode for species selection? Do we expect a difference in speciation and extinction rates ? And if so, why? Do asexual species show the same amount of species-level traits, especially emergent traits, that affect their speciation rate? Does the strength of species selection differ with the mode of reproduction? None of these questions has been satisfactorily answered yet. Nevertheless, the common prediction is that the genetic properties of sexual reproduction, in comparison to asexual reproduction, leads to a higher diversity between organisms. This potentially leads to more speciation events and therefore to a fitness benefit at the species level. Based on this causality chain, many biologists consider the evolution of sex to be the product of species-level selection for the proposed higher net-diversification rate of sexual species (Nunney 1989; Gouyon 1999; Mallet 2010) in harmony with the short term benefit of recombination (Weismann 1889; but see Otto 2009) which enables rapid adaptive responses by populations.

Although the diversity benefits of sexuality are rarely questioned, a long term prediction about the effects of sexual recombination on species diversity is, however, not as straight-forward as is often assumed. On the one hand, as already indicated above, sex allows for a higher evolutionary rate (Kimura and Ohta 1971; Rice and Chippindale 2001; Butlin 2002). Therefore, sexual species should be less prone to an accumulation of detrimental mutations (Muller 1964, 'Muller's Ratchet') and are expected to show a higher ability to fix advantageous mutations (Orr 2000) than asexual species with otherwise identical properties. On the other hand, however, time sex can also slow down evolution through constraints in genomic and

epigenetic variation (Kondrashov and Kondrashov 2001; Gorelick and Heng 2010). In a recent study Melián et al. (2012) explored these antagonistic effects of recombination and presented a model which showed that although sexual species are created in higher number, theses species are at the same time less abundant and therefore affected by a higher extinction probability. In summary, the current view on the role of sex for diversification and extinction leaves a blurry image. More research is definitely required to evaluate its importance for speciation and, in reverse, the importance of speciation for the evolution of sex.

1.7   CONCLUSION

Although Darwin's *On the Origin of Species* constitutes the foundation of all evolutionary research, the explanation for why species exist and which processes explain their origin, is far from understood. While the effects of (organismic) natural and sexual selection have been and still are under extensive scrutiny, the role of multi-level selection is, however, still widely ignored. I have argued, that selection among species is at least in theory a non-neglectable contributor to species diversity. Many organisms carry traits that are hard to explain solely on the basis of organismic selection or that only exists due to species formation as emergent features. Some of these properties have been proposed to be adaptively linked to speciation and extinction rates, but evidence is based mainly on statistical analyses of the fossil record. A better understanding of causal relations is sorely needed. Accepting species adaptations not only as a correlating factor in macroevolutionary patterns, but also as an active part in the speciation processes of organismic communities could prove to be a fruitful addition to models of adaptive speciation. This might help to understand the factors that regulate species richness across scales.

Chapter 2

Modelling Speciation at Multiple Levels

'our truth is the intersection of independent lies'

R. Levins, Strategy of Model Building in Population Biology

INTRODUCTION

Models provide representations of the world (Hughes 1997). In science we use them to reduce the world's complexity to a few ingredients we consider essential and hope to be rewarded with a better understanding of the world it represents. Although we can rarely be certain that we didn't miss something important during the construction process and that the conclusions we have drawn are true, models simply provide a more convenient, more cost-effective, better manageable substitute. This is true especially for very complex processes. In evolution, both speciation and multi-level selection fall into this category. Both theories have a long modelling history, but combining both processes into a single model has rarely been attemp-

ted. This leaves a missed opportunity for both fields, as adaptive speciation and species selection are strongly connected mechanisms.

I showed in chapter 1 that an exploration of how multi-level selection shapes species adaptations is important to fully understand the evolutionary dynamics leading to speciation events. A major challenge is that the assumed causal relationships are hard to verify. From the patterns (i.e. the product) alone, species selection is difficult to distinguish from alternative explanations, especially with empirical methods. The same is true for its outcome, adaptive speciation. Because of this, researchers have approached the two fields mainly from a theoretical perspective with the help of models. While these models were able to show the plausibility of either processes, a method which combines organismic dynamics leading to speciation and species-trait adaptations due to species selection, to my best knowledge, has not yet been reported. In this chapter, I shall first give an overview of the different methods used in both fields. Then, I shall show that the mathematical framework of 'adaptive dynamics', implemented in an agent-based model with its emergent multi-level properties, is ideal to investigate interactions between species-level adaptation and population diversification.

2.1   MODELS OF SPECIES SELECTION

Various types of multi-level selection models have been developed in the past: Statistical models, analytical models and numerical models. Probably the most important formalization was made by Price (1972) with an analytical model of fitness-character covariance over time. Although his equation, known as the 'Price Equation', was originally developed to formalize evolutionary trait changes within populations at a single level, it became popular among theoreticians interested in multi-level selection in the context of social adaptations (MLS1) at the end of the last millennium because the equation conveniently allowed a decomposition of the covariance across multiple levels (Hamilton 1975; Wilson 1975). Although a claim exist

that the Price Equation is neither a proper tool for doing statistics, nor for making models or deriving predictions (Veelen 2005, 2009), in practice, however, it is commonly used as a tool to describe organismic adaptations such as social behaviour with a MLS1 fitness decomposition in group-structured populations (Gardner and West 2006; Gardner and Grafen 2009). A modification of the Price equation which to deal with species selection dynamics (MLS2) is straightforward (Okasha 2006). To observe the change of a collective character, one simply defines it as the covariance of such a character with the collective's fitness. One problem is, however, that within-collective selection is not explicitly representable in the equation (although it can be described separately by a second Price equation), is problematic if the collective level character is not affecting particle level fitness, or vice versa. It is probably because of this missing feature that modelling approaches of the MLS2 type using the Price Equation are rare (Simpson 2013).[1]

Statistical tools that deal with MLS2 cases are for example the Binary-State Speciation and Extinction (BiSSE) model (Maddison, Midford and Otto 2007) and its extensions (a good overview is given by Ng and Smith 2014). BiSSE is a more recently developed likelihood method which attributes diversification and extinction probabilities to species depending on the presence or absence of certain biological characters. It can be used to test lineage-level consequences of species-level traits such as the mode of reproduction using phylogenetic data. Goldberg et al. (2010) found that species in the family of nightshade plants maintain self-incompatibility in favour of a higher net diversification rate, and claimed that species-level selection for obligate outcrossing is thereby offsetting organismic selection for self-fertilization. Johnson et al. (2011) observed a correlation between the loss of sexuality and increased diversification in evening primroses. BiSSE has the potential to

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[1]The same is true for the rivalling methods of Contextual Analysis and the Neighbour Approach. See Okasha (2004) for a description of these approaches.

verify a number of proposed effects of species traits on diversification and extinction. Nevertheless, although it offers a good way to show a statistical relationship between a character and its effect, it has its limitations. The number of speciation and extinction events in a phylogeny, for example, is based on the assumption of a specific species concept (Ezard et al. 2012). Furthermore, it is hard to pinpoint causal relations with a statistical approach, as it cannot deal with cross-level byproducts which are inherent to character-fitness covariations in a multi-level setting (Okasha 2006).

Simulations constitute another approach to study species selection. Reported models are primarily representations of a lineage-selection strategy, which utilizes a macroevolutionary birth-death process (Nee 2006) in combination with an assumed covariance between a species-character and its effect on speciation and extinction. One of the earliest studies that simulated such a model, aimed at explaining the success of sexual reproduction by species-level selection (Nunney 1989).[2] It was based on the following assumption: Sex is initially disadvantageous because of a two-fold reproductive loss, but sexual species are both less likely to go extinct and have speciation rate that is equal to the speciation rate of asexuals or higher. The study reported that this higher-level advantage is indeed able to maintain sexual reproduction if the transition (due to mutation) between sexuality and asexuality is sufficiently rare. In a follow-up study, Vienne, Giraud and Gouyon (2013) added ecological competition to the model, guided by the assumption of higher extinction rates in species that occupy niches close to other species. They combined this with the assumption that sexual species, because of recombination, leave child species with trait values that are further apart from their parent species. Both simulations, and models of this kind in general, share the same problem I already

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[2]Although Nunney titled his article 'The Maintenance of Sex by Group Selection', in the modern terminology which I introduced in chapter 1, he was actually referring to species selection instead of group selection.

mentioned for statistical models: Assuming explicit diversification and extinction probabilities ignores the fact, that the causal processes might be much more complicated. Furthermore, classic assumptions about character/diversification covariances, especially for asexual reproduction (Barraclough, Birky and Burt 2003), might simply be false.

2.2   MODELS OF ADAPTIVE SPECIATION

Understanding the evolution of species divergence and splitting in sympatry (without geographical isolation) is seen as one of the 'holy grails' of speciation research because it would prove that speciation is to some extent an adaptive mechanism — and eventually link microevolutionary processes with macroevolutionary patterns (Hansen and Martins 1996; Uyeda et al. 2011). Although only empirical studies are able to ultimately prove its biological plausibility, they are notoriously difficult to conduct and, as a result, uncontested cases are scarce (Coyne and Orr 2004; Coyne 2011). Therefore, an unsurprisingly vast amount of theoretical studies on speciation with gene flow between diverging populations has been developed in the past (Gavrilets 2003), with a significant increase in the past 10 years. These show that sympatric speciation is possible under biologically reasonable conditions (Gavrilets 2014).

From the conceptual point of view, existing speciation models investigated all different aspects underlying the speciation process (Kirkpatrick and Ravigné 2002). They can be broadly categorized into two groups with complementary trade-offs, as Weissing, Edelaar and Van Doorn (2011) realized. On the one hand, sophisticated genetic models with simplistic assumptions about selection and mating. On the other hand, models based on population dynamical considerations with emergent fitness, which, however, simplify the underlying genetics down to unrealistic levels. Not surprisingly, the authors predicted that more robust insights are to be expected from a pluralistic approach. The most insightful contributions to

sympatric speciation in recent years, however, have come from the population dynamics approach, especially with the introduction of a new mathematical tool termed 'Adaptive Dynamics' (AD).

