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On Agent-Based Models of Sex, Plants and Sustainability

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On Agent-Based Models of Sex, Plants and Sustainability

Dissertation

to obtain the degree of Doctor at Maastricht University,
on the authority of the Rector Magnificus, Prof. dr. Rianne M. Letschert,
in accordance with the decision of the Board of Deans,
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by

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To my beloved parents for their great support.

Contents

6 Game theory of pollution: national policies and their international effects 99

CHAPTER 1

Introduction

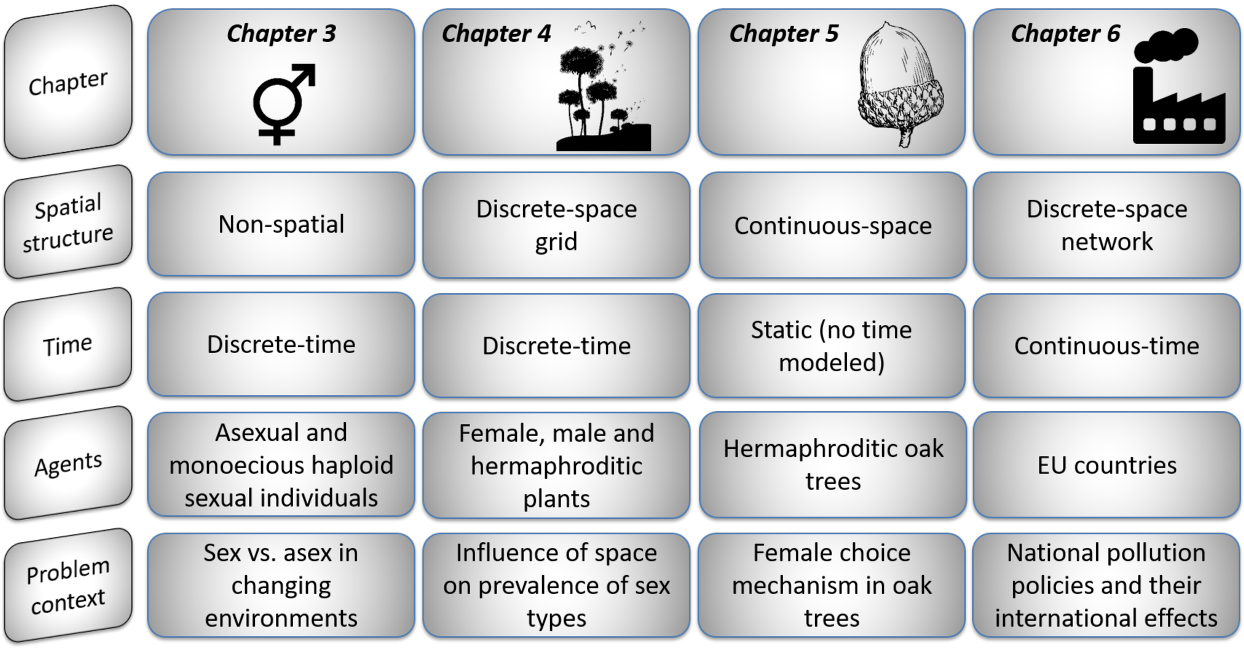
In nature, we can distinguish different forms of reproduction, such as asexual and sexual reproduction. Most bacteria, for example, split themselves asexually [Narra and Ochman, 2006]. No partners are needed and thus no genetic recombination of genes is performed. The offspring genetically is an identical copy of the parent individual. By contrast, mammals reproduce sexually, i.e., female individuals are fertilized by male individuals and genes from both mating partners are recombined to form offspring [Handel and Schimenti, 2010]. In other cases of sexual reproduction, e.g. in plants, there are individuals that have both male and female reproductive organs and as such they may on the one hand fertilize themselves and on the other hand use both male and females organs to reproduce with others. Such individuals are called hermaphrodites and they are well-studied in botany, as most higher plants are hermaphrodites [Charnov et al., 1976]. In addition, not only the form of reproduction can vary between species, but there is also a wide range of different mechanisms to proliferate and to help species to survive [Fox, 1978, Poltermann et al., 2000, Tinkle et al., 1970]. These mechanisms include strategies to attract pollinators by producing large and bright flowers [Lee, 2007, Miller et al., 2011], and strategies to attract mating partners by having a colorful plumage [Järvi et al., 1987, Saetre et al., 1994], or by performing a birdsong [Eriksson and Wallin, 1986, Gottlander, 1987]. Moreover, they also include strategies used by plants to prevent self-fertilization to increase the quality of offspring [Darwin, 1877], and mechanisms involving individuals changing their sex during lifetime to be more successful in spreading their genes to the next generations [Ghiselin, 1969, Munday et al., 2006]. All these different forms and strategies of reproduction co-exist in nature. According to Darwin

[1859], though, only the most successful strategies survive. Thus, by the fact that we observe various reproduction strategies co-existing in nature, the question is raised why one strategy is more advantageous for some species, whereas another strategy apparently is better for other species.

Sexual reproduction can be seen as a mechanism for the exchange and improvement of successful strategies since it recombines genes with the purpose of forming better offspring thereby increasing the fitness of a population. Less successful strategies eventually will be outcompeted due to natural selection. Recombining genes to form offspring can be viewed as partially copying and mixing the parents' strategies, which are transferred to individuals of a new generation. However, not only during reproduction individuals copy strategies of other individuals. Imagine for example an engaged discussion between two humans, which affects and influences their opinions. Each one of them will arrive at a new and more refined opinion, by keeping a part of the original opinion while replacing and extending another part by new insights based on the discussion. In this case, new strategies (opinions) are not simply transferred to another individual in a new generation, but the individuals themselves partially change their strategies. We can also think of individuals copying complete strategies of other individuals. Learning strategies of human babies, for example to achieve speaking or walking, consist largely of mimicking the behavior of others [Meltzoff and Moore, 1983, Termine and Izard, 1988]. Copying another one's behavior, especially if this behavior appears to work well, may be a successful strategy to improve fitness or chances of survival of an individual and of a population. In all these examples, good strategies are spread amongst individuals either by reproduction or by other interactions, to new generations or between the same individuals, and either completely or partially.

In this thesis, we examine different real-world phenomena to achieve a better and deeper understanding of the process of exchanging and spreading good strategies: in the field of reproduction (Chapters 3-5), but also in economics and sustainability science in relation to air pollution and emission control (Chapter 6). We use concepts and modeling approaches from the field of game theory, complemented with mathematical simulation techniques. While the specific problem settings vary from chapter to chapter, virtually all models in this thesis are agent-based. They do differ with respect to their structural properties. Figure 1.1 shows an overview of both the problem settings and the model properties for each chapter. Here, the first row lists the chapter number and its topic, the second and third rows show the underlying spatial and time structures, the fourth row presents the type of individuals the models consider, and in the last row, the problem setting is briefly described. In the following, for each chapter, the problem setting is described in more detail together with the accompanying research question that gets addressed.

Throughout this thesis, each chapter presents a mathematical model for a certain problem together with an accompanying agent-based simulation set-up. Then it shows and discusses the simulation results to obtain answers to the research questions of interest. While the current chapter gives an overview of the applications and their interconnections, Chapter 2 provides a general background on both the modeling techniques and on the related biology. The research questions of Chapters 3-6 are presented in the next section.



Chapter	Chapter 3	Chapter 4	Chapter 5	Chapter 6
Spatial structure	Non-spatial	Discrete-space grid	Continuous-space	Discrete-space network
Time	Discrete-time	Discrete-time	Static (no time modeled)	Continuous-time
Agents	Asexual and monoecious haploid sexual individuals	Female, male and hermaphroditic plants	Hermaphroditic oak trees	EU countries
Problem context	Sex vs. asex in changing environments	Influence of space on prevalence of sex types	Female choice mechanism in oak trees	National pollution policies and their international effects

Figure 1.1: This thesis at a glance: overview of the commonalities and differences between the topics and agent-based modeling approaches per chapter. The first row shows the topic, the second row the spatial aspect in the model, the third row the time aspect, the fourth row the investigated types of individuals and the fifth row the problem context.

Chapters and their Research Questions

Chapter 3:

The question “Why sex?” has puzzled many researchers in biology, but as yet remains unanswered to complete satisfaction. In stable environments, it is observed that asexual populations are able to very quickly increase their fitness, while sexual populations usually need more time to reach the same or a better fitness level [Edhan et al., 2017]. However, from the Darwinian principle that evolutionary processes favor fitter populations and mechanisms, sexual reproduction would go extinct unless it is advantageous for some species and under certain circumstances in one way or another. When environments change slowly, populations are generally able to slowly adapt and change along. But when encountering sudden environmental changes, we hypothesize that populations need genetic diversity to react quickly to survive in the new environment. Reproduction mechanisms therefore need to provide a balance between selecting for successful genotypes and being robust against environmental changes.

Research questions: *What are the differences in the mean viability development of sexual populations compared to asexual populations in fixed environments? How can a population be more robust against environmental shocks?*

In Chapter 3, a non-spatial, agent-based simulation model is used to compare the two reproduction methods in more detail. Populations of either sexually or asexually reproducing individuals undergo mating and death processes. Instead of modeling a certain species in a specific environment, we keep the model abstract and as simple as possible to gain insight into the general advantages and disadvantages of both forms of reproduction. Tracking the genetics of the individuals in the simulated populations allows for understanding the underlying mechanisms in a fixed environment. Furthermore, the simulations allow to examine what happens if an environment suddenly changes. In these situations, overall long-term population fitness faces a trade-off between keeping genetic diversity to achieve robustness against such changes, and fast specialization by selecting for successful genotypes to improve population fitness during intervals when environments do not change.

Chapter 4:

Plants can have male flowers producing pollen, or female flowers producing ovules that can be fertilized by pollen, or hermaphroditic flowers that are able to produce both pollen and ovules. Furthermore, a plant is not necessarily restricted to one type of flower. There are many plants with both male and female reproductive organs, also known as hermaphroditic plants. These hermaphrodites can allocate percentages of available resources to male and female reproduction. It is well-known that this sex allocation of hermaphroditic plants has an impact on the prevalence of sex types (males, females, and hermaphrodites) in a plant population [Charnov et al., 1976]. However, most of these models do not take into account any spatial aspects. They rather assume populations to be well-mixed and without restrictions on pollen flow distances.

Research question: *How do spatial effects, like competition for space or varying pollen dispersal distances, influence the prevalence of males, females, and hermaphrodites within a plant population?*

In Chapter 4, we present a discrete-space, agent-based model considering annual plants that are either completely male, completely female or hermaphroditic. Male and hermaphroditic plants spread pollen and fertilize ovules produced by other female and hermaphroditic plants, giving rise to the next generation of offspring. Next to modeling a broad variety of scenarios, this model allows us to investigate the frequency dynamics of the different phenotypes “male”, “female” and “hermaphrodites”, considering many generations. Thus, we are able to track which types go extinct, depending on the sex allocation of hermaphrodites and on available resources. We use this information first to examine the impact of plant spacing in contrast to a well-mixed population, and next to investigate the influence of increased seed/pollen dispersal distances and of introducing regions where no seeds can germinate on the prevalence of sex types.

Chapter 5:

Oak trees are hermaphroditic plants that can produce both pollen and ovules. Interestingly, oak trees produce six ovules per flower, but only one matures to an acorn, even when all ovules are fertilized. Thus, many fertilized ovules are aborted. Moreover, contrary to other species, long-distance fertilization is common in stands of oak trees and nearby oak trees are often absent as pollen donors. These observations cannot be explained by commonly used simple pollen flow models where the probability to fertilize a tree declines with distance. Therefore, the hypothesis is raised that oak trees evolved a female choice mechanism in such a way that the oaks choose ovules from rare pollen donors to mature to an acorn, instead of randomly choosing one ovule within a flower.

Research question: *Can the female choice hypothesis in oak trees explain the observed fertilization patterns of these trees?*

In Chapter 5, a continuous-space agent-based model is used to test the hypothesis that oaks choose an ovule for maturation to an acorn that is fertilized by a father that has fertilized the least number of ovules within that flower. This implies that rare fathers are favored. The oaks in our model have positions in continuous space and produce both pollen and ovules. We use a two-step lottery model to simulate the hypothesized female choice mechanism: In the first step, a pollen flow model is used to decide which ovules are fertilized by which fathers, and in the second step, the female choice mechanism is implemented. Next to examining the consequences of this mechanism, we validate whether our hypothesis on female choice in oak trees fits better actual field data on oak tree fertilization than a random choice hypothesis.

Chapter 6:

Pollution caused by industrial production is a critical environmental problem worldwide. It needs to be understood what drives countries to accept or reject environmentally friendly policies to produce their goods. Once this is well understood, effective policies can be designed which stimulate environmentally friendly behavior. In Chapter 6, we focus on EU countries affecting the pollution behavior as well as the pollution stock of neighboring countries.

Research question: *What are potentially effective policies that would lead to a more environmentally friendly goods production throughout the European Union (EU)?*

Chapter 6 uses an agent-based model, where the countries of the EU are the agents that can decide on how much they invest in clean policies. The borders of the countries define the spatial network structure, as well as whose air pollution is influencing whom. We analyze three different scenarios: (1) each country chooses its investment into clean policies such that its expected costs are minimal, (2) countries imitate the investments into clean policies of their neighbors without taking the neighbor's success concerning their costs into account, and (3) each country imitates its neighbors' investments into clean policies only if this behavior seems to bring a profit to the country. For each of these scenarios, we examine under which conditions the countries have incentives to act environmentally friendly.

Chapter 7:

In Chapter 7, we reflect on the work done in the four content chapters (Chapters 3-6). In this broader context, we summarize our results by answering the research question, evaluate the modeling techniques used in this thesis and discuss future research directions.

CHAPTER 2

Background

2.1 Modeling background

In this thesis, simulation models are used to get insights into real-world phenomena. Usually, it is not possible to capture all details of a phenomenon in a model [Marion and Lawson, 2008]. Reasons for that can be that information of the system under consideration is missing, or the system is too complex to be described completely. However, a model can serve as an abstract description of the phenomenon. The level of abstraction depends on the described system and on the purpose of the model [Crouch and Haines, 2004, Dym, 2004, Marion and Lawson, 2008]. For some model applications, a simple model might be reasonable, while for other applications, a high accuracy of the description is necessary. Models with a low abstraction level are often very complex, while simpler models may still be analyzed analytically, e.g., by solving model equations. In the analytic case, it is possible to obtain exact information on the investigated phenomena under the model assumptions [Law and Kelton, 2007]. Most often, however, models of real-world phenomena are too complex to aim for an analytic solution [Marion and Lawson, 2008]. Then, computer simulations are useful to get insight into the investigated phenomena. This thesis focuses on such real-world phenomena that are too complex to aim for analytic solutions. We use agent-based model simulations to examine the research questions presented in Chapter 1. The models in this thesis have various structural properties. In the following, a further categorization is shown.

2.1.1 Model properties

In this thesis, we focus on models that consider agents that interact with each other or with the environment. Agents in this sense can be living organisms, such as animals [Arnold and Cook, 1984, Heppner and Grenander, 1990], plants [Bawa, 1980, Charnov et al., 1976, De Jong et al., 2008] or cells [An et al., 2009, Staňková et al., 2019, You et al., 2019] as well as non-living objects such as cars [Nagatani, 1993, Nagel and Schreckenberg, 1992] or particles [Sinclair and Jackson, 1989, Zhou et al., 2010]. In the following, we will refer to these modeled objects as either agents or individuals. The interaction of these agents can also be of various forms: they may have pairwise interactions leading to reproduction, make decisions influencing others, follow physical laws, etc.

In addition, the models can have several structural properties. They may, for example, differ in the way how time or space is modeled. Both time and space may be modeled in an explicit or implicit way. Furthermore, there are many models where time and space aspects do not play a role at all. Here, we describe the model properties most relevant for this thesis.

Deterministic vs. stochastic models

Models without any random variables are called deterministic models [Law and Kelton, 2007]. Applying inputs to such a deterministic model will always lead to the same results or outputs [Marion and Lawson, 2008, Renard et al., 2013, Rey, 2015]. The model presented in Chapter 6 is an example of a deterministic model. There, simulating pollution in a network of countries in combination with the same set of inputs always leads to exactly the same outputs. In some situations, however, it would be very dangerous to neglect stochasticity in the process. In models of queuing systems, for example, variations in processing time can enormously influence the delays and thus the analysis of a given queuing system [Law and Kelton, 2007]. Models, where (at least some) parameters are described by random variables or distributions, are referred to as stochastic models [Rey, 2015]. Due to stochastic elements in these models, model outputs may differ per simulation run, even when using the same inputs [Garrido, 2009]. Simulating stochastic models many times provides output distributions rather than (mean) output values only. The advantage of output distributions is that they provide information not only on the average but also on the variance of the results. Except for the pollution model in Chapter 6, all other models used in this thesis are stochastic models. They all contain stochastic elements, such as random mating partner choice or random recombination of genes.