AD is a mathematical framework to describe the changes of a trait distribution over time in a population of interacting organisms (Metz et al. 1996; Dieckmann and Law 1996). It was developed to observe frequency- and density-dependent changes of phenotypes within a population. Since then, it has been successfully used to describe various types of evolutionary dynamics. Adaptive diversification, of which sympatric speciation is one possibly outcome (Rueffler et al. 2006), is, however, probably its most prominent research application (Dieckmann and Doebeli 1999; Doebeli and Dieckmann 2000, 2003; Doebeli 2005, 2011). AD models were able to demonstrate that frequency-dependent ecological interactions can easily provide the selective conditions for speciation with gene flow. The most simple models use a continuous quantitative trait associated with an ecological resource exploitation in an environment with a limited capacity. Through frequency-dependent interactions between any consumer and its environment (the environment's capacity and plus other consumers) it produces evolutionary branching points at which the population splits into distinct clusters, i.e. species.

Despite being a powerful analytical tool, results generated by AD should be taken with caution. AD is confronted with a good amount of critique for its genetic assumptions (Gourbiere and Mallet 2005; Bürger, Schneider and Willensdorfer 2006, but see above for the pluralism counter-argument towards speciation models), its implementation of assortative mating (Kopp and Hermisson 2008) or the assumed distribution of resources (Polechová and Barton 2005). Indeed, evolutionary branching was found to be less likely than the first implementations suggested. Nevertheless, the theoretic plausibility of adaptive speciation due to frequency-dependent selection is far from dismissed (Weissing, Edelaar and Van Doorn 2011), and AD has proven itself as one of the most promising approaches in this field.

2.3   THE SYNTHESIS: MULTI-LEVEL DYNAMICS IN AGENT-BASED MODELS

In chapter 1 I stated that a previously neglected but necessary extension to the theory of adaptive speciation is an incorporation of species selection. I developed the idea that there are several ways how selection at the species level can influence the three different speciation requirements listed above. For this task, I see AD as a promising approach. As an analytical framework it allows developing generalizable conclusions (Gavrilets 2003, 2014) and has successfully been used as such to gain novel insights into adaptive speciation, as I just reviewed above. Furthermore, a feature of AD is the possibility to implement the underlying dynamics using agent-based modelling (ABM) of a stochastic birth-death process (Dieckmann and Law 1996).[3] While this transformation increases the specificity of the results, it allows us to add a feature which is required to incorporate species selection: The ability to observe the emergence of system-level properties from the adaptive behaviour of its constituting individuals (Railsback 2001; Strand, Huse and Giske 2002).[4]

ABM is a mature bottom-up simulation modelling approach, where a system is constructed from multiple, interacting entities, called agents. The agents are constructed by assignment of context dependent behaviour strategies, from which the system dynamics emerge. Railsback and Grimm (2011) summarize, that the often criticized property of computer simulations in general, the limitation of mathematical tractability, is also a benefit, as it allows addressing problems that require less simplified models. As the main benefit of ABM in particular, they name its usefulness for problems of emer-

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[3]'Agent-based modelling' and 'individual-based modelling' are synonymous terms. While the latter is used more common in ecology, the first is used more broadly across fields and therefore preferred.

[4]For the following I prefer the term 'individual' instead of 'particle', contrary to chapter 1, as it is less prone to confusion in the context of ABM but more commonly used than the latter. Nevertheless, I shall use it with the same meaning.

gence because of their *across-level* nature. Furthermore, they highlight that a standard protocol has been developed to describe ABMs in publications with the aim to make these models understandable and reproducible (Grimm et al. 2006, 2010), which addresses some proclaimed concerns about using simulations for research (Gavrilets 2003). These properties make ABM well-suited to complement analytical studies of species selection and adaptive diversification, which are prototypic examples of an interaction between two adjacent hierarchical levels.

Traditionally, ABM is used to 'observe' the emergence of system-level properties. While a simple observation is sufficient in most cases, an explicit feedback from these properties to the individual agents is easily implemented as well. Including the group level as a possible effector on the lower-level dynamics has gained increasing interest in recent years under the label 'Multi-Level Agent-Based Modelling' (ML-ABM) and has been applied to various fields, including social science, physics, medicine and ecology (Morvan 2012). This also applies to evolutionary dynamics in a hierarchical setting, especially in the context of adaptive dynamics. For example, if we encapsulate the emerging trait clusters as agents, we are able to add higher-level selection on cluster properties to the system, i.e. species selection.

Modelling with the Greyfish Simulation Framework

The greyfish simulation framework, in the following simply referred to as greyfish, is an ABM tool I implemented in the Java programming language (See appendix section 2.A for a detailed description). One of the main design goals of greyfish was a modular architecture to maximize application flexibility. Furthermore, a strict separation of the core from model specific development allows a rapid transformation of novel ideas into algorithm.

In greyfish, each agent is equipped with a set of *properties* and *actions*. They define in combination the agents context-dependent behaviour. Properties can either be static and hold assigned values, or dynamic and reflect different time specific states, including the agent's environment. The actions trigger events which can modify these properties. They can be linked to the state of any agent that is currently active in order to make the action conditional. An *environment* connects all the agents; it schedules the execution of their tasks and serves as an interface for the interactions between them. The central control unit is an *experiment*, which creates the agents, places them into the environment, and defines the overall simulation structure.

Evolutionary dynamics are easily introduced into a simulation by defining a 'birth' action that adds new offspring-agents to the environment and a 'death' action that removes an agent. To generate variation in the birth-death process, the execution of at least one of the two actions must be made conditional on a 'trait'-property, which defines a mutation and recombination function, in addition to the actual trait value itself. These traits can range from a simple decimal number to some complex genetic architecture.

In addition, greyfish provides the necessary structures to model agents on multiple hierarchical levels and add an interaction between these levels. This feature is not exclusive to greyfish. Other recent frameworks have introduced similar features and termed the higher-level agents 'macro-agents' (ibid.). Whereas these frameworks fo-
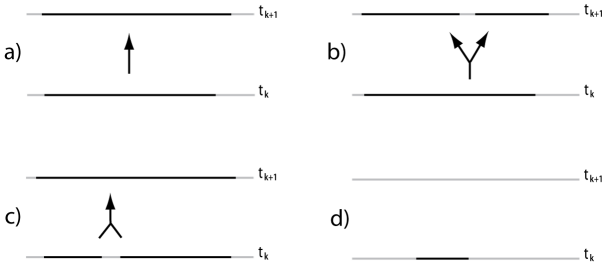
Figure 2.1 The four possible transitions of clusters with one or more individuals, represented as a one-dimensional quantitative trait range, between any two steps t_k and t_{k+1} in a simulation. A cluster can a) remain in a stable state (except for updated boundaries), b) split into multiple offspring clusters, c) merge with one or more sister clusters or d) stop to exist. In macro-evolutionary terms a) can be seen as stasis, b) as the splitting of lineages, c) as hybrid speciation including 'despeciation' (cf. Mallet 2007) and d) as extinction.

cused on predefined spatial hierarchies, in greyfish it is also able to define macro-agents which can represent *emergent* interaction structures of lower-level agents. In the following I shall exemplify this, by showing how to add such macro-agents on top of a simple model of asexual diversification. Here, the macro-agents represent clusters of ecologically competing organismic agents, based on a similarity measure between different values of a single continuous trait. Therefore, in contrast to hierarchies defined by explicit environmental (e.g. spatial) factors, the group boundaries are dynamic and must be continuously updated.

A Proof-Of-Concept Implementation

In the following, I shall present a simulation of AD including 'cluster' macro-agents, which demonstrates the basic principle of how to model emergent individual units. Such an agent possesses (1) a property that holds the state of the represented cluster and (2) an
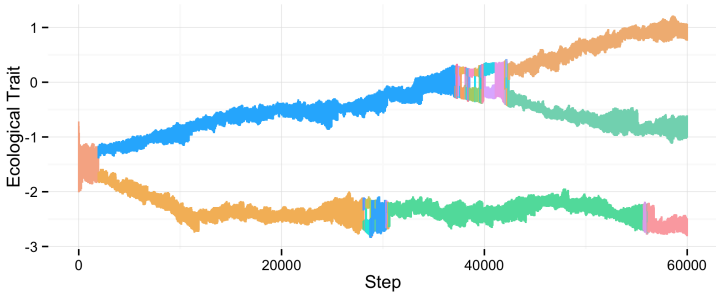
action that compares this state from step t_k to the set of clusters newly identified in step t_{k+1}. This results in the four possible transition events illustrated in figure 2.1: Stasis, extinction, split and fusion. The action will respond accordingly by (a) updating the value of the property if the cluster remained static (only the boundaries changed); (b) with the production of offspring agents followed by its own removal in case of a split into multiple new clusters or (c) a fusion with sister clusters; the last alternative (d) is its immediate removal in case the cluster disintegrated.[5]

This 'cluster' agent strategy should work with any clustering algorithm at hand. For the case of the one-dimensional continuous value that I shall use in this demonstration model, I evaluated and compared different algorithms and chose DBSCAN (Ester et al. 1996) for its good performance (time complexity is $\mathcal{O}(n \log n)$ if an indexing structure is used and for not requiring an a priori assumption about the number of clusters to search for.[6]) DBSCAN stands for density-based spatial clustering algorithm with noise. It groups spatial objects based on their reachability distance and classifies them according to the group size either as a true cluster or noise (For applications where noise is not desirable, as in our case, these elements can be treated as true clusters as well).
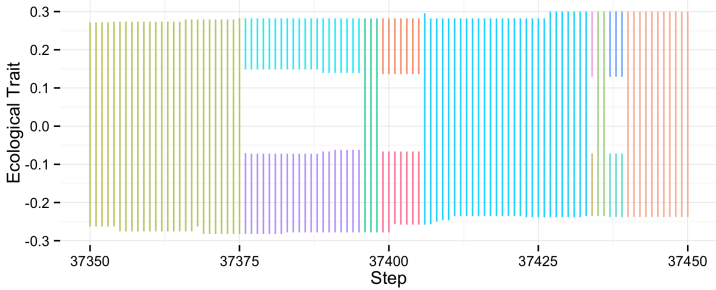
For my prove-of-concept experiment I modified a simple AD model of asexual diversification due to ecological resource competition (see appendix 2.A). Frequency dependent interactions are determined by a single continuously varying trait inside an environment defined by a quartic function $K(x) = 150 \exp(-\frac{1}{2}(4.0x)^4)$. The competition between individuals, which affects their survival, is introduced by a Gaussian function of their ecological similarity ($\sigma_\alpha = 0.75$). The birth rate of each individual is fixed at 0.04. Offspring receive a trait value drawn from a normal distribution centred

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[5]This resembles the Hennigian view on the lifetime of species (Meier and Willmann 2000), which assumes the extinction of the ancestral species at bifurcation.

[6]Indexing structures are data structures that allow efficient range or nearest neighbour queries.