Static vs. dynamic models

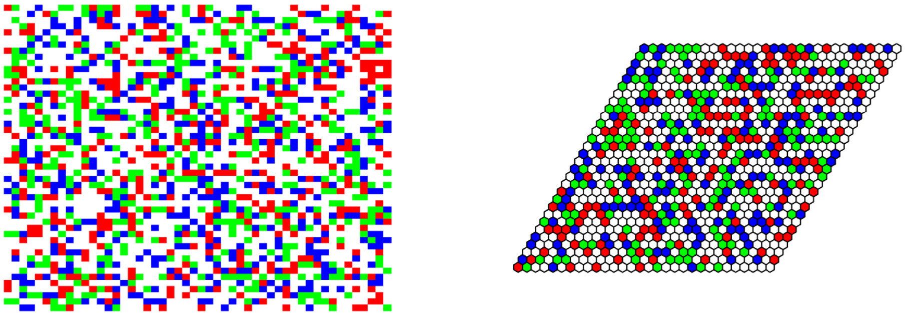
In a static model, time is not considered explicitly [Law and Kelton, 2007]. Variations of parameters over time are disregarded. In these models, (equation) parameters and all inputs of the model define a set of results. An example of a static model is a model of the mechanical stress of a bridge where the constructors want to find out whether this bridge can support a required weight. Some weight distribution can be used as an input for the model, and the output then shows if the construction of the bridge is strong enough for these inputs or a new design of the bridge is needed. In such a static model, time-varying effects like traffic or wind are either neglected or oversimplified. However, time-varying aspects may well affect the results. In order to include such time-dependent effects properly, a dynamic model is needed [Jørgensen et al., 2007, Li and O'Donoghue, 2012]. For example, when modeling how populations evolve, time naturally plays an explicit role. Generations are a natural choice to express time when examining population dynamics including death and birth processes. In this thesis, Chapters 3 and 4, for example, use dynamic models to examine how populations evolve from generation to generation.

Discrete-time vs. continuous-time models

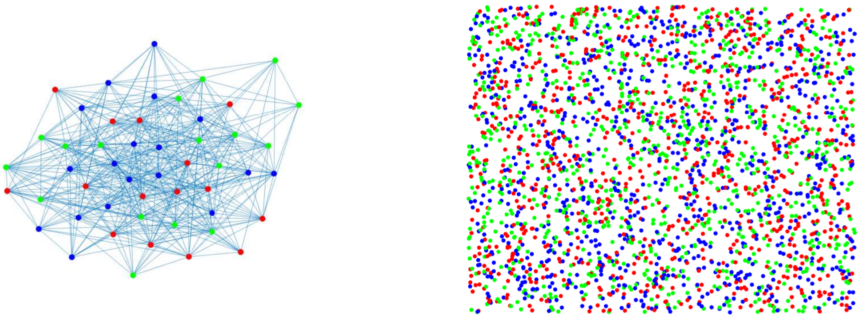
When modeling the evolution of species, usually time is measured in generations. They change in discrete steps of equal length. Models, where time is expressed explicitly, and changes occur in discrete steps, are called discrete-time models [Law and Kelton, 2007]. When the dynamics of a model do not change in every time step, but rather at (irregularly) occurring events, the model is referred to as an event-based model. Queuing systems are a typical example of such models as people usually arrive at a queue irregularly. The model presented in Chapter 3 is a hybrid model. In general, hybrid models combine different model characteristics. In Chapter 3, it combines discrete-time generations and irregularly events. There, sexual and asexual populations evolve over (discrete) generations and, environmental shocks arrive in some of these generations (events). Models where time progresses continuously, are called continuous-time models [Law and Kelton, 2007]. Often, such models are described by differential equations that express the changes of variables over time. When computer simulations are used to analyze the model, they have to be discretized, because a computer program can only evaluate a system at discrete time steps. Numerical methods like Runge-Kutta methods can be used to approximate the solution of a differential equation in case they cannot be solved analytically [Butcher, 2016, Wanner and Hairer, 1996]. Furthermore, there also exist hybrid models combining a continuous-time approach with a discrete-time one [Stéphanou and Volpert, 2016]. However, in this thesis, we consider either continuous-time models (Chapter 6) or discrete-time models with (Chapter 3) and without occurring events (Chapter 4). In Chapter 5, time is not modeled explicitly.

Spatial vs. non-spatial models

In many real-world phenomena, spatial aspects can influence the behavior (i.e., strategy, decision, or development) and/or the success of agents. These spatial aspects can vary from the agents' positions over geographical structures in the environment to spatially restricted interactions. Especially when examining biological phenomena such as the reproduction of plants and animals, spatial aspects often play an important role. Although present in the real-world scenario, many models neglect spatial aspects. They assume well-mixed populations and no spatial restrictions on the interaction of agents. However, examples show that results from this non-spatial approach may differ from results achieved by modeling the same scenario assuming a heterogeneous population without individual aspects like aging or local competitions for space [Kerr et al., 2002, Laird, 2014, Schüller, 2014, Schreiber and Killingback, 2013, You, 2018]. Nevertheless, spatial aspects should only be included in the model if they have an impact on the modeled phenomenon, as spatial models are usually harder to analyze than their non-spatial variants. In general, there are two main approaches to apply spatial models. First, one can consider reaction-diffusion processes by means of partial differential equations. These can either be solved analytically, or be discretized to be solved numerically, or be approximated by agent-based models. In the latter case, agents usually disperse randomly in space, and the model dynamics are obtained by expanding ordinary differential equations by a diffusion term. Second, the model can assume a continuous or discrete space as the underlying spatial structure, and the agents are distributed on this structure. Discrete-space structures can for example be modeled by rectangular lattices (Figure 2.1a) [Nakamaru et al., 1997, Nowak and May, 1992, Reichenbach et al., 2007], hexagonal lattices (Figure 2.1b) [Birch et al., 2007, Uyttendaele and Thuijsman, 2015] or graph/network structures (Figure 2.1c) [Barthélemy, 2011, Hauert and Szabó, 2005]. Both discrete- and continuous-space structures can be modeled as a field without (rectangular field) and with periodic boundary conditions (torus field). In Chapter 5, for example, we can run simulations for trees spread over both field forms. When considering a torus, pollen leaving the field on the left/right side enters the field again on the right/left side. Pollen leaving on the top/bottom border enters again on the bottom/top border, respectively. On a torus, no tree experiences any boundary effects. Often, interactions between agents in such a spatial structure are restricted to interactions between neighbors [Cardillo et al., 2012, Kerr et al., 2002, Killingback and Doebeli, 1996, Sysi-Aho et al., 2005]. Depending on the spatial structure, the number of neighbors may differ. Considering a rectangular lattice (Figure 2.1a), for example, the number of direct neighbors of a focal individual can either maximally be four or eight, depending on whether or not diagonal cells are assumed to be direct neighbors as well. The concrete number of neighbors depends on how many neighboring cells are occupied. In a graph or network structure (Figure 2.1c), direct neighbors are those individuals that have a direct connection to an individual. However, both on a lattice and a graph, the neighborhood of a focal individual may not only be restricted to direct neighbors but may instead contain all individuals within a certain distance. In discrete-space structures, different distance measures defining which individuals are within a neighborhood are possible, while in continuous-space structures, a radius defines a circular neighborhood of an individual. In Chapter 4, for example, rectangular regions of different sizes around a focal individual define the neighbors that can be reached by pollen of the focal individual. The above-described examples only consider two-dimensional space. However, spatial models can also be multi-dimensional. In three-dimensional space, e.g., interaction areas can be defined similarly and have a spherical or cubic shape. In this thesis, we will focus on the two-dimensional case only.



(a) Rectangular grid structure *(b) Hexagonal grid structure*



(c) Network structure *(d) Continuous-space field*

Figure 2.1: Different two-dimensional spatial model structures.

2.1.2 Agent-based modeling

To model real-world problems dealt with in this thesis, we mainly focus on agent-based models (ABMs). These are used to analyze *interactions* between *agents* and are usually analyzed by means of *simulations*.

Agent-based models are often contrasted by equation-based models [Rahmandad and Sterman, 2008, Van Dyke Parunak et al., 1998], but also combined with these to use the advantages of both approaches [Bobashev et al., 2007]. Equation-based models are also referred to as classical models, and they capture the change of a system over time (e.g., by ordinary differential equations) or over time and space (e.g., by partial differential equations) [Füllsack, 2013] in a macroscopic way. In contrast to that, agent-based models capture the diversity of the agents in the system and their interactions on a microscopic level. Both forms of models describe or simulate a certain system by first building the model and then executing it. However, the two common approaches differ in the modeling form as well as in their execution [Van Dyke Parunak et al., 1998].

Introduction to agent-based modeling

The classical modeling approach is to describe a certain system by means of equations. However, Grimm and Railsback [2005] argue that this approach may not be the best for all applications. In physics, for example, many phenomena like the flow of an electric current or the motion of an object can be examined by equation-based models, although the properties of atoms and their interaction influence the properties of the complete system. In contrast to atoms, the agents in ecological models are living organisms like plants, humans or animals. These organisms have a life cycle full of development: They mature, reproduce, die, and interact with the environment as they need resources for example. Furthermore, these organisms may differ from each other a lot. They have individual characteristics, and these characteristics influence the strategies and/or the success of these strategies. The interactions among individuals contribute to the reproduction success of the entire population. Thus, to understand development on a population level, one may want to include the individual interactions. Therefore, in ecology, the use of agent-based models – or individual-based models as they are often referred to – is popular, because these models can capture the diversity of individuals and their interactions on a microscopic level. Furthermore, while the classical approach allows for direct analysis that may require deep mathematics, ABMs usually need simulations as analysis tool. Therefore, no deep understanding in mathematics is needed to analyze ABMs. ABMs belong to the group of computational models, which may require huge computational resources to study complex scenarios with the help of computer simulations [Melnik, 2015]. Computer simulations are often needed when the non-linear and adaptive interactions between agents are too complex to be analyzed analytically [Srbljinović and Škunca, 2003].

In spite of their growing popularity, no strict, universally accepted definition for ABMs exists [DeAngelis and Mooij, 2005, Grimm and Railsback, 2005]. In this thesis, we adopt the definition by DeAngelis and Mooij [2005] saying that ABMs “simulate populations or systems of populations as being composed of discrete agents that represent individual organisms or groups of similar individual organisms, with sets of traits that vary among the agents”. According to this definition, all models used in this thesis are agent-based models: the models examined in Chapter 3 to 5 simulate populations of genetically diverse individuals that reproduce. The model in Chapter 6 studies a group of individual countries that decide how much to invest in environmentally friendly policies. In the following sections, we give more insight into agent-based modeling, its development and its (dis-)advantages.

Advantages of ABMs

Some applications may be easier described by ABMs than by classical models [Adami et al., 2016, Grimm and Railsback, 2005]. In particular, ABMs can more easily deal with a great diversity of individuals without becoming too complex. In modeling ecological and evolutionary processes, DeAngelis and Mooij [2005] identified five categories in which agents can individually differ from each other: spatial, ontogenetic, phenotypic, cognitive and genetic:

- *Variability in Space*: Classical models may contain implicit spatial aspects, but they cannot typically model distinct individuals that create local nonuniformity in populations. Many authors could observe differences between predictions of spatially explicit and non-spatial models [Chesson, 1981, Durrett and Levin, 1994, You, 2018].

- *Variability in Ontogeny*: Some variation in ontogeny can be modeled by classical models. Already in the 1940s, Leslie [1945, 1948] presented models that included individual age structures. However, in order to investigate a more detailed life cycle and its influence on individual interactions (like foraging processes), ABMs have proved to be a more useful tool to handle the complexity caused by these variations [Schüller, 2014].
- *Variability in Genetics*: ABMs are often able to capture the genetic changes in real populations much better than classical models. When modeling genetics in populations, individuals can differ a lot from each other. Furthermore, introducing gene mutations or genetic drift, for example, increases the diversity among individuals and their development. This variety of individuals, strategies, and development can usually be captured well by ABMs.
- *Variability in Phenotypes*: Even when considering genetically identical individuals, phenotypic differences between them can influence the population dynamics. Resource availability is one major factor. Animals finding enough food, for example, can grow more and are stronger than genetically identical animals lacking these resources. Size and strength of an animal determine the surviving success in changing environments as well as in fights against predators. These individual differences can be addressed very easily with ABMs.
- *Variability in Cognition*: Learning processes are in part individual experiences as they include individual memories. These processes can often focus on learning from other individuals and sometimes on learning from the environment. Especially the first one is influenced by interactions with other individuals, which affect the phenotype and, thus, the fitness of an individual. ABMs can be set up to include this.

It may be possible to include some of these aspects in classical models, but when all the individual variety needs to be included in a model, then a classical approach quickly becomes too complex, while an ABM is still able to capture the diversity. Especially when individual behavior is very complex and can only be characterized by discrete “if-then” rules, ABMs may be advantageous over classical models. Discreteness in individual behavior is difficult to capture in differential equations [Bonabeau, 2002]. Agent-based modeling often gives more freedom to choose many individual parameters. Furthermore, an ABM is usually defined by simple rules for the interaction between individuals. These interaction rules are motivated by observations in nature and, thus, are often intuitive. In contrast to classical differential equation models, where often deep mathematics is needed to analyze the model, ABMs usually need simulations for analysis and thus, can also be analyzed by a less technical audience [Bonabeau, 2002, Ellner, 2001, Gilbert and Troitzsch, 2005, Wissel, 2000].

When to use ABMs?

While we discussed the advantages of ABMs in the previous section, ABMs bring disadvantages as well [Grimm and Railsback, 2005]. One main point of criticism on this type of modeling is that the execution is often computationally expensive. This also holds for the models examined in Chapter 3 and Chapter 4 of this thesis. However, the great genetic diversity (Chapter 3) and the spatial competition (Chapter 4) are hard to capture with a classical model. Due to the stochasticity in these models, many simulations with the same initial conditions had to be performed in order to get reliable results. We use a computing cluster where many simulations can be run in parallel to reduce the waiting time.

ABMs often define interactions on an individual, microscopic level that are documented by means of words rather than by means of equations. Although transferred into code, the interactions of agents in ABMs are often described by if-then-rules in the literature. These descriptions need to be very precise in order to ensure that the model can be compared to other models and that results of ABMs can be reproduced [VDI/VDE 2653-1, 2010]. In some research fields like in industrial automation, there already exist guidelines regarding the description and use of ABMs [VDI/VDE 2653-1, 2010]. These guidelines even give suggestions in what automation applications ABMs may be used [VDI/VDE 2653-3, 2010].

In order to standardize the description of ABMs especially in ecology, Grimm et al. [2006] introduced the ODD protocol tested by 28 modelers. The protocol consists of three large parts that contain in total seven elements:

- Overview: 1) purpose, 2) state variables and their scales, 3) process overview and scheduling
- Design concepts: 4) design concepts
- Details: 5) initialization, 6) input, 7) submodels

Within this protocol, the overview part should provide the information needed to create the framework of the ABM in an object-oriented language. In the design concepts part, general underlying concepts including the interaction among individuals are described. The details part includes all the details that are not described in the design concepts part but are necessary to be able to completely re-implement the ABM. In 2010, the ODD protocol was updated as it was misunderstood in some parts [Grimm et al., 2010]. Therefore, element 2) was renamed to “Entities, state variables, and scales” and element 6) to “Input data”. Furthermore, Grimm et al. [2010] included more topics to specify in the design concepts part. While in this thesis, we do not completely commit to the ODD protocol, we implicitly follow its structure: First, we state the purpose of the model, followed by the description of the characteristics of the agents, their interactions and, if time plays a role in our model, which processes take place during one generation. Design concepts like fitness are defined afterwards. The setting of the simulations including the initialization of parameters and the input data are presented before each experiment. With this approach, our models and results are still reproducible.

The advantage of a great freedom of parameters at the same time brings a big challenge. When setting up a model, all these parameters have to be defined properly and in an overall consistent and coordinated manner. This parametrization ideally should be aligned with data and observations. Often, such data is not available in full. However, data or information requirements are not only a big challenge when using ABMs, but also for classical models. In the model examined in Chapter 5, for example, we use data from three published field studies to validate our model. Furthermore, current pollution data is used as input in the model of Chapter 6. In these models, real data can be used as the models describe a concrete species (Chapter 5) or a concrete competition scenario (Chapter 6). By contrast, the use of data in the other models of this thesis is difficult, as they describe general processes rather than capturing a specific real-world scenario.