(a) Full View

(b) Detailed View

Figure 2.2 Evolution of 'cluster' agents in a model of asexual ecological diversification. Each agent is represented by a distinct colour (colour assignments differ between the two plots). Panel (a) shows the full time span of the experiment with stasis as the predominant state interrupted by two main diversification events with multiple split/fusion events. Panel (b) zooms into a small frame of the upper right diversification event and shows a fast reproduction cycle due to multiple splits and fusions of clusters.

at the value of their parents ($\sigma_\mu = 0.01$). DBSCAN was parameterized with a reachability threshold of 0.2 and a reachability minimum no. of points equal to 5. Initially, I inserted 500 organismic agents with their ecological trait values drawn from a normal distribution with mean -1.5 and standard deviation 0.2 and a single 'cluster' agent containing all organismic agents.

The evolution of the 'cluster' agents during the following 60 000 steps of a single run is visualized in figure 2.2 with distinct colours assigned to different agents. From a simple visual inspection we can see that, except for extinction, all possible transitions occur in the simulation. The full view (Fig. 2.2(a)) reveals that stasis is the predominant state, interrupted by four diversification phases of which two resulted in two distinct descendants, and two resulted in a single descendant with a similar trait range. The detailed view (Fig. 2.2(b)), however, shows that a bifurcation is preceded by multiple reversed diversification attempts. In combination, these results suggest that a persistent split of a lineage occurs rarely while clusters are constantly splitting and fusing at certain phases. Thereby, they describe a pattern which resembles the speciation dynamics envisioned by the 'ephemeral speciation model' (Rosenblum et al. 2012).

As I already mentioned, the described simulation serves as a prove-of-concept implementation for multi-level selection models. Although it shows how emergent groups can be represented, it lacks the final step to complete a multi-level selection scenario: selection at the cluster level. This would additionally require the introduction of a birth rate in the 'cluster' agent dependent on the cluster history (e.g. stability) and a costly trait in the lower-level agent with an influence on the diversification tendency. Biological relevant traits of such type can be found in the literature, especially in models of adaptive dynamics. For example, Doebeli (2011) used meta-populations to incorporate the evolution of dispersal rates, a trait which has repeatedly been identified to increase diversification (Phillimore et al. 2006).

2.4   CONCLUSION

In this chapter I have reviewed existing modelling approaches addressing adaptive speciation or species selection. These ranged from statistical analyses of macro-evolutionary patterns with model selection approaches such as BiSSE to the hierarchical decomposition of selective forces using the Price Equation and adaptive diversification due to frequency dependent selection using adaptive dynamics. All of them are excellent tools and have been successfully applied to diverse issues in their respective fields, but none of them directly offers the possibility to investigate an adaptive feedback from species selection on speciation processes which I requested in chapter 1. A simultaneous focus on multiple layers of a problem induces an increased level of complexity, which is often hard to handle with mathematical tools. As demonstrated above, this gap is filled by agent-based modelling, as it provides the opportunity to investigate emergent group formation, group level fitness and selective feedback from the collective to the particle level.

While advocating its use, I do not claim that ABM is an inherently better modelling tool compared to alternative approaches. I am aware of the fact that the benefits of agent-based models are counterbalanced by the risk of being intractable (Weissing, Edelaar and Van Doorn 2011). Like all simulation techniques, however, ABM is not made to draw generalizable conclusions about the system that is studied, but to show 'how the world would look like, if it really did work the way in which [we] think it does', as Peck (2004) formulated it. In this respect I think that ABM offers a great value to support challenging investigations of the connections between hierarchical levels in evolution, such as the long standing question about the link between micro and macroevolutionary patterns, which statistical comparative analyses have yet failed to answer (Ng and Smith 2014).

2.A   APPENDIX: GREYFISH

Greyfish is an ABM framework I designed to quickly implement simulation models without constraints to flexibility (Hösler 2015). It was developed especially with issues in evolution and ecology in mind, but its abstraction does not prevent an application to different fields. Written in the Java programming language, greyfish can be executed on numerous platforms, from your local desktop to a high performance cluster. To allow for a maximum performance, parallelization and scalability haven been further development guidelines.

Basic Software Design Concepts

The basic structure of greyfish is visualized as a class hierarchy in figure 2.3. The main entry point to greyfish is an *experiment*, which contains the rules of the simulation construction, its execution and the data collection logic. Any simulation consists of *agents* that are structural clones of a defined prototypes, which is defined by a set of *components*. These components describe the agents behavioural actions and its properties, some of which are evolvable traits with a custom genetic basis. All agents are situated in an *environment*, which makes the agents aware of each other and defines their behavioural constraints as well as their evolutionary context.

In the most simple case, an experiment consists of an environment with discrete time and without any spacial properties. The simulation process with such an environment is described by algorithm 2.1. After initialization, the environment is repeatedly instructed to step forward. In response, it first increases its time by one unit. Then, the state of each agent and the environment is updated according to the events of the previous step. Last, each agent is asked to select a maximum of one of its actions to execute, which in turn might enqueue modifications of the environment or the properties of any agent. The delayed update strategy prevents perception
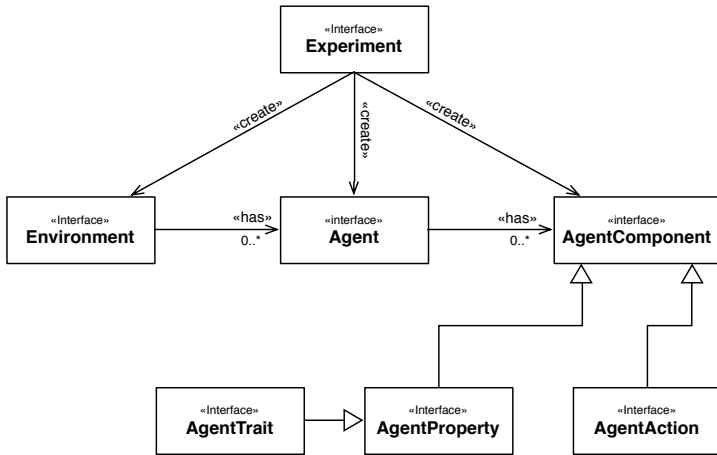
Figure 2.3 Basic simplified class structure of the greyfish modelling framework

or knowledge differences between agents that are executed in the same step. The state of the environment and all other agents is held constant. With such a discrete step environment it is an easy task to implement an evolutionary birth-death processes which provides the foundation of an adaptive dynamics simulation as described above.

Sample Implementations of Ecological Diversification

In the following I shall walk through the steps to build a greyfish simulation of an adaptive dynamics model. I shall illustrate this process with two sample implementations that reproduce results described in the book *Adaptive Diversification* by Doebeli (2011). There, in two of its chapters, the author introduces AD models of adaptive diversification due to resource competition in asexual and sexual populations. The underlying evolutionary force, frequency dependent selection, is generated by assigning each modelled individual a fixed rate of proliferation and a varying rate to die, which

```
initialization;
while experiment not finished do
    step();
end
Function step()
    increment time;
    apply enqueued modifications;
    foreach agent in environment do
        execute(agent)
    end
end
Function execute(agent)
    foreach action a of agent do
        success = trigger(action);
        if success then break;
    end
end
Function trigger(action)
    if conditions met then
        enque modifications in environment
    end
end
```

Algorithm 2.1 Experiment loop with a basic environment

is a result of the individuals experienced density generated by its ecological competitors, and the carrying capacity of the environment. Next to the deterministic formulation for infinite populations he describes a Gillespie algorithm (Gillespie 1977; Erban, Chapman and Maini 2007) to verify the results for populations of finite size, which is basis for the following agent-based implementation.

All ecologic interactions between the individuals are based on a single quantitative trait and a continuous resource distribution, defined by the carrying capacity function $K(x)$, which is used to calculate the population density for an individual i with trait value x_i.

We can imagine arbitrary shapes for this function but for simplicity here we assume a Gaussian function with

$$K(x) = K_0 \exp\left[\frac{-(x-x_0)^2}{2\sigma_K^2}\right]. \qquad (2.1)$$

The population density for individual i is calculated by dividing the effective population size $N_{\text{eff}}(i)$ for that individual by the capacity for individuals having trait value x. The effective populations size sums up the competitive impact of all other individuals j on individual i:

$$N_{\text{eff}}(i) = \sum_{j \neq i} \alpha(x_j, x_i), \qquad (2.2)$$

This competitive impact is based on the function $\alpha(x, y)$, the 'competition kernel', which returns a value representing how strongly an individual with phenotype x competes for the same resources with an individual of phenotype y. Again, for simplicity, we assume a simple Gaussian function here:

$$\alpha(x, y) = \exp\left[\frac{-(x-y)^2}{2\sigma_\alpha^2}\right]. \qquad (2.3)$$

With the competition kernel (2.3) and the capacity kernel (2.1) at hand, a death rate d_i can be assigned to each individual i:

$$d_i = b_i \frac{N_{\text{eff}}(i)}{K(x_i)}. \qquad (2.4)$$

The right hand side of the equation is the product of the individuals birth rate b_i and the ecological competition it faces due to the density effect which I have described above. The birth rate b_i is assumed to be equal among all individuals, so that $b_i = b$ for all i. Variation in the death rate is therefore solely based on the ecological viability.

The ecologic trait value of the offspring produced by an asexual individual is generated by applying a mutation function $\mu(x)$ to the

parents value. A reasonable common assumption is to draw values from a normal distribution with the value of the parent as the mean and a standard deviation σ_μ. In the case of sexual reproduction, we additionally require a method to combine the phenotype of two parents, the segregation kernel $S(x, y)$. A reasonable assumption for quantitative traits, when genetic details are not of interest, is to simply calculate the arithmetic mean $(x + y)/2$.

At this point we have defined all what is needed to observe the diversification of an asexual population into distinct clusters.[7] For generating similar effects in sexual populations, the system requires that offspring are generated from non-randomly mated parents. In the simplest scenario, this kind of assortative mating is introduced by a preference function based on the ecological similarity of two mating partners. In the following I use the Gaussian function

$$A(x, y) = \frac{1}{\sqrt{2\pi}\sigma_A} \exp\left[-\frac{(x - y)^2}{2\sigma_A^2} \right], \qquad (2.5)$$

to determine the mating probability of two agents with phenotype x and y. σ_A controls hereby the strength of the assortment.