All these challenges have to be kept in mind when choosing an ABM to capture a phenomenon. It depends on both the application and the purpose of the model, whether an ABM is the best choice. In those applications where a great variety of heterogeneous individual behavior determines the population dynamics, ABMs are highly valuable [Bonabeau, 2002], because they are very well able to capture the heterogeneity while remaining transparent. Furthermore, when learning and adaptation of individuals are considered, or when individuals move through space, ABMs may have advantages over other approaches as well. [Bonabeau, 2002]. Especially in ecological studies, where living individuals with diverse properties interact with themselves and with the environment, ABMs are often used. However, the more details are included in a model, the more complex it becomes. This does not only hold for ABMs, but for classical models as well. Thus, every model needs to balance between the level of abstraction (simplicity) and detail (complexity).

Evolutionary game theory using agent-based methods

Game theory is a standard framework in economics to examine best response strategies for individuals in competitive situations. Its origins date back to 1944 when Von Neumann and Morgenstern [1944] first introduced its basics. Beginning with the seminal paper by Maynard Smith and Price [1973], there was a shift from an emphasis on models with rational individuals, choosing fixed optimal strategies against other individuals' behavior, to evolutionary models [Samuelson, 2002]. The term “evolutionary game theory” includes a great variety of models describing how individuals adapt their behavior over a certain period of time. This definition covers biological models as well as learning algorithms, such as used in artificial intelligence and many more [Samuelson, 2002]. In this thesis, the models of Chapter 3, Chapter 4 and Chapter 6 all investigate the adaption of individuals over time. While classical models can predict optimal strategies in simple settings, e.g., when assuming the population of individuals to be well-mixed and large, more realistic situations with small heterogeneous populations or spatial interactions can often be examined more easily using agent-based models [Adami et al., 2016].

2.2 Biological background

Most of the models in this thesis address scenarios concerning reproduction. Two pure forms of reproduction exist: sexual and asexual reproduction. In the following, we provide an overview of different aspects of these forms of reproduction. This information is needed in Chapter 3, where we compare sexual and asexual reproduction in both fixed and changing environments. We then continue with a short background on plant reproduction. In particular, we focus on different sex types, breeding systems, and flower anatomy. These sections serve as background for Chapter 4 and for Chapter 5. However, we start this section with a glossary for the biological background in order to make the following subsections easier to read.

2.2.1 Biological glossary

- Alleles: Alternative forms of a gene at a certain locus.
- Chromosome: Part of a cell that stores genetic information. It contains DNA and many proteins.
- Diploid Organism: An organism having a pair of each type of chromosome.
- DNA: Molecule composed of two chains in double helix where genes are encoded.
- Eukaryotes: Organisms whose cells have a membrane-bound nucleus.
- Fertilization: Fusion of haploid gametes to form a diploid cell (zygote).
- Gametes: Haploid cell that fuses with another gamete during the fertilization of an individual. In females, these cells are called ovum or egg; in males, these are called sperm.
- Gametophyte: Haploid multicellular stage in the life cycle of a plant developed from a haploid spore.
- Germ Cell: Cell that gives rise to the gametes of an organism that reproduces sexually.
- Haploid Organism: An organism having a single set of unpaired chromosomes.
- Locus: Position of a gene on a chromosome.
- Meiosis: Cell division in which the chromosome number is reduced by half and in which four haploid cells are created. These resulting cells are genetically different from the initial cell.
- Mitosis: Step of the cell cycle in which the duplicated DNA is separated, and two new cells are created.

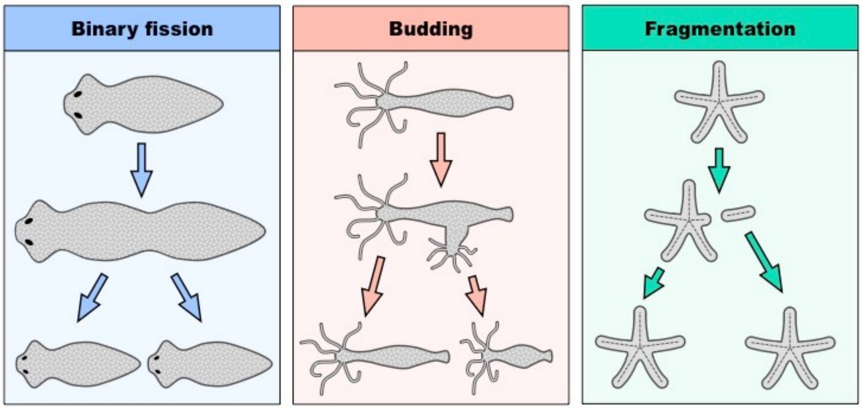


Figure 2.2: Different forms of asexual reproduction [Cornell, 2016].

- Nucleus: A membrane-bound structure that contains the cell's hereditary information and controls the cell's growth and reproduction.
- Prokaryotes: Unicellular organism without a nucleus, mitochondria, or any other membrane-bound structure.
- Sporophyte: Diploid multicellular stage in the life cycle of a plant that is developed from the zygote.
- Zygote: Cell formed by fusion of two gametes during fertilization.

2.2.2 Asexual reproduction

In asexual reproduction, one or more genetically identical individuals are formed from an adult individual. This form of reproduction can often be observed in lower life forms [Van Damme et al., 2004]. There are many different forms of asexual reproduction. The most well-known forms are: fission, budding, and fragmentation (see Figure 2.2). Fission is the division of a single agent into multiple parts. Many types of bacteria, for example, reproduce by fission [Angert, 2005]. Budding is a form of reproduction where an outgrowth develops on one side of the organism and separates when matured. Hydra, for example, are reproducing like this [Graf and Gierer, 1980, Otto and Campbell, 1977]. Many types of yeasts reproduce by fragmentation [Dombek and Ingram, 1986]. There, the organism is split into fragments, which mature to genetically identical copies. Many plants develop fragments of themselves that grow to new plants. This approach is called vegetative propagation [Harada and Iwasa, 1994, Hussey, 1978]. All these forms of asexual reproduction have in common that only one adult is involved; a mating partner is not required. This is considered a huge advantage of asexual reproduction over sexual reproduction [Archetti, 2004, Maynard Smith, 1971, 1978]. In asexual reproduction, the offspring is a genetically identical copy of the parent individual. Genetic recombination does not take place.

Most of the organisms reproducing asexually are prokaryotes. However, a form of eukaryotic asexual reproduction exists as well. Eukaryotes are organisms whose cells have a nucleus surrounded by membranes. In contrast to that, prokaryotes do not have any membrane-bound organelle. The division of a eukaryote starts with mitosis. This is the process where the membrane dissolves and the nucleus divides. The chromosomes are separated as well, such that each daughter cell receives a diploid chromosome set. The second step is cytokinesis, where the cytoplasm is divided into eukaryotic cells resulting in two identical daughter cells. As prokaryotes do not have the membrane structure, they only have to perform cytokinesis after copying the nucleus. Thus, prokaryotes reproduce asexually without any mitosis.

2.2.3 Sexual reproduction

In contrast to asexual reproduction, sexual reproduction involves two parent individuals. In the fertilization process, sex cells (gametes) of both parents combine, which results in genetically distinct offspring. This form of reproduction can be found in most eukaryotes, including humans. Some species like cacti or starfish, for example, can reproduce both sexually and asexually [Ortega-Baes and Gorostiague, 2013, Ottesen and Lucas, 1982, Willis and Ayre, 1985]. However, all sexually reproducing organisms have certain key life cycle features in common, like meiosis and fertilization. Depending on the species, these features may vary a lot. In the following, variations of these sexual life cycles are briefly introduced. This overview is taken from OpenStax [2015].

Diploid-dominant life cycle

Humans and most animals are following a diploid-dominant type of life cycle. There, the only haploid cells are the sex cells (gametes). At an early stage of the development of an organism, diploid cells (germ cells) are created in the gonads (testes and ovaries). Some of these undergo meiosis and form haploid gametes (sperm and eggs). In the fertilization process, the haploid gametes fuse to form a diploid cell (zygote). By mitosis, two new cells are formed.

Haploid-dominant life cycle

In a haploid-dominant life cycle, the single-celled zygote is the only diploid cell. Fungi and some algae are examples of organisms following this life cycle. In such a haploid-dominant life cycle, multicellular haploid structures (hyphae) are formed by mitosis. When two compatible individuals have grown towards each other, the hyphae of both individuals form a structure called zygosporangium. It contains multiple haploid nuclei from the two parents within a single cell. These haploid nuclei fuse and form diploid nuclei (equivalent to zygotes). They are carried by a cell called the zygospore. With meiosis, the life cycle is completed.

Alternation of generations

This type of life cycle is a mixture of the two previous types. Some forms of algae, for example, are following this cycle. The haploid organism creates gametes using specialized cells. As the organism is already haploid, meiosis is not necessary to form the gametes in this case. The zygote is formed by the fertilization of the haploid gametes and undergoes many rounds of mitosis. At the end of this process, a diploid multicellular sporophyte is formed. By meiosis, specialized cells of this sporophyte produce haploid spores that will develop into multicellular gametophytes.

2.2.4 Reproduction in plants

Sexes in plants

When considering human beings, we distinguish between two sexes: males and females. In plants, there are many more sexes to examine. Table 2.1 displays an overview of the sexes on flower, individual plant, and population level. Flowers can be male, female, or hermaphroditic. An individual plant can bear any combinations of these flowers. This combination determines the sex of the individual plant. The composition of different plant sexes within a population again determines the sex system (or breeding system) of that population. As hermaphrodites can produce both ovules and pollen, they may also be able to fertilize themselves, which is referred to as selfing. However, there are also lots of plants that are self-incompatible [Takayama and Isogai, 2005]. In Chapter 4, we examine under what conditions different sex systems of plant populations that are self-incompatible can be observed.

Flower anatomy

Flowers are the reproductive organs of flowering plants. The flower itself consists of several parts. Figure 2.3 shows a schematic representation of a hermaphroditic flower. The pistil is the female reproductive part of the flower consisting of the ovary containing the potential seeds (ovules), the pollen-receptive platform called stigma and the style connecting the ovary and the stigma.

When pollen lands on the stigma and germinates, it forms a pollen tube. This pollen tube growth down towards the style to transport the genetic information carried by the pollen to the ovules in the ovary [Editors of Encyclopaedia Britannica, 2018].

The stamen is the male reproductive part of a flower. It consists of the filament with an anther at the top. In the anther, pollen production takes place.

Staminate and pistillate flowers only contain the reproductive part necessary for either producing pollen or for letting the ovules be fertilized. The other parts of the flower stay the same.

Sexuality	Description
Individual Flowers	
Hermaphrodite	Bisexual flower with both stamens and pistil
Diclinous	Unisexual flowers
pistillate	Unisexual flower with pistil only
staminate	Unisexual flower with stamens only
Individual Plants	
Hermaphrodite	Only hermaphrodite flowers
Monoecious	Both pistillate and staminate flowers on the same plant
Dioecious	Staminate and pistillate flowers borne on different plants
Gynoecious	Plant bears only pistillate flowers
Androecious	Plant bears only staminate flowers
Gynomonoecious	Plant bears both hermaphrodite and pistillate flowers
Andromonoecious	Plant bears both hermaphrodite and staminate flowers
Trimonoecious	Plant bears hermaphrodite, pistillate and staminate flowers
Plant Populations	
Hermaphrodite	Only hermaphrodite plants
Monoecious	Only monoecious plants
Dioecious	Only dioecious plants
Gynodioecious	Both hermaphrodite and gynoecious plants
Androdioecious	Both hermaphrodite and androecious plants
Trioecious	Hermaphrodite, gyneocious and androecious plants

Table 2.1: Sexes in plants on flower, plant and population level [De Jong et al., 2008, Dellaporta and Calderon-Urrea, 1993]

2.2.5 Genetics

No matter whether organisms reproduce sexually or asexually, and no matter whether we talk about plants or animals, they transfer their genes to the offspring. The following brief introduction into genetics shall serve as an overview of aspects of genetics used in this thesis and is adapted from Staroscik [2018].

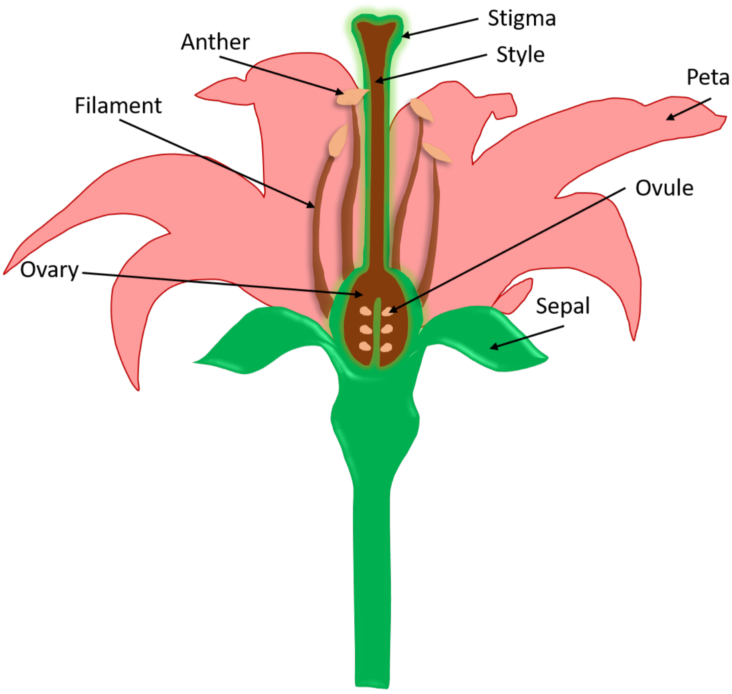


Figure 2.3: Flower Anatomy. Picture adopted from [ProFlowers, 2014]

Genes, loci, and alleles

In genetics, the transfer of heritable information is studied. Living organisms use DNA to pass the information from one generation to the next one. In the DNA, the genetic information is encoded. This genetic information is contained in discrete units that are called genes. Dependent on the species, the genes occur at certain locations on the chromosomes that contain DNA. This position of a gene on a chromosome is called locus. Alternative forms of genes at a locus are alleles. In this sense, brown, blue, and green are alternative forms of the same characteristics - namely eye color.

Genotypes and phenotypes

An organism's phenotype is its set of observable characteristics, whereas the genotype is the complete hereditary material of this organism. Genotypes of diploid organisms cannot be observed directly from the appearance of that organism. Considering, for example, the four blood types A, B, 0, and AB, which are four different phenotypes. The corresponding possible genotypes of a diploid organism are: AA, AB, A0, BB, B0, and 00. The resulting phenotype is then determined by the combination of dominant and recessive alleles. In the blood type example, allele A and allele B are both dominant to allele 0; they are co-dominant. Thus, genotypes AA and A0 lead to phenotype A, AB to AB, BB and B0 to B and 00 to 0. In a haploid organism, the genotype is directly leading to the phenotype, as the organism only has a single set of chromosomes.

CHAPTER 3

Evolutionary fitness optimization and robustness: sexual and asexual reproduction in dynamic environments

Abstract

The question of why we observe a lot of species reproducing sexually despite the fact that this form of reproduction bears many costs has long been a major challenge [Barton and Charlesworth, 1998, Muller, 1932, Siller, 2001]. To attain insight into the advantages of sexual reproduction, we consider a discrete-time mathematical model based on previous research by Edhan et al. [2017], tracking genetic parameters of individuals in simulations of both sexually and asexually reproducing populations. Although our agent-based model considers a stable environment and no mutations, we observe that sexually reproducing populations are able to attain significantly higher mean fitness levels than comparable asexually reproducing populations. Asexual populations directly increase their mean fitness at an exponential rate but converge to fitness levels lower than those of comparable sexual populations. However, sexual populations first pass through a lengthy learning phase of no fitness increase before they begin a steady climb up in mean fitness. Via analysis of our agent-based simulations, tracking genetic parameters in simulated populations, we provide explanations of the mechanisms that lead to the observed fitness advantage of sexual populations as well

as the different phases of fitness that they go through in their dynamic. In addition, we investigate the influence of several model parameters on the sexual population development dynamic and show that, without mutations, in the long run, sexual reproduction does not lead to a genetically diverse population but rather to an optimized population consisting of a uniform genotype, borne by every individual in the population. To extend the basic model, we also investigate discrete environmental changes and their effects on population genetics and fitness. In this context, we examine the trade-off between population fitness optimization and robustness against sudden environmental shocks.