Using the functions as defined above and taking the birth and death rates as probabilities, a greyfish experiment can be created in the following way. The agents are constructed with a birth and a death action, which are evaluated in this order, and an ecological trait property. At each time step the birth action of agent i is triggered with probability b_i and produces a single offspring. If it doesn't, the death action is triggered with probability d_i and removes the agent from the simulation.[8]

My ABM approach is very similar to the Gillespie algorithm. Nevertheless, it slightly differs in the birth and death rates per step.

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[7]Branching events only occur if $\sigma_K > \sigma_\alpha$ (cf. Doebeli 2011).

[8]Since actions get evaluated successively and the death action follows the birth action, the probability that the death action is triggered (d_i) is multiplied by $1 - b_i$ to retain a probability of d_i.

(a) Asexual Diversification
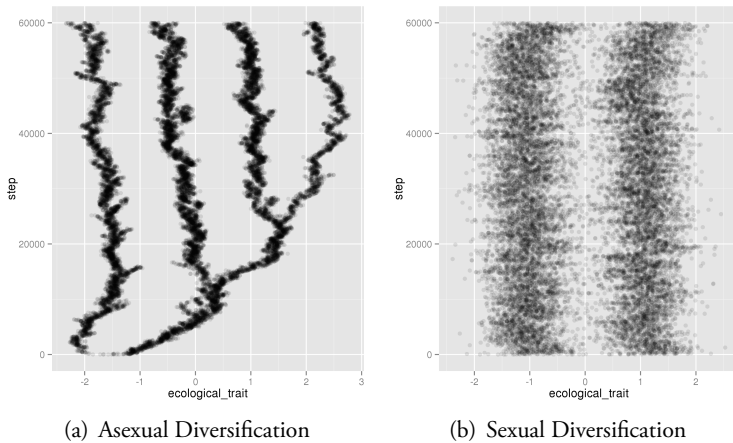
(b) Sexual Diversification

Figure 2.4 Simulation results from a sample implementation of adaptive ecological diversification models in the greyfish simulation framework. For figure (a) a Gaussian function was used for both the capacity and the competition kernel along with the following parameters: $K_0 = 200$, $\sigma_K = 2$, $\sigma_\alpha = 0.75$ and $\sigma_\mu = 0.01$. The simulation was initialized with 500 agents and normally distributed traits around -1.5 with a standard deviation of 2.0. Figure (b) was also produced with Gaussian functions and these parameters: $K_0 = 200$, $\sigma_K = 2$, $\sigma_\alpha = 1$, $\sigma_{s_x} = 0.2$ and $\sigma_A = 0.45$. Here 1000 agents constituted the initial population with traits normally distributed around 0 with standard deviation 1.

In the Gillespie case only a single birth or death event is chosen each step with a probability respecting all past events. As a result, the population size stays roughly the same over the whole experiment. In the greyfish model, however, the population size is only limited by the carrying capacity and independent of the initial population size.

For the experiment, single populations of sexual or asexual individuals with initially Gaussian distributed trait values were simulated for 60 000 steps. The evolution of the ecological trait is exemplified

in figure 2.4 by plotting the trait value of each agent at its time of birth. In the asexual case (panel (a)) a final formation of 4 distinct clusters can be observed as the result of multiple branching events. These clusters show an equal dispersal along the highly positive values of the Gaussian carrying capacity function. Panel (b) illustrates the sexual case with only two visible clusters of a higher variance, which is a consequence of a dispersal effect introduced with mating and the segregation kernel. Both patterns thereby resemble the results described in Doebeli (2011, Fig. 3.3b and 4.1b) and verify the correctness of the model implementation.

Chapter 3

Species Coexistence Promotes Sex with Assortative Mating

INTRODUCTION

I have shown in chapter 1 that macroevolutionary dynamics are re-considered as relevant processes for microevolutionary trajectories as a result of discrepancies between observations of biotic interactions and fossil record analyses. Several studies have revealed that organis-mic traits are likely to be shaped by a trade-off between organismic fitness and a positive influence on the speciation to extinction ratio (Goldberg et al. 2010; Raffaele and Kamoun 2012; Wright, Kalisz and Slotte 2013). I argued, that a better understanding of 'how traits shape trees' (Ng and Smith 2014) requires a deeper analysis on the 'how'. Many studies focus on the statistical analysis of phylogenetic data (Rabosky and McCune 2010) but this leaves room for mislead-ing conclusions about the causal processes at work. While ultimately an empirical question, studying speciation on neontological data is challenging (Jablonski 2008b). Therefore, I suggested Agent-Based

Modelling (ABM) as a compromise in my examination of different modelling methods in chapter 2.

In this chapter, I use ABM to study such a macroevolutionary feedback on one of the most interesting organismic traits, whose adaptive benefits have always puzzled evolutionary biologists: sexual reproduction (Maynard Smith 1978). While many short-term benefits have been revealed over the past decades (Schwander, Marais and Roze 2014) and initially assumed costs have been relativized (Lehtonen, Jennions and Kokko 2012), still some parts of the full picture are poorly understood. One of these is the influence of sex on speciation and extinction. Although sexual species are commonly considered to have a relatively higher net-diversification rate than asexual species (Jablonski 2008b), this is not an unchallenged assumption (Barraclough, Birky and Burt 2003; Birky and Barraclough 2009; Melián et al. 2012). I shall show in the following, that sexual reproduction indeed generates a long-term adaptive benefit in an agent-based model of adaptive diversification. My results suggest, however, that recombination is not the sole feature of sex that drives speciation, but assortative mating as a mechanism which facilitates species coexistence.

3.1   SEX SELLS — AT EVERY LEVEL

The switch from asexual to sexual reproduction is considered as one the major transitions in evolution (Maynard Smith and Szathmáry 1995, chap. 9), which all share the common property of being as fundamental to life as puzzling for the living. For sex these attributes stem from the fact that while 99.9 % of all named animal species show at least some form of sexuality (Vrijenhoek 1998), naively we wouldn't expect any sexuality at all. The main conceptual challenge is, simply stated: If mainly the female provides resources to their offspring, sexuals must produce twice as many offspring as asexuals to overcome this disadvantage — ignoring any additional costs (Williams 1975; Maynard Smith 1978; Lehtonen, Jennions

and Kokko 2012) or forms of occasional sex (D'Souza and Michiels 2010). Therefore, asexuality should always be more beneficial in the short term. This insight was originally formulated as the 'paradox of sex': Sex is ubiquitous in nature, but theoretically only half as efficient as asexual reproduction (Bell 1982). Some biologists have invested a great part of their career trying to identify the conditions and the processes that led both to the appearance and maintenance of sex; but up to now, they have only been able to highlight little fragments of the big leap.

Since the initial recognition of the problem various models have been proposed to explain the counterbalancing short-term benefits of sex; population genetic benefits of recombination in a changing environment is the most common claim (Barton and Charlesworth 1998; West, Lively and Read 1999; Otto and Lenormand 2002). Only little research, however, has been done so far to explain sex as a long-term advantage at the species level (Vienne, Giraud and Gouyon 2013), although it seems commonly accepted that sex evolved because it confers a long-term advantage to whole species (Maynard Smith 1978; Gouyon 1999; Mallet 2010). From a multi-level point of view, being a sexual organism does not necessarily have to be directly beneficial for the organism. By being part of a sexual species, an organism could gain an indirect competition advantage relative to the organisms of asexual species (I ignore mixed types here); if the species itself is relatively more fit due to a higher net diversification rate. If this hypothesis describes a relevant effect, then the evolution of sex could potentially be a result of higher level selection processes counteracting the within species benefit of asexual mutants: species selection.

As we have seen in chapter 1, the fitness benefits of being part of a sexual species must not necessarily materialize at the organismic level. While extinction risk of species directly affects the fitness of its constituting organisms, the reverse is not necessarily true. Therefore, aggregate or emergent species traits that increase the probability of a speciation event or lower a species extinction risk should be

selected for at the species level. However, these traits don't need to simultaneously increase the organismal fitness (in the form emergent traits, rather than aggregate, they even cannot be reduced to lower level traits).

Sexual reproduction is seen as one of the aggregate species traits linked to species fitness (Okasha 2006). First, sex effectively reduces a species extinction risk. Recombination can both break down negative genetic correlations (Barton and Charlesworth 1998) and increase the genetic variation allowing populations to adapt faster and enter new niches more quickly (Weismann 1889; Becks and Agrawal 2012). Furthermore, sex is commonly assumed as an important facilitator of speciation. For proponents of sexual speciation models, it is 'the' main cause of phenotypic discontinuities (Maynard Smith and Szathmáry 1995; Coyne and Orr 2004). Also in adaptive speciation models it is one of the major evolutionary drivers of diversification (see chapter 2). Mating, as a consequence of sex, provides the opportunity for non-random genetic associations. Positive assortment increases the variance of quantitative traits through the promotion of linkage disequilibrium between loci (Lynch and Walsh 1998). Furthermore, it stabilizes species differentiation through prezygotic isolation (Servedio and Noor 2003).

The consequences of sexual reproduction for speciation and extinction hint to an important flipside of the story: Sex could as well be a consequence of speciation and extinction. This interplay is what I am interested in here. One factor I find largely unexplored is the effect of assortative mating on species coexistence, one of the required steps in a speciation event which I described in chapter 1 (see also Weissing, Edelaar and Van Doorn 2011). As I explained above, sex does not only create variation but also constraints it and therefore facilitates isolation through ecological specialization. This favours that distinct adaptations, developed in such isolated species, to persist by preventing niche transitions. If these separately developed species traits cause organismic fitness differences, we can expect asexual species to be more prone to competitive exclusion.

While this can be beneficial in the short term as a way to displace less fit species, it should ultimately lead to a loss in trait richness, which is detrimental for the species community as a whole. It not only increases the extinction risks in a changing environment but can also reduce a species 'diversity-dependent' speciation rate (Etienne et al. 2012; Rabosky 2013).

To investigate sex as a kind of resolution to this conflict at the species level, I developed a simulation model describing a possible scenario where sexual reproduction produces a species-level benefit over asexual cloning through the effects of assortative mating. Previous studies that tried to model evolutionary benefits of sexual reproduction with explicit consideration of multi-level selection, assumed either predefined differences in extinction and diversification rates for sexuals and asexuals (Nunney 1989; Vienne, Giraud and Gouyon 2013) or a neutral model of community diversity (Melián et al. 2012). But as described above, the mode of reproduction and the tendency to diversify are complexly linked species properties. Therefore, simultaneously accounting for selection effects on the organismic and the species-level might drastically change the expected evolutionary dynamics of such a model.

Here, I do so by creating an agent-based simulation based on adaptive dynamics (AD) (Metz et al. 1996). AD is a mathematical framework, which has been successfully used in the past to investigate different evolutionary questions (Waxman and Gavrilets 2005) and especially to demonstrate the plausibility of sympatric speciation as an outcome of ecologic competition (Dieckmann and Doebeli 1999). I build on the frequency-dependent dynamics of AD to generate 'sympatric' demes from a single ancestral population, inside which a secondary diversification can evolve. Using this, I explore how the reproductive strategy of the agents — sexuality with different strengths of assortative mating against asexuality — affects the formation and the stability of 'sympatric' demes and results in deme diversity differences, a proxy for a reduced average extinction risk. I compare the expected diversity differences under a broad range

of ecological competition levels, a parameter which determines the chance of hybridizations by affecting the proximity of neighbouring clusters.

3.2   METHODS

The model is implemented with the greyfish simulation framework. As described in chapter 2 on modelling multi-level selection and speciation, greyfish agents have a modular design based on a set of properties and actions. They are part of an environment which schedules their (asynchronous) execution and the (synchronous) modification of state variables. For this study I designed the agents to mimic the birth-death process that is used in numeric simulations of AD. In an environment with a carrying capacity, a population evolves due to frequency-dependent selection on one or more heritable traits, a constant reproduction rate and a differential probability to die.

Model

To create the birth-death process that produces the evolutionary dynamics, the agents in this model consist of two actions, reproduction and death. These initiate the reproduction of a single offspring, preceded by mating in sexuals (explained in detail later on), and their removal from the environment respectively. As described in chapter 2, in the greyfish framework, the actions are sequentially evaluated at each step until the first is 'successful' or no action to evaluate remains. In this model, death is triggered after reproduction and their positive evaluation is associated with a certain probability.

An agent's birth rate b is fixed at a constant value, irrespective of the reproductive mode ($b = b_{\text{sex}} = b_{\text{asex}}$). The death rate equals the birth rate multiplied with two different factors and hereby defines an agent's fitness. Its first factor is determined by the agent's ecological phenotype in relation to the phenotypes of all other agents and the

carrying capacity $K(x)$ of the ecological environment:

$$e(i) = b\frac{1}{K(x_i)} \sum_{j \neq i} \alpha(x_j, x_i). \tag{3.1}$$

The function $\alpha(x_j, x_i)$, known as the competition kernel, defines the ecological competition between two individuals i and j. Here it is assumed to be a Gaussian function, centred at 0 with peak 1 and standard deviation σ_α. The carrying capacity was modelled by a quartic function $K(x) = K_0 \exp(-\frac{x^4}{2\sigma_K^4})$ with $K_0 = 150$ and $\sigma_K = 4.0$. Using this density dependent death rate simulates logistic growth and resembles the classical model of adaptive diversification due to ecological competition (Doebeli 2011). The ecological phenotype in my model is a discrete quantitative trait representing the ecological niche x_i of the agent i in an environment with the carrying capacity $K(x_i)$. The expressed value is determined by a set of L_e additive loci with two alleles, 0 and 1, encoded as a bitstring.[1] The function $\rho(x)$ projects the cardinality $c(x)$ of the bitstring x onto discrete values of a predefined contiguous interval $]a, b]$:[2]

$$\rho(x) = a + c(x)\frac{b - a}{L_e}. \tag{3.2}$$

The second factor influencing the death rate of agent i is the state of an assumed modifier trait y_i that is used to generate the desired second level of diversity between the emerging ecological clusters ('sympatric' demes). It is designed as a categorical trait and determined by a single gene with L_m nucleotides having strong epistatic interactions. Each nucleotide is either 0 or 1. The different alleles of this trait, 2^{L_m} in total, are used to calculate a factor $m(y)$, which also depends directly on the cardinality $c(y)$ of the underlying

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[1] A bitstring is a binary vector, e.g. $x = (1, 1, 0, 0, 0, 1, 0, 1)$.

[2] The cardinality of a bitstring is the number of bits that are set (value equals 1).

bitstring:

$$m(y) = \begin{cases} 1 - \frac{1}{L_m}\text{ffs}(y)\phi & \text{if } c(y) = 1 \\ 1 & \text{else} \end{cases} \qquad (3.3)$$

A cardinality of 1 reduces the factor by a fraction of $0 \leq \phi \leq 1$; linearly increasing with the position of the first least significant set bit ($\text{ffs}(y) \in \{1, 2, \ldots, L_m\}$); different cardinalities leave it unmodified. All else being equal, this effectively creates L_m local fitness maxima with linear increasing peaks. Furthermore, since the Hamming distance between the strings at two different maxima is 2, transitions between any of these maxima require at least two inversions. If mutations are rare and epistasis strong, a population that reaches one random maximum is constraint to evolve to a different (possibly better) maximum, since mutated offspring will likely end up in a fitness valley most of the time. Therefore, each cluster randomly fixates one of the different modifier trait alleles and the distribution of these fixations can be used as a measure of diversity between the clusters.

The final death rate d_i for individual i is then a combination of the ecological competition as defined by equation 3.1 and the modifying factor of equation 3.3:

$$d_i = e(\rho(x_i))m(y_i). \qquad (3.4)$$

Variations in the ecological trait and the modifier trait are created by applying functions on the parental trait values during reproduction. In the sexual (biparental) case, offspring trait generation starts with a segregation kernel which picks one of the two parental bitstrings, after recombining it with the second. Recombination results from applying a uniform crossover function on the chromosome pair, which swaps the bits of the two given strings at equal position with probability χ_e and χ_m respectively. Afterwards, this segregated trait value and the values of asexuals are processed equally with a mutation kernel. I modelled mutations as a bit-flip function, which

inverts each bit in the bitstring with probability μ_e for the ecological trait and μ_m for the modifier trait.

For sexual reproduction, the reproducing agent picks one 'sperm donor' out of a pool of possible mating partners. These candidates are sampled for each reproductive event by randomly selecting M out of all agents (excluding the choosing agent). Mate choice is assortative, defined by absolute mating preference function (Lande 1981):

$$A(x_i, x_j) = \frac{1}{\sqrt{2\pi}\sigma_A} \exp\left[-\frac{(x_i - x_j)^2}{2\sigma_A^2}\right]. \qquad (3.5)$$

This function maps the distance in the ecological trait of the two mating partners, x_i and x_j, to a mating probability and acts as a filter on the set of potential mating partners for a reproducing agent. Here I used a Gaussian assortment kernel with mean 0, peak height 1 and standard deviation σ_A. Therefore, the probability that two individuals are compatible decreases symmetrically from 0 (i.e. identical genomes); the lower the value for σ_A the faster the decease.

Experimental Design

For each simulation run, an ancestral population was generated by initially adding 500 agents to the environment. The ecological trait of the founding agents was initialized with a string of 10 000 bits, each set with probability 0.48. With a projection interval of $I_e = \,]-40, 40]$, the initial (projected) value distribution has a binomial shape with mean -1.6. The segregation kernel was parameterized with $\chi_e = 0.5$, which simulates free recombination (the bit at each position is inherited independently; cf. Dieckmann and Doebeli 1999). Each bit of the ecological trait was mutated with probability $\mu_e = 2 \times 10^{-4}$. This configuration allows the mutation kernel to generate a distribution of the projected trait values (Eq. (3.2)), which is approximately Gaussian.

The values of the modifier trait were initialized with a length of $L_m = 10$, with only unset bits and a mutation probability of $\mu_m = 10^{-5}$. As described above, this trait was designed for multiple local optima with transitions between them requiring at least two mutations. Therefore, to prevent recombination from bypassing the adaptive valley, I disabled it in this trait with $\chi_m = 0$ (see discussion section). Because the allele providing the highest fitness value would quickly invade a directly competing population, I let the founder population diversify into distinct subpopulations during the first $t_{\mu_m 0} = 100\,000$ steps with the identical modifier trait value (all bits unset; maps to the grey colour in figures 3.1 and 3.2).

Choosing values to test for assortment strength (σ_A) was guided by two considerations. First, the range for this value should by restricted to values which do not prevent any diversification to occur (irrespective of the competition strength which can partially compensate for weak assortment). This happens for either too small or too large values (Doebeli 2011). Second, in a recent meta-analysis on assortative mating in natural populations, Jiang, Bolnick and Kirkpatrick (2013) reported that most animals show a tendency towards weakly positive assortment (mean correlation between mates was at 0.28). Taking these two facts, values for σ_A that allowed for branching events to occur and showed a reasonable mating partner correlation coefficient (inside single clusters) fell roughly between 0.2 and 0.3.

I set up a two factorial experiment in which I tested different reproductive strategies, namely asexual reproduction against sexual reproduction with three different strengths of assortative mating ($\sigma_A \in \{0.2, 0.25, 0.3\}$), under multiple competition scenarios ($\sigma_\alpha \in \{0.45, 0.5, \ldots, 0.75\}$). All parameters of the experiment configuration are listed in table 3.1. I let all populations evolve for 500 000 steps. Each parameter combination was repeatedly simulated 20 times.

Table 3.1 The parameter set used for the experiments.

Symbol	Definition	Values
σ_α	strength of ecological competition	$0.45, 0.5, \ldots, 0.75$
$r \times \sigma_A; r \in \{\text{sex, asex}\}$	reproductive strategy	asex $\times$ NA, sex $\times$ 0.2, sex $\times$ 0.25, sex $\times$ 0.3
K_0	peak of the capacity kernel	150.0
σ_K	standard deviation of the capacity kernel	4.0
b_{sex}	birth rate of sexuals	0.04
b_{asex}	birth rate of asexuals	0.04
N_0	initial population size	500
ϕ	maximum impact of the modifier trait	0.7
M	number of matings	30
L_e	chromosome length of the ecological trait	10 000
χ_e	crossover probability of the ecological trait	0.5
μ_e	mutation probability of the ecological trait	2×10^{-4}
I_e	projection interval of the ecological trait	$]-40, 40]$
L_m	chromosome length of the modifier trait	10
χ_m	crossover probability of the modifier trait	0.0
μ_m	mutation probability of the modifier trait	10^{-5}
$t_{\mu_m 0}$	activation step of mutations in the modifier trait	100 000

Data Analysis

For each simulation, I identified the number of emerged clusters, the within cluster variance and the distance between cluster means. Furthermore, I calculated the richness and the diversity of the whole cluster population as described in the following. All data analyses were conducted using *R* (R Core Team 2014).