3.1 Introduction

In nature, we can observe both sexually and asexually reproducing individuals. Both forms of reproduction seem to have advantages for their own circumstances as otherwise, we would expect that one of them goes extinct.

Sexually reproducing species have a two-fold disadvantage in comparison to asexually reproducing species, simply due to the fact that they need two individuals to produce offspring [Maynard Smith, 1978, Williams, 1975]. Furthermore, these individuals may need to invest a significant amount effort in finding mating partners: depending on the species, this investment varies from spending time in locating a partner [Anstensrud, 1992, Dewsbury, 1982], performing dangerous fights [Bateman, 1948, Le Boeuf, 1974] or changing appearance [Haselton et al., 2007]. The mating process itself involves difficulties as well: during contact between two different individuals, diseases or parasites may easily be transmitted [Anderson et al., 1991, Lockhart et al., 1996, Thrall et al., 2000]. In addition, the recombination of genes may destroy successful gene combinations such that two very successful parent individuals may well produce less good offspring [Turner, 1967].

By contrast to these disadvantages, the main hypotheses forwarded in the literature to explain the prevalence of sexual reproduction in nature include: (1) sexual reproduction as a process of DNA repair [Bernstein et al., 1981, Felsenstein, 1974, Maynard Smith, 1978], (2) decreasing competition amongst offspring due to genetic diversity between offspring [Bulmer, 1980, Maynard Smith, 1976, Taylor, 1979], (3) boosting the probability of producing “better” genotypes that increase mean population fitness [Marais and Charlesworth, 2003], (4) accelerating the rate of evolution by natural selection [Crow and Kimura, 1965, Maynard Smith, 1968] and (5) promoting genetic variation to ensure populations are robust against extreme environmental changes [Bonner, 1958, Daly, 1978]. The model and simulations presented in this chapter focus on hypothesis (3) and investigate aspects of hypotheses (4) and (5) within this context.

Much research about the reproductive advantage of sex focuses on the relationship between genotypes and fitness. Understanding this relationship can be used to examine the mechanisms of species' adaptations and speciations [Fragata et al., 2019]. In this context, the concept of fitness landscapes is often used. These fitness landscapes map a genotype to a fitness value resulting in points that define locations in the landscape. By way of reproduction and mutation, populations aim to reach the fitness optima in the landscapes. The structure of a fitness landscape can vary from flat (where all genotypes have the same fitness) to extremely rugged (where the genotypes' fitness values vary a lot). Kauffman's Nk-model can be used to examine the hill-climbing of populations by way of mutation [Kauffman and Weinberger, 1989]. The parameter k models the structure of the landscape, where $k = 0$ leads to a smooth and $k = N - 1$ to the most rugged landscape. The model considered in this chapter can be seen as the last case as we consider genotypes with random fitness values from the complete interval $[0, 1]$. However, we furthermore increase the complexity by not considering mutation as the driving force in our population dynamics but unbiased uniform crossover [Culberson, 1994].

Edhan et al. [2017] use a mathematical model to compare the sexual with the asexual form of reproduction. In their work, evolution is presented as a form of learning: the reproducing population is essentially learning a given environment, with an objective function of attaining maximal mean fitness. This learning process is greatly limited by the fact that only small samples of the genotype space are made available. An asexually reproducing population rapidly identifies the locally optimal genotype within the one and only sample it has (at least until mutations can change that). The chances that this sample from the immense genotype space contains a globally optimal genotype are exceedingly small.

Sexually reproducing populations, in contrast, are engaged in constant exploration of the genotype space, with a new sampling of the genotype space available in every generation by virtue of genetic recombination. This exploration, however, is not purely a random walk through the space. The sexual reproduction algorithm also includes a "regret minimization" element that enables the population over time to shed under-performing alleles and hence concentrate on steadily better genotypes. In this way, it eventually identifies genotypes that provide higher mean fitness than could be expected from a parallel asexual population starting from the same founding population. This holds true in both fixed and changing environments, without mutations.

Edhan et al. [2017] present simulations to compare the mean viability in sexual and asexual populations in fixed environments, where the mean viability is defined as the weighted average of all genotype viability values in the population. Genotype viability, in turn, is defined as the probability that a certain genotype survives to reproductive maturity and mating. Interestingly, the simulations of Edhan et al. [2017] show that the mean viability of a sexual population starts to increase only after it has passed through a kind of learning phase during which the expected mean viability does not rise at all, while in contrast the mean viability of an asexual population strongly increases at an exponential rate directly from the start. However, the simulations of Edhan et al. [2017] do not track the genetics of individuals in the population and thus do not provide an explanation for this phenomenon.

The main focus of this chapter is to compare the sexual and asexual reproduction forms in more detail and in both fixed and changing environments. Based on the model of Edhan et al. [2017], we use simulations to answer open questions of their work by explaining the observed patterns described in the previous paragraph. Furthermore, we examine how population dynamics change in both sexual and asexual populations when environments suddenly change. Our model is kept as simple as possible. Instead of modeling a concrete species in a concrete environment, we focus on modeling the reproduction mechanisms and rather drastic environmental changes. With this approach, we can observe the impact of these abrupt changes on the population dynamics without any influences of other factors.

In Section 3.2, we provide a description of the underlying model and a more detailed definition of sexual and asexual reproduction. Next, we define fitness in our model and its relation to mean viability. In our simulation-based case studies, explored in Section 3.3, we observe that the mean viability of a sexual population converges to a certain maximum level. The reason is that the sexual population, like the asexual one, ends up in a single-genotypic population. This contradicts simple textbook biology claims that sexual reproduction promotes genetic diversity [Fester Kratz, 2017].

Furthermore, we investigate the influence of several model parameters such as genome size, controlled by both the number of loci and the number of alleles per locus, on the duration of the initial learning phase of the sexual population and on how long it takes until it reaches its maximal level of mean viability. The results show that more complex species need a longer initial learning phase and reach the maximum level of mean viability later than genetically simple species.

Next, we explore the trade-off between fitness optimization and robustness to changing environments by studying the effects of sudden environmental shocks on the mean viabilities of various reproducing populations. In this context, we first investigate at what stage of evolution a sudden disaster has the least impact on the mean viability. Secondly, we study what influence the genome size has on the impact of a disaster at a certain point in time. Bentkowski et al. [2015] have found that the genome length is influenced by the variability of the environment. Their results show that changing environments lead to large genomes because these seem to be more robust against disasters in the environment.

Our results show that at the very beginning of our simulations, species are still robust against environmental shocks, while they have not yet been successful in improving their population fitness. After some more generations, however, they have specialized to a narrow set of successful genotypes and are no longer able to adjust to environmental shocks. Thus, a single disaster has the least impact on the development of the population if it happens very early in the process. If we consider recurring disasters, then a population has to increase its fitness between two disasters but still needs to maintain robustness against sudden environmental shocks. It thus faces a trade-off between robustness against environmental changes and optimization of the population fitness. Section 3.4 concludes the chapter with a discussion of possibilities for further research.

3.2 The model

In this section, we introduce the model used for the simulations described in Section 3.3. It is based on the work by Edhan et al. [2017], who set up a mathematical model to answer the question of why sexual reproduction can be observed in nature despite all the costs associated with this form of reproduction. We consider a discrete-time mathematical model in which we track the genetics of individuals in a finite population.

Each individual is associated with a genotype g that consists of a string of p alleles. The position of an allele within this string is known as a locus. For each locus l, define the finite set of possible alleles as $A_l = \{a_{l1}, a_{l2}, ..., a_{lq}\}$, with q being the number of different alleles possible per locus. Then the set of all possible genotypes is $A_1 \times A_2 \times ... \times A_p$. For simplicity, we assume that all genotypes consist of the same number of alleles. In our simulations, we also assume that each initial population contains all possible alleles, but not necessarily all possible genotypes and that in each generation t, all the individuals of the population reproduce. This “mating” by either one or two individuals, depending on the form of reproduction, is called *interaction*. Each interaction results in two offspring individuals. This number is fixed no matter which genotypes the interaction partners bear. In the sexual case, an individual can transfer its genes to the next generation in two ways (see Section 3.2.1). First, all individuals are selected to reproduce and thus recombine their genes with a random mating partner. Second, individuals can be selected as mating partners (independently of whether or not they already produced offspring).

The genotypes of the offspring depend on the form of reproduction. In an asexual population, each offspring is an identical genetic copy of the parent individual, whereas in a sexual population, the offspring genotype is a recombination of the parent genotypes (see Section 3.2.1 and 3.2.2). The individuals of generation t die and the population of generation $t+1$ is formed by only newborn individuals that pass through a viability selection: each genotype g is associated with a certain viability v_g, which can be interpreted as the probability that an individual bearing genotype g will survive to reproductive maturity. Note that there is no necessary correspondence in the viability values between different genotypes, even if the genotypes are ‘similar’ in the sense that they share the same alleles in most, or even almost all, of their loci. The viability values of different genotypes are completely independent of each other.

The population of generation $t+1$ is thus formed by those individuals generated as the offspring of generation t that survive the viability selection.

During each run of our simulations we tracked the mean viability of the population. For a population P with $n[t]$ individuals at generation $t \in \{0, 1, 2, 3, ...\}$, the mean viability is defined as

$$\bar{v}[t] = \sum_{g \in P} \frac{n_g[t] v_g}{n[t]}, \tag{3.1}$$

with v_g being the viability for genotype g and $n_g[t]$ the number of individuals of genotype g at time t.

3.2.1 Sexual reproduction

In our model of sexually reproducing populations, we consider populations of haploid monoecious individuals. Haploid individuals have only one member of each pair of homologous chromosomes. We may consider monoecious individuals as having both female and male sex organs. We will therefore not distinguish between males and females in our simulations. Examples of such species include some form of algae [Klinger, 1993] and the yeast Saccharomyces cerevisiae [Edhan et al., 2017]. In each sexual interaction, two different individuals are involved, and the newly formed offspring genotype is a recombination of both parent genotypes; hence this form of interaction is also called *recombinational* [Grande and Brown, 2010]. In our model, for each locus of an offspring, an allele is randomly chosen from the corresponding locus of one of the parents. For example, parent individuals with genotypes $a_{12}a_{23}$ and $a_{11}a_{22}$ can create four genetically different offspring individuals, namely $a_{11}a_{23}$, $a_{11}a_{22}$, $a_{12}a_{23}$ and $a_{12}a_{22}$. In this case, genotypes have a length of two, which means that alleles from two different loci form a genotype.

3.2.2 Asexual reproduction

In asexual reproduction, only one individual is involved in the creation of new offspring. The offspring is a genetic copy of the parent individual. Thus, the offspring bears exactly the same alleles as the parent individual. This means that a parent individual of genotype $a_{11}a_{23}$ can only produce offspring individuals of the same genotype $a_{11}a_{23}$. This form of reproduction is also known as *nonrecombinational* [Grande and Brown, 2010]. Typical examples for this form of reproduction can be found in most single-celled organisms, like bacteria.

3.2.3 Fitness

In our model, we define the fitness of an individual to be the expected number of offspring that survive to reproductive adulthood. In our model, each mating results in two offspring individuals. However, they still need to pass through a viability selection before being included in the population of the next generation. Thus, the fitness depends on both the viability v_g of the offspring bearing genotype g and the fixed number of offspring per mating. The fixed number of offspring per mating is equal in our model for all individuals, no matter which genotype they bear. Hence, in order to compare the fitness of two individuals, it is important to examine the viability values of possible offspring.

In an asexually reproducing population, the offspring of an individual is always a genetic copy of the individual. Thus, both the genotype viability of the individual and the genotype viability of the offspring are directly associated with the fitness of an individual. During a simulation without any changes in the environment, this viability is fixed, since it does not depend on other individuals in the population. Thus, the fitness of an individual is fixed as well.

In a sexually reproducing population, the genotype of an offspring of an individual is a recombination of the genotypes of that individual and its mating partner. Thus, the offspring viability does not only depend on the reproducing individual itself but also on the possible mating partners. These are the other individuals in the population. This means that the genotype distribution in the population may change relatively rapidly.

Evolutionary game theory deals with the questions: which genotypes will outcompete other genotypes, and will this competition lead to a stable genotype population distribution? The genotypes that 'win' by outcompeting others are those with higher fitness values relative to the population distribution, in accordance with Charles Darwin's theory of the survival of the fittest.

Imagine a population with n_t individuals at time t with genotypes of length two and the viability values displayed in Table 3.1, where entry (a_{1i},a_{2j}) for $i,j \in 1,2,3$ defines the viability for the genotype built by alleles a_{1i} and a_{2j}. For simplicity, let us assume that all genotypes are present equally often in the population at time t.

Locus 2 Locus 1	a_{21}	a_{22}	a_{23}
a_{11}	$v_{a_{11},a_{21}} = 0.48$	$v_{a_{11},a_{22}} = 0.50$	$v_{a_{11},a_{23}} = 0.54$
a_{12}	$v_{a_{12},a_{21}} = 0.51$	$v_{a_{12},a_{22}} = 0.52$	$v_{a_{12},a_{23}} = 0.50$
a_{13}	$v_{a_{13},a_{21}} = 0.50$	$v_{a_{13},a_{22}} = 0.51$	$v_{a_{13},a_{23}} = 0.48$

Table 3.1: Viability values example for genotypes with two loci with three alleles each

In an asexually reproducing population, the viability values directly define the fitness of an individual, i.e., the fitness of an individual of type (a_{1i}, a_{2j}) is twice the viability of that genotype in our model. An individual bearing genotype (a_{11},a_{23}) has the highest fitness of all genotypes in the population and will thus outcompete the other genotypes as we do not consider mutations in our model. In the long run, the population thus will only consist of individuals bearing this genotype.

In a sexually reproducing population, it is not easy to determine which genotype will outcompete the others. In Table 3.1, $v_{a_{11},a_{23}}$ and $v_{a_{12},a_{22}}$ are the global and local maxima in the viability landscape. We would expect the sexual population to approach the global maximum as the asexual population does. However, due to the influence of stochasticity in the model (random mating and random re-combination to produce offspring), it may well be that the sexual population converges to the local maximum. In order to show that sexual populations indeed may end up in different maxima, we performed 1000 simulations runs using the viability values displayed in Table 3.1 assuming that all genotypes are present 20 times in the initial population of 180 individuals. In 663 of the simulation runs, the population ends up in the global maximum (only with individuals bearing genotype a_{11}, a_{23}), and in 337 of the runs, they end up in the local maximum (only with individuals bearing genotype a_{12}, a_{22}). For scenarios with more loci and more alleles per locus, we are able to solve the multidimensional optimization problem to determine the local and global maxima. However, due to the stochasticity, we do not know in advance, which will be the outcompeting genotype in a sexually producing population.

However, also in the sexual case, we can compute the fitness of an individual in any particular generation, provide we know the population distribution:

Let $q_g(t)$ be the fraction of individuals of genotype g in the population at time t, implying that $\sum_g q_g(t) = 1$ for all t. Then the expected fitness of an individual of type $g = (a_{1i^*}, a_{2j^*})$ at time t in the two loci example, indicated by $f_g(t)$ or $f_{a_{1i^*},a_{2j^*}}(t)$, is given by

$$\begin{aligned} f_{a_{1i^*},a_{2j^*}}(t) = & \sum_{i,j} q_{a_{1i},a_{2j}}(t) \\ & \cdot [0.5 \cdot v_{a_{1i^*},a_{2j^*}} + 0.5 \cdot v_{a_{1i^*},a_{2j}} \\ & + 0.5 \cdot v_{a_{1i},a_{2j^*}} + 0.5 \cdot v_{a_{1i},a_{2j}}]. \end{aligned}$$

3.3 Simulations and Analysis

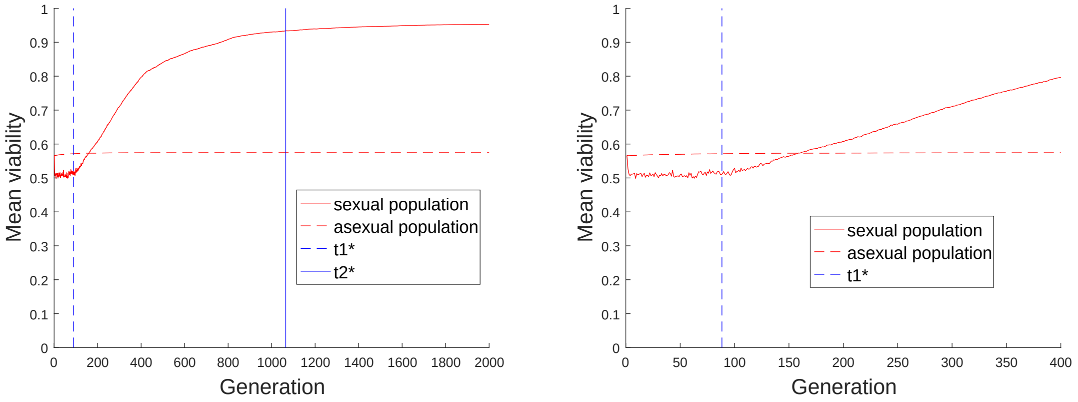
3.3.1 Initial parameters

In our simulation software, we have the capacity to adjust several parameters. Most importantly, we are able to set the number of loci and the number of alleles per locus. Thus, we can simulate both genetically simple individuals and more complex ones. Furthermore, we can change the viability values for each genotype; this gives us the possibility to simulate different environmental conditions. Additionally, we can adjust the initial population size and the number of individuals per initial genotype in the population at the beginning of the simulation.