To partition the diversified agents into clusters I used the implementation of the density based cluster algorithm DBSCAN (Ester et al. 1996) that is available in the *fpc* R-Package (Hennig 2014). For the distance measure I used the Euclidean distance of the ecologic trait value. The reachability threshold was set to 0.2, a value I identified to work equally well among all different values for σ_α.[3] I limited the cluster analysis to agents born inside a small time range of 100 steps at the end of the simulation ($[499\,900, 500\,000]$).

For each cluster the frequency of each modifier trait allele was identified and the most common one used as the aggregate state of that cluster (the design of the trait inevitably results in one dominant allele per cluster). The sum of all unique aggregates was taken as the richness of the cluster set for the time range under consideration.

To quantify the diversity of the cluster set based on this aggregate trait, I used the *Simpson Diversity Index* (Simpson 1949), a measurement respecting both the richness and the evenness of the sampled elements. It calculates the probability that two randomly sampled elements out of a finite set can be assigned to the same group and equals $D = \sum_{i=1}^{R} p_i^2$ where R is the total number of distinct elements (richness) and p_i the proportional abundance of element i. Translated to the presented model it transforms the number of distinct cluster traits and the total number of clusters into

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[3]Using random 100 steps time frame samples, I compared the algorithmic results with counts from a visual exploration under different reachability distances (0.1 to 1.0 by 0.1). For most values (0.2 to 0.8) the algorithm reported the predicted number of clusters, so that choosing a common small value of 0.2 for all different scenarios seemed a reasonable choice. Figure 3.A in the appendix shows the clustering results for this value.
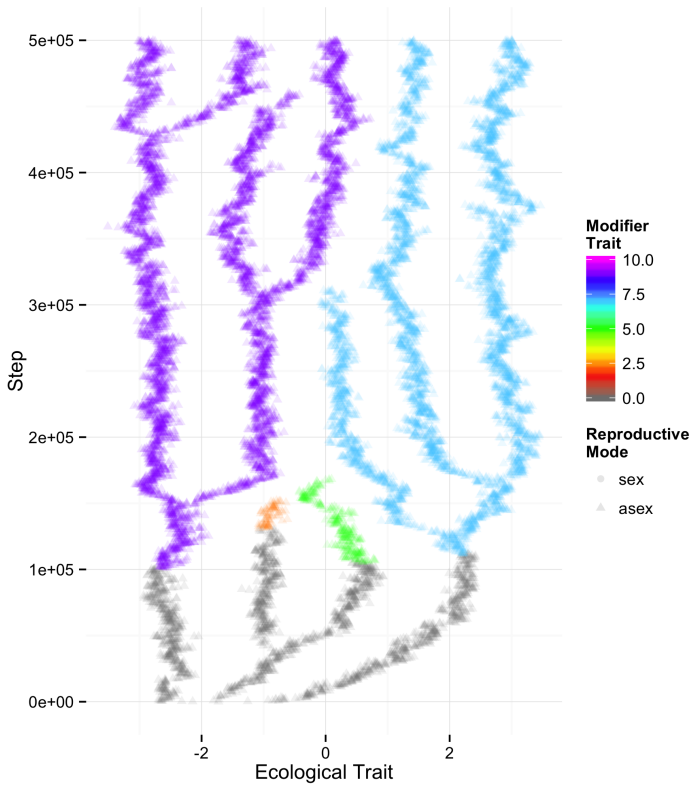
Figure 3.1 Sample result from simulating the model with a purely asexual population and $\sigma_\alpha = 0.75$. The discrete bitstring values of the modifier trait were mapped to a continuous scale using the $\log_2$ value of its integer representation increased by one: $y_c = \log_2(\text{int}(y) + 1)$. The higher the scale value the stronger the effect of the modifier trait (the lower the result of $m(y)$).

a single quantity. For convenience, D was transformed to $1 - D$, which increases with the number of distinct adaptations and the more the trait frequency resembles a uniform distribution.
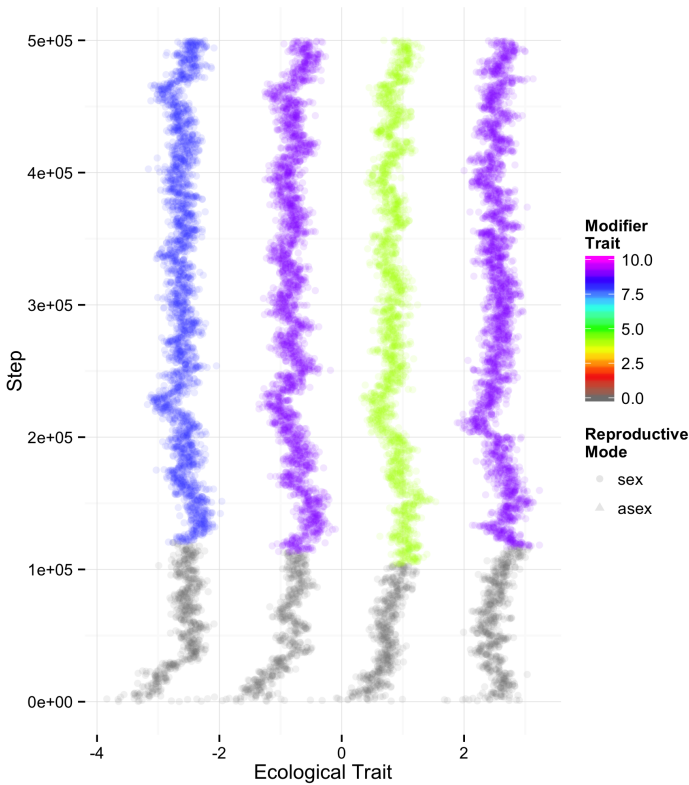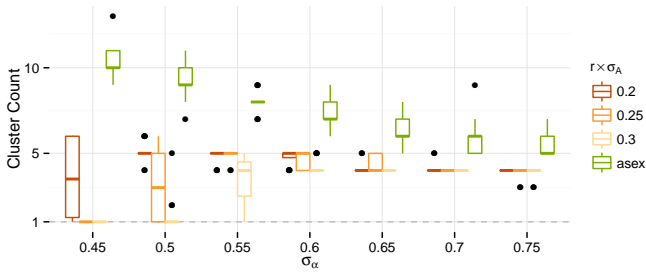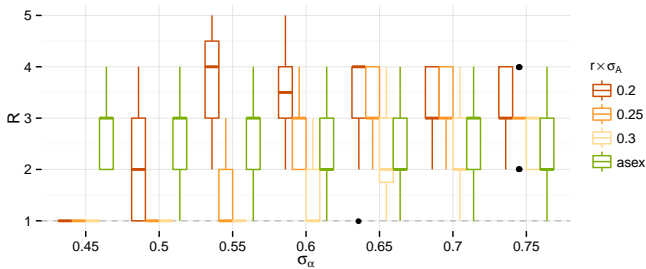
Figure 3.2 Sample results from a sexual population with $\sigma_A = 0.25$. All other parameters are the same as in figure 3.1.
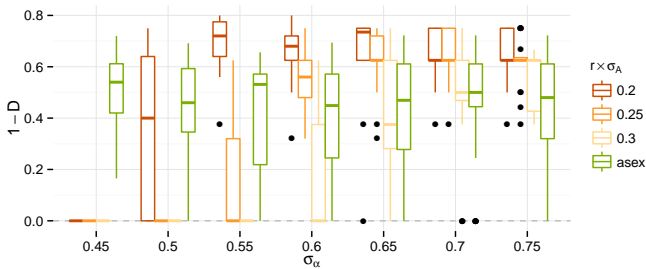
3.3   RESULTS

The simulations confirmed the expected difference of cluster number, richness and therefore diversity depending on the reproductive strategy. Sexuals show a generally smaller number of emerging clusters than asexuals (Fig. 3.3(a)). This is a direct result of recombination. It generates both, a higher variance in the ecological trait
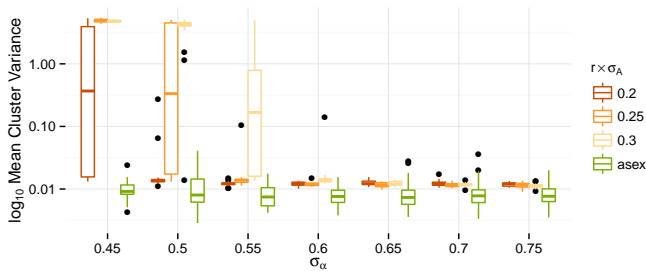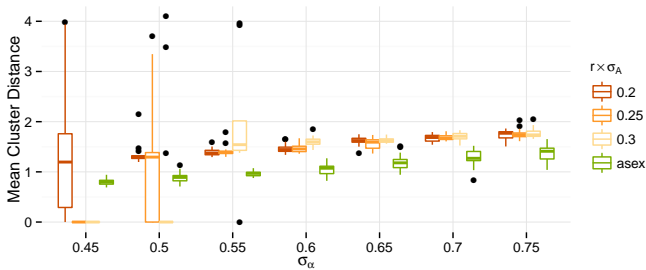
(a) Cluster Count

(b) Richness

(c) Simpson Diversity Index

Figure 3.3 Shown are (a) cluster count, (b) richness, (c) Simpson Diversity Index, (d) within cluster variance in the ecological trait and (e) the mean distance between the the ecological trait means of two adjacent clusters.

(d) Cluster Variance

(e) Cluster Distance

Figure 3.3 (continued) Values are taken from independent simulations with different reproductive strategies (asexual or sexual reproduction, the latter mode under consideration of different values for σ_A) for a broad range of ecological competition strengths (σ_α). Each parameter combination was simulated 20 times. Boxes visualize 50% and lines 95% of the results. The median is indicated by a bold horizontal bar. The dashed horizontal grey lines show the baseline, which is equal to the results expected for sex with random mating.

within clusters (Fig. 3.3(d)) and a higher distance between the ecological trait means of two adjacent clusters (Fig. 3.3(e)). Simply speaking, the wider the average cluster width and the more space between them, the fewer clusters will fit into a limited space. Furthermore, the cluster count of the two reproductive modes responds

differently to a change in the ecological competition strength. The
mean number of clusters in asexual populations decreases linearly
from 10 to 5 with increasing σ_α. Sexual populations show no cluster
differentiation when competition is below a σ_A dependent threshold.
Above this threshold, the mean cluster count for all three assort-
ment strengths increases rapidly to its maximum (4 to 5) at medium
competition strength and slowly decreases thereafter. The visual
exploration of the effects of competition and reproductive mode on
richness (Fig. 3.3(b)) and diversity (Fig. 3.3(c)), shows a major con-
tribution of both factors. While asexual populations have a nearly
constant mean diversity index over all tested competition settings
(≈ 0.5), sexual populations show an interesting variation. Starting
with 0 diversity, if competition is too low to generate a (stable) differ-
entiation into clusters, diversity increases with competition pressure
up to a plateau with values significantly higher in comparison to
asexuals. Further, the pattern for sexual populations seems to get
shifted to the right (towards higher competition) with decreasing
assortment strength.

A statistical analysis of the diversity supports the visual impres-
sion. Analysis of variance for linear mixed models with the repro-
ductive strategy nested inside competition as a random effect reports
a significant effect of the reproductive strategy ($F_{3,556} = 31.74$;
$p < 0.001$). Model selection reveals that the full model, including
the reproductive strategy, competition and their interaction as fixed
effects, explains the data best. Taking only the high competition
subset of the data where $\sigma_\alpha > 0.6$, however, leaves a different pic-
ture. The reported differences are still significant ($F_{3,236} = 22.19$;
$p < 0.001$), but the model with only reproductive strategy as fixed
effect, can not be significantly improved by adding competition
($p = 0.1335$) or its interaction with the reproductive strategy as
fixed effects ($p = 0.2854$). Performing a Tukey HSD PostHoc Test
on the subset reveals that if assortment is strong enough, the diversity
index for the sexual strategies is significantly higher than for asexuals
($\sigma_A \in \{0.2, 0.25\}$: $p < 0.001$). Weak assortment ($\sigma_A = 0.3$)

shows no difference in diversity to the asexual strategy.

Invasion Analysis

In the presented simulations, I considered sexual and asexual reproduction separately, because preliminary studies showed that sexual populations should get quickly invaded by asexual mutants. An invasion should consequently lead to a diversity drop to the asexual level. To verify this assumption, I extended the previous model by adding a trait with two alleles determining sexual or asexual reproduction. Initialized with the 'sexual' allele, mutations of this trait were activated after an initialization phase of 250 000 steps. This was implemented using a transition probability $\mu_{\text{rep}} = 1^{-5}$ between the two alleles in each offspring (different values would just alter the speed of the dynamics). After running the simulation for 1 000 000 steps (twice the duration of the previous setup), I analysed the data from agents born inside different time intervals of 100 steps width beginning with the activation time of mutations. For these sampled agents, the diversity was measured as in the previous part and compared between the different stages of the simulation. I limited the observations to the two extremes of the ecological competition values from the previous results where the difference in the SDI between the two reproductive modes was largest: the low competition setting with $\sigma_\alpha = 0.45$ and the high competition setting with $\sigma_\alpha = 0.75$.

Within the low competition environment, asexuality invades the unimodal distributed sexual population quite quickly and dominates the ecological space almost completely after a few thousand steps (Fig. 3.4(a)). Because the invaded sexual population did not differentiate into clusters, all asexual agents inherited the same modifier trait allele. Therefore, although the cluster number increased with invasion, richness did not, and diversity remained unaffected (Fig. 3.4(c)). Interestingly, the emergence of asexual clusters sometimes enabled a formation of long standing sexual clusters at both borders of the carrying capacity. This is caused by the combined in-
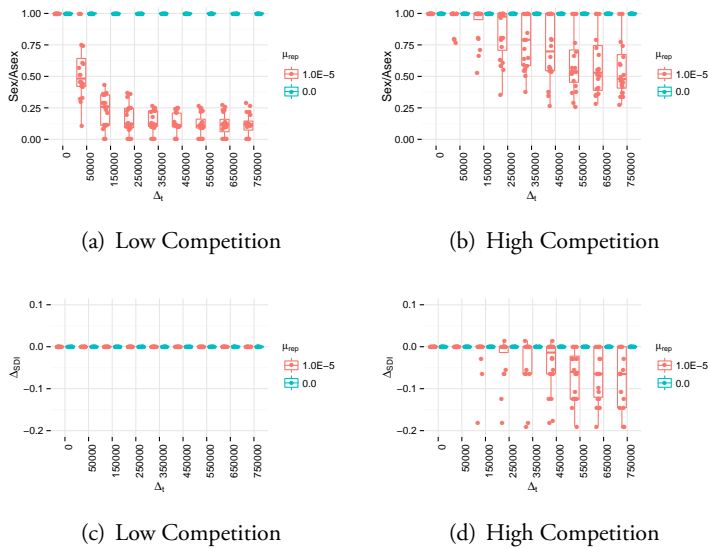
(a) Low Competition

(b) High Competition

(c) Low Competition

(d) High Competition

Figure 3.4 Change in the composition of the trait determining reproductive mode and of the Simpson Diversity Index Δ_{SDI} in simulations allowing for transitions between sex and asex after an initial diversification phase of 250 000 steps. Values were measured at different time offsets after the initial phase (Δ_t) for different mutation (transition) probabilities (μ_{rep}) in a low ($\sigma_\alpha = 0.45$) and high competition ($\sigma_\alpha = 0.75$) environment with medium assortment ($\sigma_A = 0.25$). All other parameters equal those used in the previous setup.

fluence of the vanishing mating pool on the side of asexual invasion and the lack of competitors on the side of the dropping capacity, which is an edge effect of the carrying capacity function. Simulations with high competition left a different picture. Invasions happened much more slowly. On average, asexual agents made up only half of the overall population after whole 1 000 000 steps (Fig 3.4(b)). As expected, diversity responded with a continuous decrease because of the newly formed asexual clusters replacing their sexual competitors.

3.4   DISCUSSION

Sexual reproduction is commonly believed to increase a population's ability to diverge into new species because of the increased genetic variation generated by recombination and segregation (Bell 1982). Asexual populations, as a consequence, should be limited in this ability. More recent findings, however, suggest that asexuality is by no means an evolutionary dead end. Theoretically, asexuals have the same ability to diversify into discrete entities (Barraclough, Birky and Burt 2003) and under certain conditions show even more diversity than sexuals (Johnson et al. 2011). The above results support a differentiated picture of the link between reproductive mode and diversification. The reproductive strategy and its differential response to varying ecological competition shows a strong influence on the expected species diversity. While the number of clusters in asexual populations outnumbered clusters in sexuals, if the degree of assortment fits to the strength of ecological competition, sexual reproduction enables species to reach higher diversity levels than cloning.

This rather surprising result can be explained by looking at the dynamics in single experiments. In figures 3.2 and 3.1 we can see that while each sexual cluster is mostly able to maintain its modifier trait value through time, irrespective of the variation in their fitness effects, asexual clusters with lower gains are prone to become extinct if directly neighbouring clusters with a higher gain are present. This situation can be interpreted as a form of competitive exclusion (Hardin 1960): If two sympatric and non-interbreeding species occupy the same niche have differences in their reproduction rate, the faster reproducing species will displace the other. In the simulations assortative mating not only generates the 'sympatric' demes, but also prevents a secondary contact at which such an exclusion could happen.

The results of the invasion analysis support the destructive effect of asexuality on the diversity measure. In the high competition en-

vironment, diversity decreased approximately by 0.1 after 1 000 000 steps. This is the same value we would expect from the previous results, as it is roughly the difference between the diversity in sexuals and asexuals with the corresponding parameters. The data exploration of the low competition setting also meets the expectations. The unimodal distributed sexual population is not able to provide multiple distinct clusters as the source for a diversity in the modifier trait between asexual clusters. This deficiency and the design of the genetic architecture prevents an otherwise possible diversity increase with the differentiation into clusters during invasion.

The results are of course only valid in the boundaries of the chosen functions and parameters. These choices, however, were made carefully under a tradeoff between feasibility a biological similarity. The maximum richness in the simulations is obviously limited by the number of clusters that are able to emerge, which is in turn primarily limited by the environmental constraints of the carrying capacity.[4] For the given parameter settings, in sexual populations, the cluster count rarely exceeded 4 to 5. Although this resulted in rather minor richness differences (Fig. 3.3(b)), it was nevertheless sufficient to observe significant differences in the diversification measure.

Assortment in sexual populations was based on a simple phenotype matching rule (cf. equation (3.5)). This is a common assumption in adaptive diversification models but might not reflect empirical reality (Verzijden, Lachlan and Servedio 2005). Furthermore, the model assumes no costs for assortative mating. Although this poses an unlikely scenario, their addition would not change the resulting diversity difference between sexuals and asexuals, as they were studied in isolation. Asexual invasion, however, would indeed be facilitated. Although it has been shown, that even medium costs of assortment would prevent its evolution in an adaptive diversifica-

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[4]For capacities wider than we used here, an additional constraint poses the genetics of the ecological trait, as the bit-flip mutation function drives the cardinality towards $\frac{1}{2}L_e$, which makes the origination of extreme traits unlikely. In this case, increasing the bitstring size or an alternative mutation kernel could be an option.

tion scenarios (Schneider and Burger 2006; Kopp and Hermisson 2008), empirical studies on assortative mating prove, that weakly positive assortment is expressed in the majority of species in the animal kingdom (Jiang, Bolnick and Kirkpatrick 2013). So while I am aware that selection for assortative mating is rather weak in speciation models, I ignore the question of how assortment evolved in the first place and take it as a fixed adaptation at a strength that matches empirical findings (with the awareness, that the measurements were taken from animals not directly comparable to the isogamous sexuals used in the model).

The genetic architecture of the agents is one of the main prerequisites for the results I present here. My design of the ecological trait was inspired by the work of Dieckmann and Doebeli (1999) on sympatric speciation (Similar genotypes have been used in other recent studies (Rossberg, Rogers and McKane 2013)). The authors used the count of '+' alleles from many binary '+/−' loci to determine the trait value and also assumed free recombination. Although architectural choices have a considerable impact on the outcome of adaptive diversification models (Bürger, Schneider and Willensdorfer 2006), I didn't consider effects of alternative designs since I used the ecological trait only the establishment of clusters and was not interested in the conditions under which ecological diversification is generally possible. Apart from the ecological trait, the secondary diversification inside the clusters required especially the assumed intragenic epistasis in the modifier trait gene and its low mutation rate. This assumption, however, is not unrealistic if (unlike in the ecological trait) the bits of this trait are seen as nucleotides rather than alleles, between which recombination rates are generally lower but epistatic interactions strong, numerous and likely to generate local optima (Watson, Ficici and Pollack 2002).