In order to limit the population size and thus the time a simulation takes to be performed, we define a maximal population size limit of 10000 individuals. If this limit is exceeded at any generation during a simulation run, half of the population is randomly eliminated. By using a randomized elimination process, we on the one hand lower the population size but on the other hand maintain the distribution of types.

In an asexually reproducing population, there are already sufficiently many individuals per genotype present in the population when such an elimination process takes place to ensure that the probability of eliminating all individuals of one genotype is very low. In a sexually reproducing population, it might be that some genotypes are completely removed from the population under this elimination if only a small number of individuals bear this genotype. However, it is unlikely that an allele is entirely removed, such that the individuals in the population are able to create the removed genotype again out of the remaining alleles. The influence of the elimination process on the outcome of our simulations is thus extremely minor. A simulation run ends when a pre-defined number of generations has been reached. Both the number of generations and the number of simulation runs is restricted by computation time resource bounds. For each scenario, we have to make a reasonable choice such that on the one hand we run enough simulation runs and, on the other hand, we limit computation time to make the best use of our computation resources.

3.3.2 Phases of the mean viability dynamics



(a) Mean viability dynamics with three different phases

(b) Zoomed version of Figure 3.1a to visualize the initial phase

Figure 3.1: Example for mean viability dynamics for both a sexual (solid red line) and asexual (dashed red line) repdroducing population both starting with the same initial population.

In Figure 3.1, the results of a single simulation run as an example for the mean viability dynamics $\bar{v}$ of both a sexually (red curve) and an asexually reproducing population (red dashed curve) are displayed. We present the results of a single run to show the characteristics of the mean viability dynamics without any smoothing effects that are obtained by taking averages. The results presented later in this section are based on multiple simulation runs and their averages. While Figure 3.1a shows the results until generation 2000, Figure 3.1b shows the results of the same simulation until generation 400. Both scenarios start with exactly the same initial population. In this example, the genes have a length of 200 loci, and each of these loci has four alleles. The viability values for each possible genotype are chosen randomly from the interval $[0, 1]$ as they represent the viabilities of the individuals bearing these genotypes to survive to adulthood. For such a large number of possible genotypes it is impossible to store values separately. Thus, we divided each genotype into 20 substrings of 10 loci each. For each substring, we generated a table by assigning a uniform random value between 0 and 1 for each possible choice of alleles. To get the viability of any complete genotype, we took the average viability of the corresponding substrings. Initially, we start with a population with four different genotypes and 50 individuals for each genotype. The simulation run contains $T = 2000$ generations, and in each generation, every individual is reproducing.

The mean viability of the asexually reproducing population increases very rapidly directly from the first generation until it reaches a plateau. In contrast to this, the mean viability of the sexually reproducing population initially has an unsteady phase before it starts to increase. Compared to the very fast increase of viability in the asexual population, the mean viability in the sexual population increases much slower. Remarkably, despite this slow start, in the end, the mean viability of the sexually reproducing population far exceeds the mean viability of the asexually reproducing population. (Keeping in mind that in our model here we consider fixed environments and mutation-free reproduction).

The development of the mean viability of the asexual population can be easily explained: The simulations start with a population consisting of four different genotypes. The individuals have no possibility of creating new genotypes in asexual reproduction. Genotypes of lower viability have lower chances of surviving to adulthood. Therefore there are fewer and fewer of them in the population as time goes on compared to the genotype with the highest viability. At the end of the process, the population only consists of individuals bearing the genotype with the highest viability.

We may divide the graph of the mean viability $\bar{v}$ of sexually reproducing populations into three phases, as displayed in Figure 3.1. In the first phase, the mean viability appears to follow a random walk. It goes up and down a bit but stays within a certain bandwidth around the initial value. At point t_1^*, the mean viability suddenly starts to get past the bounds of this bandwidth. After this increase, the mean viability reaches a plateau at a second point t_2^*.

For the sake of exploring what parameters influence these two ‘phase change’ points, we need to define them properly. To do so, we first implement a moving average low pass filter from 30 simulations as described in detail in Law and Kelton [2007]. Afterwards, we apply a piecewise linear model for trend change detection [Liu et al., 2010, Tomé and Miranda, 2004]. With this piecewise linear function $f_1(x)$, we approximate the filtered mean viability. Let $f_1(x)$ be defined as

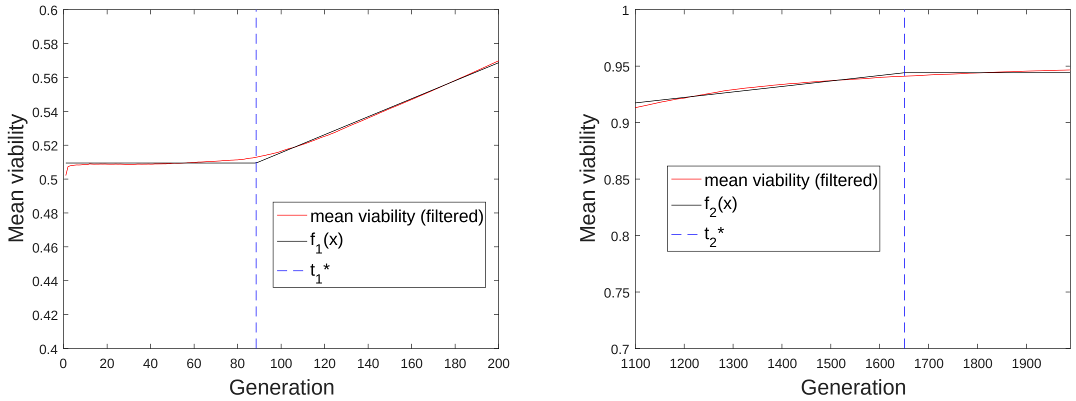
$$f_1(x) = \begin{cases} a & x < t_1^* \\ b(x - t_1^*) + a & t_1^* \le x \le r \end{cases}$$

with a, b and t_1^* being parameters determined by a least squares fitting such that $f_1(x)$ best fits the pre-processed mean viability values. In order to find t_1^*, we only consider the first r mean viability values for approximation. This value r can vary depending on where we expect t_1^* to be, since on the one hand, $r > t_1^*$ needs to be satisfied, but on the other hand the approximation is more accurate if we do not choose r too large. Furthermore, we assume that the mean viability value from $t = 0$ to $t = t_1^*$ stays in a certain bandwidth. Therefore, we use a horizontal line to approximate the initial random walk phase. An example is shown in Figure 3.2a.

Using a similar approach, we determine t_2^* by approximating the last s values of the filtered mean viability values by a piecewise linear function $f_2(x)$ defined by

$$f_2(x) = \begin{cases} c(x - t_2^*) + d & s \le x \le t_2^* \\ d & x > t_2^* \end{cases}$$

with c, d and t_2^* being parameters determined by a least squares fitting such that $f_2(x)$ best fits the last pre-processed mean viability values. Again, we assume that the mean viability



(a) Example for piecewise linear approximation for the first $r = 200$ viability values

(b) Example for piecewise linear approximation for the last $s = 990$ viability values

Figure 3.2: Examples for piecewise linear approximation for both the first and last viability values after applying a moving average low pass filter from 30 simulations with window size 10. Both Figures are taken from the same simulation runs.

values from $t = t_2^*$ until the end of the simulation $t = T$ do not increase (as a plateau has been attained). We therefore use a horizontal line to approximate the plateau phase. An example can be found in Figure 3.2b.

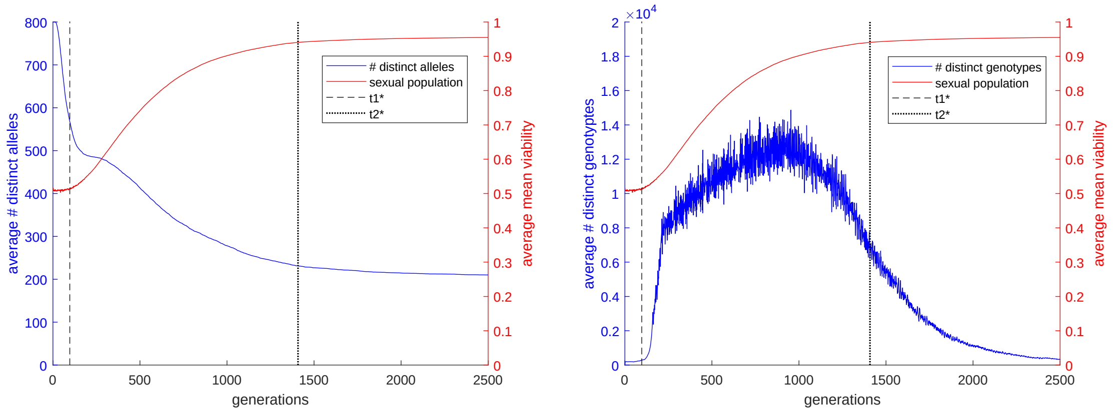
In what follows, we will refer to these three phases, respectively, as the '*Random Walk Phase*', the '*Fitness Increase Phase*', and the '*Plateau Phase*'.

The random walk phase

The random walk phase is characterized by small fluctuations of the mean viability around a certain value. In this phase, a rapid loss of alleles can be identified (see Figure 3.3a). At the beginning of a simulation run, we start with $4 \cdot 200 = 800$ different alleles, which implies 4^{200} possible distinct genotypes. Each such genotype is randomly assigned a viability value in the interval $[0, 1]$. Due to the fact that in each generation, every individual in the population is reproducing, selection occurs rapidly, and genotypes with low viability disappear very quickly. This makes alleles also go extinct rapidly as well, yielding the fast loss of alleles of Figure 3.3a. The fluctuations of the mean viability at the beginning of the simulations can be explained by the combination of a great variety of possible genotypes and a relatively small number of individuals.

The fitness increase phase

At generation t_1^*, the mean viability of the sexually reproducing population suddenly starts to increase. At the same time, the number of different genotypes increases very fast (see Figure 3.3b), while the decrease of number of the alleles slows down (see Figure 3.3a). The large fluctuations in the number of genotypes are due to a population size limit of 10000 individuals. If this number is exceeded, half of the individuals are eliminated. This fact also



(a) Mean viability dynamics and the number of alleles

(b) Mean viability dynamics and the number of genotypes

Figure 3.3: Average mean viability dynamics from 10 simulation runs for both a sexual and asexual repdroducing population with settings: 200 loci, 4 alleles per locus, 4 initial genotypes with 50 individuals each, viability values from $[0;1]$. *Both figures show results from the same simulation runs.*

explains the small plateau after about 200 generations in the curve displaying the number of distinct alleles in Figure 3.3a. At this point, unsuccessful alleles have been eliminated, such that the remaining alleles form genotypes with a higher viability. This makes both the population size and the number of genotypes grow. Simultaneously, the mean viability steadily increases because those alleles resulting in genotypes with low viability have already been eliminated. Hence, the strong randomness in the process is reduced since the relation between the remaining possible genotypes and the population size is much more even. In this phase, we can observe competition between the remaining genotypes. This competition process is much slower than in the asexual case since in a sexually reproducing population, beneficial gene combinations are frequently broken down again due to recombination.

The plateau phase

After the increase phase at point t_2^*, the mean viability reaches a plateau. Remarkably, at the end of each simulation run, we observe only 200 alleles (Figure 3.3a). Thus, in the end, only one allele per locus remains in the population. These are the 'winners' of the allele competition within each of the loci.

Hence, just as in an asexual population, only one genotype remains uneliminated at the end. This single genotype will not be broken down again by recombination, and therefore the mean viability will remain at this level. This winning genotype does not necessarily need to be the same genotype as the genotype that remains in the end in the asexual population (see Section 3.2.3). In most cases, it almost certainly will not be the same genotype since the sexual population generally attains higher mean viability than the asexual population). However, even if we start the simulation with populations in which all the genotypes are present, we may still end up with different winning genotypes in the sexual and asexual populations. In the asexual population, the genotype with the highest viability will always win, while in the sexual population, it cannot be predicted in advance which specific genotype will succeed (see Section 3.2.3).

3.3.3 Parameters influencing the dynamics

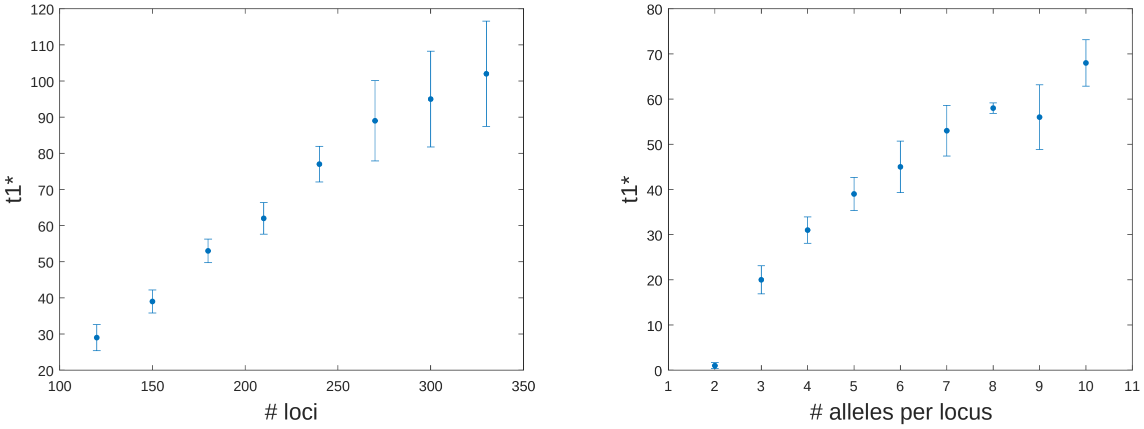
In this section, we investigate the influence of different initial parameters on the dynamics of the mean viability in the sexual reproduction dynamic. We focus here on both t_1^* and t_2^*, the points at which the phases change. More specifically, we explore the dependence of the mean viability dynamics on the number of loci, the number of alleles per locus, the variance of individual viability values, and on the initial number of individuals per chosen genotype. To test the influence of each individual parameter, we change that parameter and keep all other settings fix. As default settings, we chose: 200 loci, four alleles per locus, an initial population size of 200 individual, and four initial genotypes. When increasing the number of alleles, we had to increase the initial number of genotypes as well, since an assumption in our model is that all alleles have to be used at least once in the initial population. In all other cases, we only modified the parameter being tested.

In Figure 3.4, the influence of the above mentioned parameters on t_1^* is shown, while Figure 3.5 shows the influence on t_2^*. To give more insight into the accuracy of t_1^* and t_2^*, the errorbars in the figures show the standard deviation of the estimated parameters. 30 simulations are split into three times ten simulations and for each block, t_1^* or t_2^* respectively is computed as described in Section 3.3.2. From these three values for t_1^* and t_2^*, the mean and the standard deviation are determined and presented in Figures 3.4 and 3.5. While the standard deviation of t_1^* seems to increase with a higher value for t_1^*, we cannot observe similar behaviour for the standard deviation of t_2^*.

We observe a linear increase in the length of the random walk phase with an increasing number of loci (Figure 3.4a). This is due to the fact that with an increasing number of loci the number of possible genotypes increases exponentially. Thus, in the random walk phase – due to greater randomness – it takes longer to eliminate deleterious genotypes.