3.5 CONCLUSION

With the reasonable assumption that species diversity can be used as a proxy for species fitness, the first take-home message from the experiment is a strengthening of a well known theory: If species selection is an effective force in the evolution of species traits, which I think is the case (see chapter 1 on this topic), then it is possible to envision a scenario in which sexual reproduction is maintained by it, despite the relatively high costs that sex imposes. The interesting twist of the story, however, is that the benefits of recombination are not necessarily the primary driving component of sex which is responsible for a positive selection gradient. Assortative mating, as a mechanism which aids sympatric speciation by isolating 'sympatric' demes and the avoidance of competitive exclusion, is not unlikely to play a major role as well. While the importance of non-random mating for organismic fitness has been recognized (Michiels et al. 1999), here I emphasize its influence on inter-species competition. This supports the idea, that species-level selection both operates against adaptations that weaken the competitive ability of species (Rankin et al. 2007) and promotes adaptations that strengthen it, such as sexual reproduction (Ciros-Pérez, Carmona and Serra 2002).

The results further suggest for the competition between sexual species, that stronger degrees of assortative mating increase a species competitive ability. A conclusion which integrates well with empirical evidences for the general importance of assortment in species (Schuett, Tregenza and Dall 2010). A recent study on Eastern Bluebirds for example, reports that high interspecific competition might select for assortative mating (Harris and Siefferman 2014). What to keep in mind is that in the model I used an absolute mating function (Eq. 3.5), which assumes that mate choice is expressed only in the choosing sex. It has been shown, however, that assortative mating can arise from various behavioural or ecological processes and can be more complicated than I model it here (Jiang, Bolnick and Kirkpatrick 2013).

While I have shown that selection for sex at the species level has a solid theoretical justification, a confirmation from an evolution experiment would be necessary to ultimately prove the biological relevance of this process. Although experiments were able to document the plausibility of adaptive diversification in the laboratory (Linn et al. 2003; Maharjan et al. 2006; Herron and Doebeli 2013) and in the field (Barluenga et al. 2006; Savolainen et al. 2006; Ryan et al. 2007), evidences of species selection are only available on the basis of a statistical analysis of fossil records (Goldberg et al. 2010; Simpson 2013). The increased interest in this topic over the recent years (Rabosky and McCune 2010), however, rises the hope that neontological support might appear in the near future (Jablonski 2008b). I hope that the kind of theoretical studies I did describe here, will be useful to guide this research and contribute to a better understanding of the processes that shaped the diversity of life on earth.

3.A   APPENDIX: SUPPLEMENTARY DATA
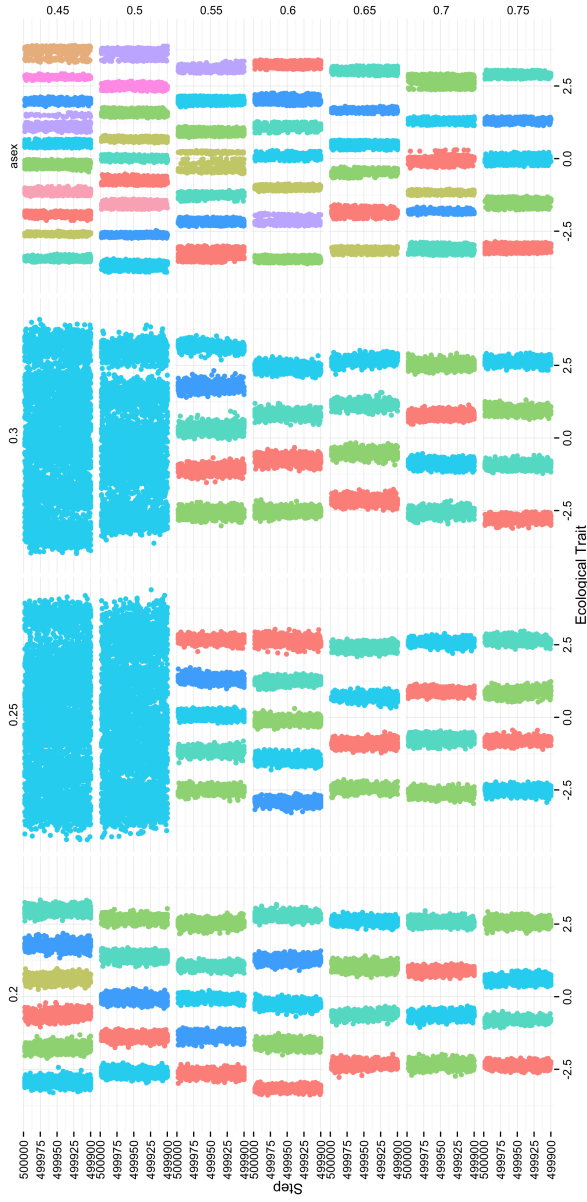
ACKNOWLEDGEMENTS

Figure 3.5 DBSCAN (Ester et al. 1996) clustering results (reachability threshold = 0.2; reachability minimum no. of points = 5) from single randomly chosen experiments for each combination of σ_α and $\{sex, asex\} \ni r \times \sigma_A$ used to compile the cluster count reported in figure 3.3(a). Each colour in a single panel denotes a single cluster. Equal colours across different panels have no special meaning and are coincidental.

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Deutsche Zusammenfassung
(German Summary)

Natürlichen Selektion gilt als universelles Modell zur Erklärung biologischer Vielfalt. Ihre vorhergesagten Auswirkungen scheinen jedoch häufig den beobachtbaren Phänomenen der Natur zu widersprechen. Insbesondere können einige makroevolutionäre Muster, die unter anderem aus Fossilien rekonstruiert wurden, nicht mit den Beobachtungen von mikroevolutionären Dynamiken in Einklang gebracht werden. Eines der großen Ziele der synthetischen Evolutionstheorie bleibt damit bisher unerreicht. Ein möglicher Grund für die Unstimmigkeit liegt im hierarchischen Aufbau der Natur. Dieser ist sowohl ein Resultat evolutionärer Mechanismen, als auch eine Quelle prozessverändernder Faktoren. Die Prinzipien der Selektion sind nämlich nicht nur auf Organismen anwendbar. Sie gelten gleichermaßen für Arten, indem man Artbildung mit Reproduktion und Aussterben mit Tod gleichsetzt und einen Einfluss von den Merkmalen einer Art auf die Wahrscheinlichkeit der jeweiligen Ereignisse annimmt. Merkmale mit positivem Einfluss auf Artbildung und Merkmale mit negativem Einfluss auf die Wahrscheinlichkeit auszusterben werden somit durch Artenselektion bevorzugt. Dass Arten mit dieser Sichtweise nicht nur Ansammlungen von Organismen darstellen, sondern auch adaptive Einheiten, ist zwar eine

Perspektive, die unter Biologen weitaus akzeptiert scheint, jedoch in Überlegungen zu Artbildungsprozessen oft übergangen wird.

Meine Arbeit hat das Ziel, diese Interaktion genauer zu beleuchten, um letztendlich den unterschiedlichen Theorien aus Ökologie, Evolution und Paläontologe zu einer Harmonisierung zu verhelfen. Im ersten Kapitel beginne ich daher zunächst mit einer Beschreibung der theoretischen Fundamente zur Mehrschichten-Selektion im Allgemeinen und zur Selektion auf Artebene im Besonderen. Folgend werde ich versuchen diese Konzepte mit der Theorie der adaptiven Artbildung zu verweben. Ich werde zeigen, wie Merkmale von Arten bestimmte Faktoren im Artbildungsprozess unterstützen können und damit nicht nur ihre bedeutungsvolle Rolle in der Makroevolution begründen, sondern auch den Einfluss von Mehrschichten-Selektion auf ihren Entstehungsprozess hervorheben.

Ausgehend von diesem konzeptuellen Kapitel, werde ich eine Analyse methodischer Ansätze anschließen, mit deren Hilfe das Dargelegte theoretisch untersucht werden kann. Zu den beiden beleuchteten Teilaspekten (Mehrschichten-Selektion und adaptive Artbildung) sind in der jüngeren Vergangenheit richtungweisende Modellierungsansätze entwickelt worden. Ich werde zeigen, dass viele dieser Methoden jedoch evolutionäre Zusammenhänge nur statistisch, aber nicht kausal erfassen können oder eine mathematische Verallgemeinerung der Einbeziehung komplexerer Zusammenhänge Vorzug gewähren. Gerade die synchrone Betrachtung von Prozessen auf mehreren Ebenen verlangt jedoch genau dies. Ich werde erläutern, und beispielhaft demonstrieren, dass die Agenten-Basierte Modellierung eine exzellente Alternative darstellt, um die Interaktion von Art-Merkmalen und Artbildung zu untersuchen.

Im letzten Kapitel dieser Arbeit werde ich schließlich die Schlussfolgerungen der beiden vorhergegangenen Kapitel in der Untersuchung eines speziellen Merkmals anwenden: Sexuelle Reproduktion. Ihre Entstehung und Erhaltung wird als eine der bedeutendsten aber gleichzeitig rätselhaftesten evolutionären Errungenschaften angesehen. Der Grund hierfür liegt darin, dass sie sich aus theoretischer

Sicht nie gegen asexuelle Reproduktion hätte durchsetzen dürfen und dennoch weit verbreitet ist. Die Kosten übersteigen, naiv gesehen, den Nutzen bei Weitem. Um diesen Widerspruch aufzulösen, wurden verschiedenste konzeptuelle Erweiterungen der Evolutionstheorie zu Hilfe genommen, jedoch konnten diese auch in Summe keine lückenlose Erklärung liefern. Eine davon ist Selektion auf Artebene, da mit sexueller Reproduktion sowohl eine gesteigerte Aufspaltungsrate in Unterarten als auch eine reduzierte Wahrscheinlichkeit von Aussterbeereignissen assoziiert wird. Die Schwierigkeit, diese Annahme durch empirische Belege zu untermauern, erfordert eine ausgedehnte theoretische Herangehensweise. Mit Hilfe eines Simulationsmodells werde ich zeigen, dass sexuelle Reproduktion in ihrer einfachsten Form eine erhöhte Diversität zwischen Arten begründen kann. Als wesentliche Ursache hierfür werde ich die nicht zufällige Paarung von sexuellen Organismen identifizieren, da sie zu einer Vermeidung von zwischenartlicher Konkurrenz führt und damit die generierte Diversität stabilisiert. Mit der Annahme, dass unter dem Einfluss von Artenselektion Diversität vorteilhaft ist, zeigen meine Resultate letztlich einen direkter Zusammenhang zwischen Artenselektion und der Evolution von sexueller Reproduktion.