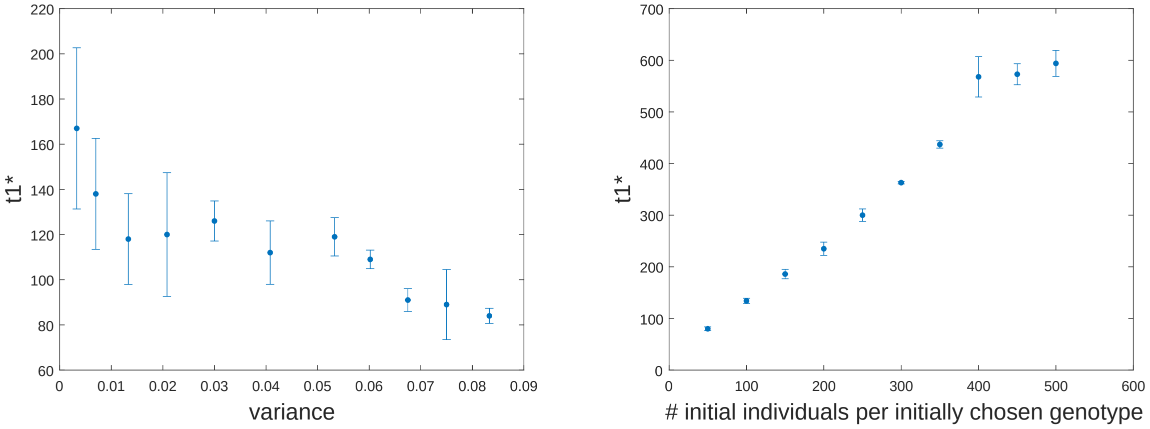
The same linear relationship exists for the length of the random walk phase and the number of alleles (Figure 3.4b). This is due to the fact that the alleles are competing with each other within each of the loci. When there are more alleles per locus, both the number of competitions and the number of possible genotypes increase. This increases the selection pressure on valuable genotypes and thus the random walk phase. We observe a decrease in the length of the random walk phases with increasing variance in the individual viability values (Figure 3.4c). From the results, it is difficult to tell whether this decrease is linear or exponential. However, a smaller variance of the viability values decreases the difference between beneficial and deleterious genotypes and therefore lengthens the selection phase. The dependence of t_1^* on the number of initial individuals per chosen genotype is again linear (Figure 3.4d). With more individuals per genotype in the initial population, it takes longer to eliminate a certain genotype.

The dependence of t_2^* on the four parameters is similar: We observe a linear increase with increasing number of loci (Figure 3.5a), with increasing number of alleles (Figure 3.5b) and with increasing number of initial individuals per chosen genotype (Figure 3.5d). The dependence of t_2^* on the variance of individual viability values is linear: it takes longer to reach t_2^* with decreasing variance (Figure 3.5c).



(a) Dependence of t_1^* on investigated number of loci[1]

(b) Dependence of t_1^* on investigated number of alleles per locus



(c) Dependence of t_1^* on investigated variance of viability values

(d) Dependence of t_1^* on investigated initial number of individuals per genotype

Figure 3.4: Dependence of t_1^* on different parameters: The figures show the mean of three values for t_1^* computed each from 10 simulation runs with different initial populations. The error bars display the corresponding standard deviation of these three values.

3.3.4 Changing environments

So far, we have investigated scenarios under the assumption of perfectly fixed environments. This is not very realistic. In this section, we explore the effects of sudden discrete changes in the environment. In our model, the viability is the fitness for each genotype, and the fitness

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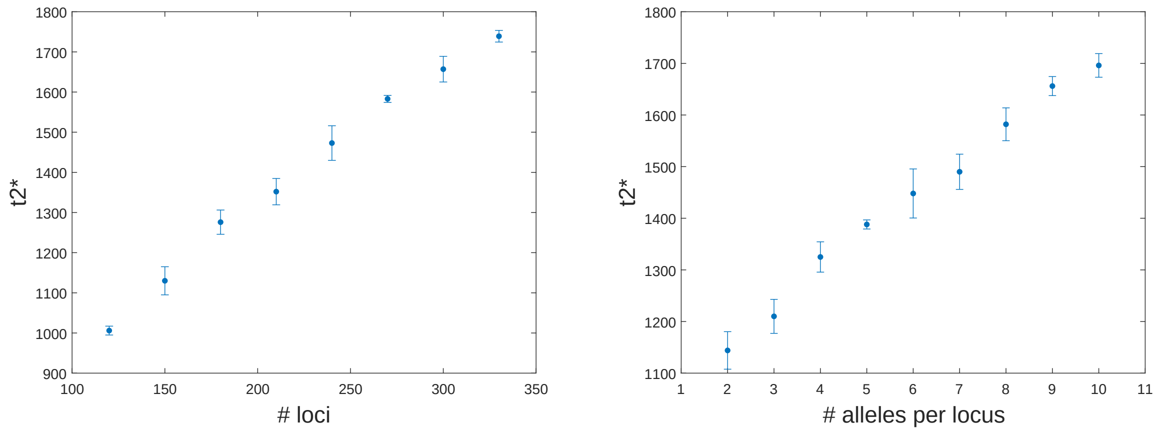
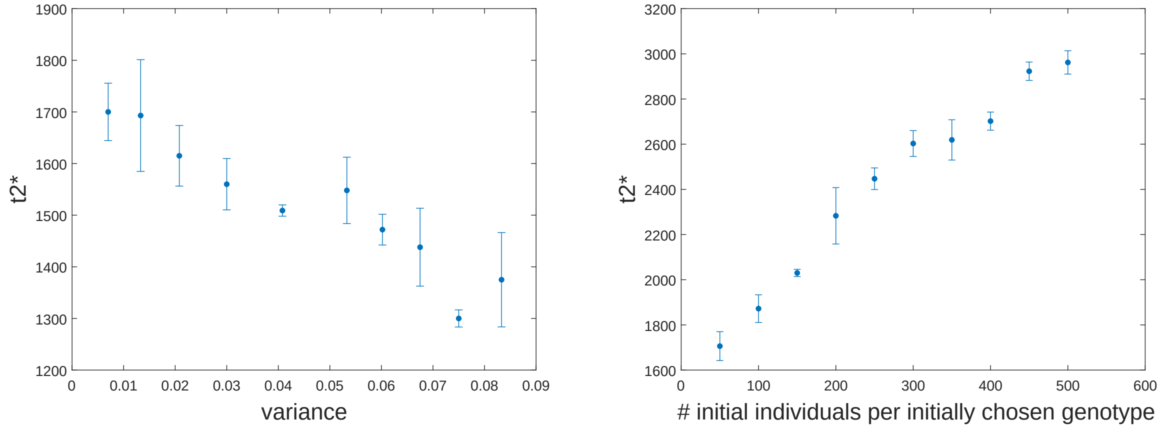
[1] For these experiments, we used 30 substrings instead of 20 substrings as the number of loci is not divisible by 20.



(a) Dependence of t_2^* on investigated number of loci[1]

(b) Dependence of t_2^* on investigated number of alleles per locus



(c) Dependence of t_2^* on investigated variance of viability values

(d) Dependence of t_2^* on investigated initial number of individuals per genotype

Figure 3.5: Dependence of t_2^* on different parameters: Figures show the mean of three values for t_2^* computed each from 10 simulations with different initial populations. The errorbars display the concerning standard deviation of these three values.

defines how well an individual is adapted to the environment. Hence, in order to model a change in the environment, we randomly generate new viability values for each genotype at certain generations. This sudden change can be compared to a natural disaster, nuclear accident, or abrupt climate change. All other model assumptions stay the same.

Note that alleles that were beneficial alleles prior to the environmental shock may at once become liabilities, while deleterious alleles that the population dynamic had previously sought to shed may equally instantly become high-valued. The population must begin learning anew after such a shock.

To obtain an initial intuition regarding the influence of sudden changes, we conducted ten simulation runs with 3000 generations each and investigate 200 loci with 4 alleles in each locus. Initially, we started with 4 genotypes and a population size of 200. For each simulation run, we randomly choose viability values from the interval [0,1].

The sudden change is simulated by randomly choosing new viability values from the same interval. In Figure 3.6, the effects of sudden discrete changes of the environment are shown. Figure 3.6a displays the results if the viability values for each genotype are randomly changed in generation 40, while Figure 3.6b shows the results of a sudden change in generation 300.

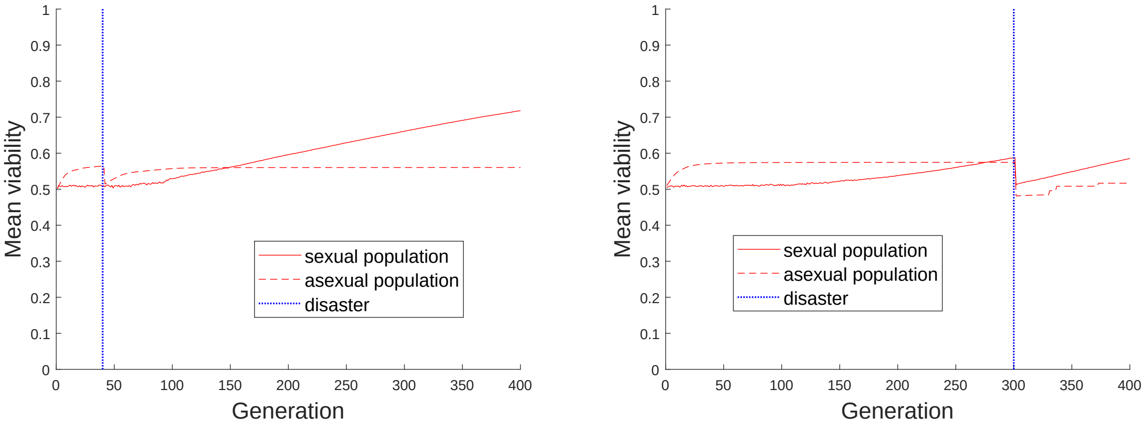
In the first case, the change is in the middle of the random walk phase and does not seem to have any impact on the sexual population. In this phase, most alleles are still present, such that most of the genotypes can still be created by recombination. Thus, the influence of the sudden change of environment in this early phase is limited. In contrast to this, the mean viability of asexually reproducing populations decreases directly after the change, prior to increasing again and reaching a plateau level of mean viability. However, it may not necessarily attain the same level of the phase before the environment changed. Depending on the genotypes in the population and the new environment, the new level might be different from the old level. If the environment changes, the success of the population is completely random, since asexual populations are stuck with the genotypes in the founding population and cannot recombine to other genotypes. Of course, the success probability in case of a sudden change of environment increases the greater the number of different genotypes in the population.

In the second case, the change occurs during the increase phase, and we observe a direct effect on the mean viability of the sexually reproducing population. At first, we observe a fall in the mean viability of the population. This is due to changes in the genotype viability values. In this phase, the sexual population has already sorted out some alleles, and the remaining genotypes have a high viability. After the disaster, these viability values change randomly, and thus, it is likely that the mean viability drops.

Remarkably, in this case, after a disaster, the random walk phase does not start again (despite what one might expect since the environment has been completely ‘reset’ and it might appear everything reverts to the first stage) but rather the increase phase is continued after the disaster. This shows that the sexual population can use the advantage of having sorted out alleles and does not need to start from the beginning. The asexually reproducing population on the other hand does not seem to recover from a sudden environmental change. The mean viability drops further after some more generations. One might expect a more smooth decrease of the mean viability after the disaster. The stepwise behavior can be explained by the fact that this curve shows the average of 10 different simulation runs. In four of these simulation runs, the population died out. In the generation, where the population goes extinct, the mean viability immediately drops from a positive value to zero, which influences the average mean viability. If we exclude mean viabilities of zero when computing the average, we observe a stepwise increase in the averaged values when populations die out.

When does a disaster least impact the population development dynamic?

The results of the previous section raise the question: when does a sudden environmental shock have the least discernible impact on the development dynamic of a sexual population? In other words, can we identify conditions under which a sexually reproducing population



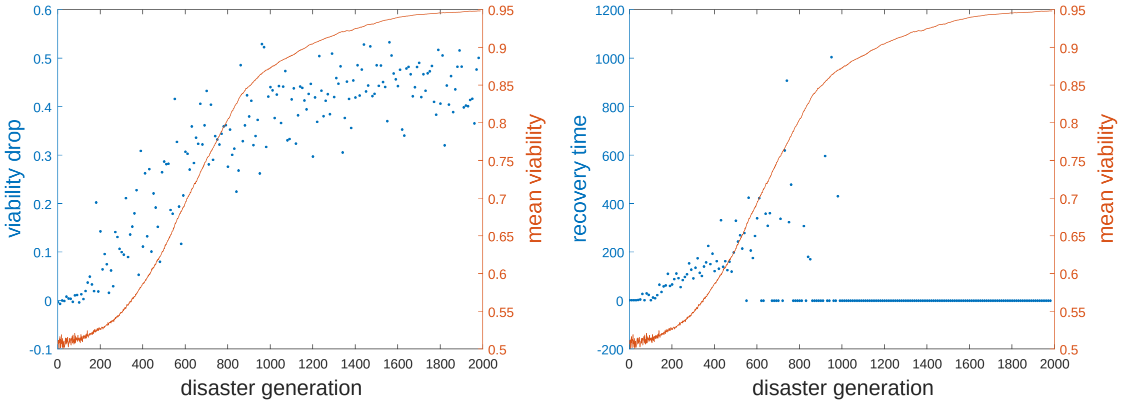
(a) Mean viability with a sudden change of viability values in generation 40

(b) Mean viability with a sudden change of viability values in generation 300

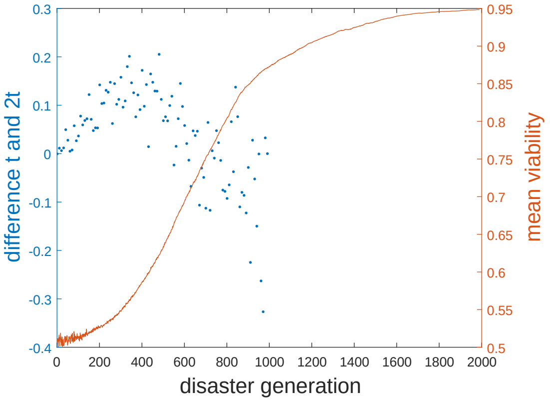
Figure 3.6: Mean viability average of 10 simulation runs with a sudden and random change of viability values

can most readily 'shake off' an environmental disaster and resume its mean viability climb almost as if nothing had disturbed it? If a disaster occurs 'late', meaning after the sexually reproducing population has begun strongly converging on a single genotype, the population is similar to a plateaued asexual population, in the sense that it cannot produce a sufficiently variable set of new genotypes to search the genotype space efficiently. It will then exhibit sub-optimal mean viability. In contrast, if the disaster occurs at a very early stage, only some alleles have been eliminated and the population can then react nearly optimally to the sudden change of environment. The resistance of the population to disasters is much more robust in early generations.

To analyze the effects of sudden environmental shocks on population development, we ran the following experiments: we began with an initial population consisting of 200 individuals with five different genotypes. The genotypes all consisted of 200 loci with four alleles in each locus. The viability values were taken from the interval $[0,1]$. Based on these settings, we ran 2000 generations with fixed viability values, i.e., simulation runs that included no disasters. Afterwards, we used the same initial settings, the same initial populations, and the same viability values, but this time implemented a single disaster at different generations $g_d \in \{0,10,20,...,2000\}$. In other words, during each simulation run, the disaster happens at a different generation g_d, while all the settings stay the same. The disaster is again modeled by changing the viability values randomly at a certain generation. In all experiments, both sets of viability values are the same, no matter in which specific generation g_d the disaster happens.



(a) Drop   *(b) Recovery time*



(c) Mean viability $2t - t$

Figure 3.7: Reactions on disasters at different generations of a sexual population

To analyze the results, we consider two different measures indicating how well a population can react to environmental changes:

- Drop in mean viability: This measure gives the difference between the mean viability immediately before and after the disaster

- Recovery time: The recovery time represents the time a population needs until it has the same mean viability it attained before the disaster. If it does not reach the same mean viability until the end of the simulation, we mark the recovery time as -1.

The results of these simulations are presented in Figure 3.7. In Figure 3.7a the drops in the mean viability dependent on the disaster generation are presented, with Figure 3.7b showing recovery times. Furthermore, in the same figures, the mean viability dynamics for simulation runs without any disaster are displayed. The results shown in Figure 3.7c are explained later.

We can observe that mean viability drops are quite small in the earliest generations. In the middle generations, the drops increase, and at the end, the drops seem to be constant again. This behavior is very reminiscent of the mean viability dynamics, which are characterized by a random walk phase, increase phase, and plateau phase (see Section 3.3.2). The magnitudes of the drops are smallest and stay constant in the initial phase, increase during the increase phase, and level off at the end of the process.

Recovery times behave in a pattern similar to that of the magnitudes of the drops: at the beginning, recovery time is negligible; a gradual increase is then noticeable. If the disaster occurs too late (after 600 generations or more), there is a significant chance that population will not recover at all. Note that if the disaster occurs before generation 1000, the population still has enough time to recover. Hence recovery is not restricted by the number of simulated generations remaining; something else is preventing recovery. If the disaster occurs, for example, at about generation 600, some simulation runs do exhibit mean viability recovery, with a recovery time that does not exceed 500 generations. Thus, there is still enough time left for the populations to recover again. Furthermore, the graph shows that the sexual population can use the advantages it attained before the disaster. The slope of the regression line through the dots is smaller than one. For example, if the disaster happens at generation 200, the population does not need another 200 generations to achieve the same mean viability as before the disaster.

In a model in which disasters arrive at recurring time points (e.g., according to a Poisson distribution with arrival rate λ), populations need to balance two somewhat competing objects: increasing their mean fitness between disasters whilst maintaining their robustness against environmental shocks (which will tend to decrease as the genotypic variability in the population decreases with increasing mean fitness). This prompted us to measure not only the difference between mean viability before and after a shock but also to consider the increase of the mean viability between consecutive shocks.

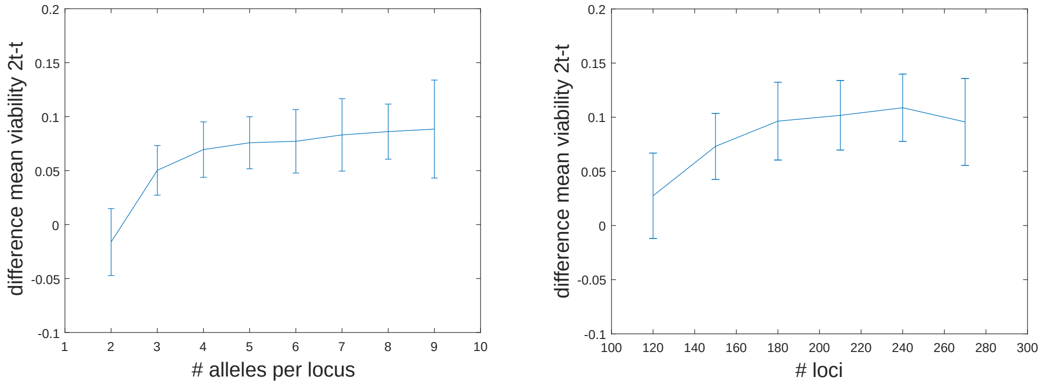
We therefore introduce a third measurement of how well a population can react to environmental changes:

- Difference between mean viability at $2t$ and t: This measures the difference between the mean viability at generation $2t$ and t if disaster strikes at generation t. If this value is negative, it means that the population has not yet recovered at generation $2t$.

Figure 3.7c shows the difference between the mean viabilities at generation $2t$ and t for a sexually reproducing population in the previously described simulation case studies. If we consider the difference in the mean viabilities before the disaster and at the generation at which we expect the next disaster, we observe behavior that differs from the behavior recorded in measurements of the size of the drop and the recovery time. From a population perspective, the greater the difference between the two mean viability numbers the better, as this indicates robust recovery to disaster. Figure 3.7c shows that the optimal time for a population to suffer a disastrous blow is when it is in the increase phase of the sexual reproduction dynamic. If a disaster occurs during the random walk phase, the population is robust against an immediate drop in mean viability but is not likely to optimize its fitness. If disaster strikes late in the increase phase or during the plateau phase, the population is generally not robust to changes in the environment.

What is the optimal number of alleles/loci to have when disasters occur?

The previous section shows that it is better for a sexual population to be in the early increase phase if recurring disasters happen. However, populations cannot control the time of arrival of a disaster shock. We therefore investigate in this section what is the optimal number of loci and the optimal number of alleles per locus to have if disasters happen at certain generations. Figure 3.8 shows the difference between the mean viability of a sexual population at generation $2t$ and t if the disaster happens at generation $t = 400$ for different values for both the number of alleles and of loci. We conducted 70 simulation runs with different initial populations and viability values for each number of loci and number of alleles. The figures display the average difference of the mean viability and the standard deviation of these 70 runs. The simulations with varying numbers of loci investigate four alleles per locus and initially 200 individuals with four distinct genotypes. The simulations with varying number of alleles were conducted with ten different genotypes in the initial population and 200 loci.



(a) Difference of mean viability at generation 800 and generation 400 for different numbers of alleles

(b) Difference of mean viability at generations 800 and generation 400 for different numbers of loci

Figure 3.8: Difference of mean viability at generations t and $2t$ for $t = 400$ for different numbers of alleles and different numbers of loci

According to Figure 3.8a, we observe that the difference between the mean viability at generations $2t$ and t increases with the number of alleles per locus. However, having more than seven alleles per locus does not seem to bring any further advantage. If the number of alleles is too small, the population is effectively already in the late increase phase. If disaster strikes at this stage, the population generally cannot react well. As the number of alleles per locus increases, the increase phase starts later (see Section 3.3.3) and thus, the population is effectively shifted towards an earlier point of the increase phase. Referring to the results of Section 3.3.4, the population at this point, has still the flexibility to react to the disaster but is also already optimizing its fitness. Figure 3.8b shows similar results. The difference between the mean viability at the two measured generations is increasing for an increasing number of loci. In contrast to the previous results, we observe here a maximum at 240 loci before the difference decreases again. In this case, the increasing number of loci shifted the phases of the mean viabilities such that the population is still in the random walk phase and thus, referring to the results of Figure 3.7c, is not at an optimal balance between optimizing fitness and reacting flexibly to disasters.

3.4 Conclusions

3.4.1 Discussion

In this chapter, we elaborate on results by Edhan et al. [2017]. They presented a model of reproduction in both sexual and asexual populations. One of their results showed that sexual populations may have an advantage in both unstable and stable environments. Furthermore, they identified a typical fitness development path in both types of populations. In greater detail, the authors of that study observed, in sexually reproducing populations, an initial phase resembling a random walk, a learning phase of steadily increasing mean fitness, and finally a plateauing. Here, we elaborate on explanations for their observed phenomena.

We therefore present results that grant more insight into what happens in the allele space as the sexual reproduction dynamic proceeds. With these results, we can explain the typical fitness development path alongside examining aspects of both the genotype and allele space in the long run. Our simulations reproduced exactly the same overall typical fitness development in sexual populations as Edhan et al. [2017]: in the beginning, there is a random walk in which mean fitness on average remains approximately constant, after which a learning phase initiates leading to increased mean fitness. We explain this behavior by the loss of alleles that occurs in the initial phase of the dynamic as revealed by our simulations: the population needs to remove most of the deleterious alleles (relative to the environment) before it can begin to increase the mean viability. Due to the immense size of the potential genotype space compared to the number of individuals in the population in any single generation, there is a great deal of randomness inherent in the recombination of genotypes dynamics. This is the reason for the observed random walk in the initial phase. After a large number of poorly performing alleles have gone extinct, the mean viability can begin to increase from a certain point onwards.

However, we observed that this point t_1^* can vary significantly. We therefore explored what parameters influence the location of this point amongst the possible generations. For identifying t_1^*, we first used a moving average filter to reduce the influence of randomness in our simulations. We then approximated the first mean viability values by a piecewise linear function. We tested four parameters, namely, the number of loci, the number of alleles per locus, the variance of viabilities assigned to the individual genotypes, and the initial number of individuals per genotype. In all four cases, we observed a clear dependence of t_1^* on the tested parameter. We may therefore conclude that for more complex species with more loci, and more alleles per locus, the random walk phase of the sexual reproduction strategy lasts longer than for simpler species. In simpler species, both the allele competition within the loci and the process of eliminating deleterious genotypes proceeds much faster.

From t_1^* onward, the mean viability of the sexual population increases until it reaches a plateau at point t_2^*. We observed that at the end of our simulations, only one allele per locus remained in the sexual population. This implies that the entire population only consists of individuals of the same genotype. Recombination no longer matters from that point onwards, since a genotype recombined with the same genotype always results in this same genotype. Hence a plateau results.

It may seem remarkable that the sexual population in the end homes in on a single uniform genotype, given the endless process of recombination it undergoes, which would seem to imply that gene combinations, even the most successful ones by fitness measurements, should be torn apart in every generation. Never the less, this end result is what our theoretical model indicates should happen, and our simulations all confirmed this.

An asexually reproducing population similarly ends its dynamic with a uniform genotype and attains the resultant plateau. We may therefore compare the performance of the end-point asexual genotype with that of the end-point sexual genotype in terms of speed of convergence and fitness. An asexual population will attain its plateau much faster than a corresponding sexually reproducing population. However, the slow and steady sexual population strategy eventually outperforms the asexual population in fitness. This is because by recombination, a sexually reproducing population manages efficiently to sample a broad swath of the genotype space, whereas an asexually reproducing population essentially samples only once (i.e., what it has in its initial population) and can only attain the optimum fitness of its one-shot sample. Most likely – especially for large genotype spaces – there will be genotypes outside the initial population with higher viability values than those in the initial population. This gives the sexual reproduction strategy advantage over the asexual one.

It would appear that it is impossible in most cases to determine in advance which genotype will be the winning genotype in the sexual reproduction strategy and that random aspects inherent in the dynamic can have unpredictable effects pushing the population towards one or another equilibrium. This is in sharp contrast to the asexual case, in which a genotype with the highest viability with respect to the environment will inevitably win out.

The example described by Table 3.1 has two pure Nash equilibria, namely genotype $g3$ consisting of alleles (a_{11}, a_{23}) and genotype $g5$ consisting of alleles (a_{12}, a_{22}). These are Nash equilibria in the sense that the viability cannot be increased by changing the allele in only one locus, i.e., per locus, the viability is maximized. The theoretical model would predict that if there is convergence, then, since the loci are playing a coordination game of identical interests, that convergence will be to a Nash equilibrium. Indeed, we performed 1000 simulations runs, which always yielded populations uniformly bearing either genotype $g3$ (63.3%) or $g5$ (36.7%), in line with the theory. However, predicting which Nash equilibrium will be attained prior to a run was not possible, and likely depends on both the initial population and many random factors idiosyncratic to each simulation run.

Sexually reproductive populations are more robust against changes in the environment than asexual ones. After an asexual population has eliminated nearly all of the genotypes in its initial population, it has in the process also eliminated nearly all possibility to adapt to changes. Unless it can make use of mutations, it is stuck with the genotypes that are in the population at the moment of change. If these genotypes are not as fit for the new environment as they were for the previous environment, the mean population fitness will decrease. In contrast to this, sexually reproducing populations do not need many genotypes to adapt. What they do need is a sufficiently wide variety of alleles in their population; with these, they are able to recombine and create genotypes that are better for the new environment. To summarise: we observed a trade-off between the rapid increase in population fitness versus robustness against changes in the environment. The asexual population on the one hand increases its mean viability quite rapidly but then cannot adapt well to changing environments. The sexual population on the other hand needs more time to begin its climb up the ladder of fitness but can then more robustly react to changes in the environment.

This leads to the question, at what stage of evolution will a disastrous shock have the least deleterious impact on mean population fitness. If a disaster occurs only once, we can measure the impact of the disaster by both the recovery time and the drop of mean viability. Based on these two measures, from the perspective of mean population fitness, the earlier a shock strikes, the better, because the population can then react most robustly. If the disaster is expected to happen repeatedly with a fixed period of t generations, it is of interest to determine the difference between the mean viability at multiples of t. Our simulation results indicate that for the population, it is most optimal to be at the beginning of the increase phase when a shock strikes. However, our simulation results include a great deal of variance. The dots in Figure 3.7a, for example, show large dispersion of results, especially with respect to shocks in the late phase. This is due to stochasticity in our simulations. For future work, it would be interesting to attempt to reduce the observed variance by simulating shocks striking after populations have attained certain mean viability levels, rather than supposing shocks always strike at a certain generation.

Combining the results of Section 3.3.3, where we observe that the genome size has an influence on the duration of the phases and the results of Section 3.3.4, which indicate that the early increase phase is optimal for recovering from shocks, in Section 3.3.4 we explore the influence of the genome size on the possibility of recovering from shocks. The genome size influences the time frame within which a sexually reproductive population will be in the early increase phase; this then has implications for recovery from disasters. The optimal genotype size may therefore depend on whether the environment is changing rapidly or slowly.

Looking forward to possible goals for future research, adding mutations to our model and simulations forms one such goal, as the asexual population would then no longer be restricted solely to the genotypes available in the initial population. Depending on the mutation rate, mutations could perhaps make asexually reproducing populations both more competitive with sexual ones and more robust to changes in the environment. These mutations can either be genotypes that are predefined in the existing genotype space or completely new genotypes. In the latter case, viabilities for new genotypes would have to be generated somehow.

Furthermore, we would like to extend our models in various ways that would bring them closer to conditions seen in nature, for example by considering diploid genotypes or by distinguishing between male and female individuals. Another possible line of enquiry could involve more complex environmental changes, such as shocks that affect only certain genotypes or alleles, or periodically repeated switches between two or more environments.

3.4.2 Summary

The main contributions of this chapter are:

1. We confirmed a clear identification of three discrete phases in the dynamics of a sexually reproducing population over many generations: an initial Random Walk phase, a Fitness Increase phase, and a Plateau phase. These phases appeared reliably in every simulation we performed, and apparently indicate a deep aspect of the sexual reproduction dynamic.

2. We confirmed that, in constant environments involving haploid genotypes without mutations, the sexual reproduction dynamic converges eventually to an equilibrium involving a single genotype that is borne uniformly throughout the population. This is in contrast to some opinions that have appeared in the literature asserting that sexual reproduction, by continually tearing down and recombining genotypes, ensures a permanent state of genetic variance in populations. As there may be several possible equilibria, however, it may be impossible to predict in advance to which equilibrium the population will settle.

3. Our simulations affirm that the greater the number of loci and/or the number of alleles per loci, the longer the Random Walk and Fitness Increase phases a sexually reproducing population will go through before converging towards a plateau. This accords with our model of evolution as essentially a process of learning an environment as represented by the fitness distribution across the genotype space. In general, the larger and more complex the genotype space, the greater the time needed for evolution to explore and learn, hence the greater the number of generations needed before increase and convergence to plateau can occur.

4. Furthermore, when considering haploid monoecious individuals without mutations, sexually reproducing populations are most robust to sudden shocks to the environment during the Random Walk and early Fitness Increase phases. The later they are in the Increase phase or the Plateau phase, the less robustness they exhibit to shocks. Asexual populations without mutations are highly non-robust to sudden shocks: their exponentially rapid convergence to a single genotype renders them unable to respond well to shocks.

5. The previous paragraph indicates a possibly fundamental trade-off in evolution regarded as a learning algorithm. The better a population is at identifying the genotypes of highest fitness, the greater the advantage in exploiting this advantage by uniformly concentrating those genotypes in populations; however, the more uniform a population, the more vulnerable it is to environmental change (reminiscent of the curse of over-fitting in machine learning). This might point to a double-fold advantage of sexual reproduction over asexual reproduction: especially in complex and large genotypes, sexually reproducing populations both attain greater mean population fitness in the long run than asexual populations, and spend greater time in the 'sweet spot' of the early to mid Fitness Increase phase, in which relatively high mean fitness is exhibited along with vigorous robustness.

CHAPTER 4

Spatial effects on sex type competition in annual plants

Abstract

This chapter examines the influence of space on the prevalence of different sex types in a sex allocation model of annual plants. In particular, we use a discrete-space agent-based model to compare the outcome of our simulations to earlier results of a non-spatial model by Charnov et al. [1976]. All types have a predefined amount of resources that they can use to produce pollen grains and ovules. While keeping the amount of resources fixed for males and females, we vary the amount for hermaphrodites. Female plants (F) can only produce ovules, male plants (M) only pollen grains, and hermaphrodites (H) can allocate any fraction of the total resources to ovules and pollen grains. All plants are located on a rectangular grid, and pollen and seeds can only be spread within a certain seed and pollen radii around the distributing plant. For our initial experiments, the pollen radius is fixed and equal for male and hermaphroditic plants, and the seed radius is fixed and equal for all female and hermaphroditic plants. Then, our simulations show that chances for each type of plants to persist depends on the sex allocation of the hermaphroditic plants. When males and females have a much higher amount of total resources than hermaphrodites, we observe that a dioecious (M+F) population prevails. When the difference between the resources is only marginally higher for males and females, hermaphrodites do not go extinct. Further-

more, they prevail in the population when they hold more resources than males and females. However, depending on their sex allocation, we also observe gynodioecious (F+H) and androdioecious (M+H) populations prevailing. With our agent-based approach, we are well able to examine the effect of the following scenarios on the prevalence of types: When increasing the pollen dispersal radius of males, while keeping the hermaphroditic pollen radius fixed, our simulations show that a dioecious population can prevail even if hermaphrodites hold more resources than males and females. The increased radius for males gives dioecious populations a reproduction advantage. Increasing the pollen area further increases the reproduction advantage for dioecious populations even more. Furthermore, we examine how the model predictions change if we assume that some of the grid cells are unsuitable for germination. Due to these cells, hermaphrodites have a reproductive advantage as they have reduced competition between siblings: In contrast to females spending all their resources on placing seeds nearby, hermaphrodites also invest in pollen that is spread far.

4.1 Introduction

Plants exhibit different breeding systems: Some species are strictly dioecious (M+F), gynodioecious (H+F), or androdioecious (H+M), and there are even trioecious species (H+F+M) (see Table 2.1 for an overview of sexes in plants). Different breeding systems have even been documented in subpopulations of the same species [Van, 1989]. Furthermore, also within individual plants, we can observe differences: hermaphroditic plants can have perfect flowers (male and female reproductive organs within the same flower) or be monoecious plants (separate male and female flowers on the same plant). Hermaphrodites that produce both pollen and ovules at the same time are called simultaneous hermaphrodites. By contrast, hermaphrodites acting as one sex and switching to the other sex during their life-time are referred to as sequential hermaphrodites. Many studies addressed the evolution of these different breeding systems both in plants and in animals [Bawa, 1980, De Jong et al., 2008, Weeks, 2012]. Separate sexes (males and females) evolved from hermaphrodites [Barrett, 2002, Bawa, 1980]. In plants, the two main pathways from hermaphrodites to separate sexes are a 1) gynodioecious pathway, where females and hermaphrodites coexist, and a 2) monoecious pathway, where hermaphrodites have separate male and female flowers [Barrett, 2002].

Charnov et al. [1976] used evolutionary game theory to determine under which conditions either a hermaphroditic, a dioecious, a gynodioecious, or an androdioecious population is evolutionarily stable. Under the assumption that males can produce N pollen, females can produce n ovules and hermaphrodites αN pollen and βn ovules, the authors suggest that a dioecious population is stable when $\alpha + \beta < 1$. For $\alpha + \beta = 1$, a hermaphroditic population is evolutionary stable if the hermaphrodite divides resources equally to pollen and seed production. Furthermore, for $\alpha + \beta > 1$, hermaphrodites can invade a population of males and females. In this case, either the males, the females, or both will be replaced by the hermaphrodites. Under these conditions ($\alpha + \beta > 1$), the hermaphrodites tend to replace the sex with which they compete most. In the extreme, hermaphrodites will displace both males and females if they can produce at least as many pollen as males and ovules as females, respectively. Several studies were done on extending Charnov's model [Brunet, 1992, Morgan, 1992, Seger and Eckhart, 1996]. Brunet [1992] categorizes these extensions based on whether they include temporal separation of sexual functions, on whether they examine plants that are able to fertilize themselves (selfing), and on whether they in- or exclude costs for building pollinator-attracting structures of the plant. Morgan [1992] presents a model where the resources also need to be used to build pollinator-attracting structures of the plant. The author examines the impact of attractive structures benefiting both male and female function, benefiting only male, or benefiting female function on the prevalence of types.

Charnov's and similar models assume a well-mixed, infinitely large population [Charnov et al., 1976, Hardy, 2002]. In contrast to these classical mathematical models, actual populations may not be well-mixed, and there are limits on how far pollen and seeds can disperse. Different assumptions on pollen flow and seed dispersal may alter predictions and create spatial patterning. Spatially-explicit, agent-based models are well suited for considering these spatial effects, finite heterogeneous populations, and biased pollen flow and seed dispersal.

As the following examples show, such models have become more popular for investigating reproduction and sex allocation. Jaffe [2008] used an agent-based model to examine conditions under which sexual reproduction in contrast to asexual reproduction is evolutionarily stable. In his simulations, Jaffe showed that four different conditions must be met for sexual reproduction to succeed over asexual: 1) selection pressure is variable, e.g., due to a changing environment 2) mate selection is non-random, but individuals more likely mate with similar phenotypes, 3) genome size is large, and 4) the population is either diploid or females are diploid while males are haploid or the population is hermaphroditic. Furthermore, De Jong et al. [2002] used a checkerboard simulation model where at most one individual can reside within a square to examine the influence of pollen and seed spread on the sex ratio of dioecious plant populations. In their simulations, they observed a female-biased sex-ratio when considering a to a short distance-limited pollen and seed dispersal. For a larger pollen spread compared to seed spread, the sex ratio was male-biased, while when considering both a pollen and seed dispersal over a large area, the sex ratio was about 0.5. Kaliszewicz [2019] used agent-based simulations to determine how resource allocation to eggs and sperm within a simultaneous hermaphrodite influence cnidarian Hydra circumcincta's fitness. Individuals of this species can be simultaneous hermaphrodites, hermaphrodites acting as females or hermaphrodites acting as males. Her model showed that under low competition to fertilize eggs, hermaphrodites acting as females and those acting as males coexist. However, in their simulated plant population, more hermaphrodites acting as males can be found. With higher competition for egg fertilization, a sex ratio of 1:1 among these types is most successful. With increasing mating competition and without any limitations on egg investment, simultaneous hermaphroditism with a female-biased sex allocation becomes the optimal strategy with respect to reproduction success.

Sex allocation theory deals with predicting and analyzing allocation to male and female function and with the evolution of sex ratios within individual populations [Charnov, 1987]. Most studies in this field have focused on finding factors influencing the allocation [Brunet, 1992]. Such factors can include selfing rates [Charnov, 1987, De Jong et al., 1999] or environmental conditions [Stehlik et al., 2008]. Furthermore, there exist models examining the optimal sex allocation in simultaneous hermaphrodites under various conditions [Fischer, 1984].

Sex allocation models generally assume that there are limited resources that can be invested in female and male functions. This is quite general, as many more sub-categories of male and female functions are possible, e.g., whether or not pollinator-attracting structures of the plants like sepals or petals (see Figure 2.3) are investigated. However, in all models, sex allocation is always defined as the proportion of complete reproductive resources allocated to male and female functions [Charnov et al., 1981, Dorken and Pannell, 2009, Schlesmann, 1988]. Models differ in emphasis and question under investigation. Some concentrate on the sex allocation at the fruit stage, i.e., pollen and seeds, others on the allocation at the flower stage (pollen and ovules) [Brunet, 1992].

In populations with simultaneous hermaphrodites, sex allocation theory examines which allocations to male and female function lead to the highest reproductive success. But, many species exhibit sequential hermaphrodites where individuals at various stages in their life can choose to switch from male to female or vice-versa. While the sex of an individual is fixed at a given point in life, this sex can change with time or circumstance. Although more common in animals, sequential hermaphroditism occurs in plants as well. For sequential hermaphrodites, sex allocation theory focuses on explaining why and when individuals switch sexes during their lifetime. Among the large literature on optimal switching strategies are the models of Ghiselin [1969] and Warner [1988]. They offer hypotheses on why some species change sex while others do not. When the relative advantage of being male or female changes with size, it may be advantageous to change sex over one's life time [Warner, 1988]. The plant Jack-in-the-pulpit (*Arisaema*) provides an example of such a change [Bierzychudek, 1982, Policansky, 1981]. In this species, small plants do not flower at all; larger plants reproduce as males and the largest as females. In addition to size-dependent switching, Freeman et al. [1980] showed that individuals with the ability to change sex have an advantage over other individuals in patchy or changing environments.

Here we develop a spatially-explicit agent-based model for an annual plant species that can function as a simultaneous hermaphrodite. We imagine a grid where each square provides a potential safe site for at most one plant to succeed during the growing season. We consider plant populations of males, females, and simultaneous hermaphrodites, where males contribute pollen, females produce ovules, and hermaphrodites have the ability to produce both ovules and pollen. Seeds and ovules can only be spread in restricted areas around the focal plant. In our model, all types have a resource limit that they can spend on the production of seeds and pollen. As the production of a pollen grain is assumed to be cheaper than the production of one ovule [Fischer, 1981], we furthermore introduce a factor that gives the number of pollen grains that can be produced for the same price as one ovule. We assume equal resource limits for males and females. However, next to hermaphrodites having the same resource limit, we implemented the possibility for hermaphrodites having either more or less resources available than males and females. Both possibilities can be explained: On the one hand, hermaphrodites may not be able to use advantages of separate male and female flowers (like a specialization in the location, shape, and space of a flower) and they may need to put more effort into their reproduction mechanisms than males and females [De Jong et al., 2008]. Both scenarios result in a decreased resource limit for hermaphrodites. On the other hand, hermaphrodites may also use parts of the flower for both ovule and pollen production. In that case, they can use more resources to invest in the production of ovules and pollen grains. This scenario results in an increased resource limit for hermaphrodites.

We are particularly interested in answering the following questions: 1) What are the effects of extending Charnov's [1976] model from a non-spatial to a discrete-space grid model on the prevalence of types in the population? 2) What are the effects on the prevalence of sex types of independently varying the dispersal radii of pollen and seeds? 3) What are the effects on the prevalence of sex types when considering cells where no seeds can germinate? To answer these questions, we allow for uneven allocation patterns of the hermaphrodites to pollen and ovule production and let pollen and ovule production be substitutable, complementary, or antagonistic functions.

The chapter is organized as follows. After the model description (Section 4.2), we present reference results where males and hermaphrodites have the same pollen radius and where females and hermaphrodites have the same seed radius (Section 4.3.1). We compare the prevalence of sex types in our model to the prevalence of types in Charnov's [1976] non-spatial version. Next, we perform case studies for an increased pollen dispersal distance for males and an increased seed dispersal distance for females and compare these results to the reference results (Section 4.3.2). Then, we start again with the settings from the reference results, but now we consider cells, in which no seeds can germinate (Section 4.3.3). In this case, the competition for space is increased as fewer cells are available where seed germination would be successful. We end this chapter by discussing the findings of this model and by giving suggestions for future research (Section 4.4).

4.2 The model

In this section, we present our model where different sexes of annual plants interact with each other. The plants are diploid and produce haploid pollen and ovules. The sex of an adult plant is determined by a single locus with three possible alleles (A, X, and Y). In the diploid state, we assume that males are XY and AY, females XX, and hermaphrodites AA, AX (see Table 4.1). In this way, the female allele (X) is recessive, the Y allele is dominant and insures maleness. Having either two A alleles (homozygous) or an A allele combined with X (heterozygous) produces hermaphrodites. YY is not possible in this genetic system.

Each square or cell of the landscape (square grid) with size 1×1 units can be thought of as a potential safe site for at most one adult plant, though the cell may at times remain empty as well. For the landscape, we assumed a torus modeled as a grid of size $\Theta = [0, 1, ..., 100] \times [0, 1, ..., 100]$ units with periodic boundary conditions, i.e., plants on the very left/top of the field are direct neighbors of plants on the very right/bottom.

Genotype	Phenotype
AA	Hermaphrodite
AX	Hermaphrodite
XX	Female
AY	Male
XY	Male

Table 4.1: Investigated Genotypes with corresponding Phenotypes

4.2.1 Seeds and pollen

Females produce ovules, males produce pollen, and hermaphrodites produce both ovules and pollen. Ovules may be fertilized by pollen and mature to seeds. In our model, we assume that all fertilized ovules become seeds and spread to new locations within the so-called seed neighborhood of a focal plant. In the neighborhood of any focal plant, we restrict the dispersal of seeds and pollen by introducing a seed and pollen radius. Each radius represents a distance threshold and defines a neighborhood around a focal cell. All cells that have a shorter distance to a focal cell than this threshold are assumed to be within the neighborhood. A cell has distance one to a focal cell if the cell can be reached by either a horizontal, vertical, or diagonal step from the focal cell. Figure 4.1 illustrates this distance for different neighborhood sizes. Blue and red cells have a distance of one and two to the green focal cell, respectively. Assuming a seed/pollen radius of one for the focal cell implies that both the blue cells and the focal cell itself lie within the seed/pollen neighborhood (9 cells total). However, as we do not permit selfing, the focal cell itself is removed from a male's or hermaphrodite's pollen neighborhood. Because we consider annual plants, the plants will die following seed production. Thus, a seed can fall and germinate within the cell of its parent. Hence, the dispersal neighborhood for seeds includes the focal plant's cell. Increasing the radius to two adds the red cells to both the seed (=25 cells) and the pollen (=24 cells) neighborhoods. In our model, the radii can be type-dependent, i.e., hermaphrodites may have a different pollen radius than males and a different seed radius than females. Also, the pollen radius may be different from the seed radius. Furthermore, the influence of a pollen donor is not restricted to the pollen donor. Although it is only able to fertilize plants within its pollen radius, the fertilized plant will use the pollen to form a seed which is spread within its seed radius. If several seeds of one of multiple adult plant land in the same cell, they will compete for which seed wins the safe site and thus, which germinates.

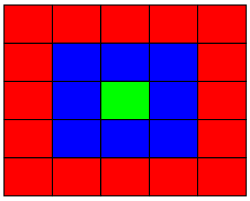


Figure 4.1: Cells with different radii to the focal plant (green). Blue (and green) cells are in the pollen (seed) neighborhood within radius 1 to the green focal plant. Both blue and red (and green) cells are within the pollen (seed) neighborhood within radius 2 to the focal plant.

We imagine that each adult plant has a resource limit, r (in units of ovules), that restricts the production of ovules and pollen grains. The pollen factor f_p gives the number of pollen grains that can be produced for the same price as one ovule. For example, if $f_p = 100$ and $r = 10$, then all females produce exactly ten seeds and males produce exactly 1000 pollen grains. Hermaphrodites can use any fraction of the resource limit to invest into ovule or pollen production. Considering the previous example with $f_p = 100$ and $r = 10$ and assuming that hermaphrodites split their resources equally to ovule and pollen grain production, then they can produce five ovules and 500 pollen grains. They also have the possibility to invest more into ovules or more into pollen grains. We allow for a continuum of resource allocations by hermaphrodites. For instance, if the hermaphrodites aim for 6.4 ovules, then each hermaphrodite plant has exactly a 60% chance to have six ovules and exactly a 40% chance to have seven ovules.

As discussed above, the hermaphrodites may see pollen and ovule production as perfect substitutes in terms of resources. In our model, we will relax this assumption. Joint pollen and ovule production may be complementary or antagonistic activities where available resources for joint production may be greater than, or less than r, respectively.

4.2.2 Interactions

Time in our model progresses in discrete generations of one year each. In each generation, every female and hermaphrodite has a chance of 40% of being selected as a focal plant that is fertilized (interaction probability), if pollen is available. If a plant is selected as a focal plant, the ovules of that plant are fertilized by pollen from males or hermaphrodites within its pollen neighborhood. If there are no males or hermaphrodites present within the pollen neighborhood of the focal plant, then no fertilization takes place. If male and hermaphroditic pollen radii differ from each other, the focal plant is fertilized by males from its male pollen neighborhood or by hermaphrodites from its hermaphroditic pollen neighborhood. If a male or a hermaphrodite is present in one of the focal individual's neighborhoods, for each ovule, one pollen grain is randomly chosen with equal probability from all available pollen grains within the pollen neighborhood. As this choice does not depend on distances between plants, we here assume that pollen from males and hermaphrodites are spread uniformly across their pollen dispersal radii.

Next, in accordance with Mendelian genetics, the genotype of a seed (fertilized ovule) is determined by a random draw of one allele from each parent's pair of alleles. This is done independently for all fertilized ovules and determines the type of the new plant. An overview of possible genetic combinations is displayed in Table 4.2.

Interaction	Seeds
AA + AA	100% AA
AA + AX	50% AX, 50% AA
AA + XY	50% AX, 50% AY
AA + AY	50% AY, 50% AA
AX + AX	25% XX, 50% AX, 25% AA
AX + XY	25% XX, 25% XY, 25% AX, 25% AY
AX + AY	25% XY, 25% AX, 25% AY, 25% AA
XX + AA	100% AX
XX + AX	50% AX, 50% XX
XX + XY	50% XX, 50% XY
XX + AY	50% AX, 50% XY,

Table 4.2: Interactions with corresponding offspring percentages.

We assume that seeds disperse uniformly across the cells of a focal plant's seed radius. The cells into which the seeds fall are chosen randomly and with equal probability from all cells within the seed neighborhood of the focal plant. Following seed dispersal, all adult plants die, no matter whether they have reproduced or not. At this point, all cells are empty and available to the seeds that have fallen within each cell. If a cell has no seeds, then it will remain empty until the next generation. If a cell has just one seed in it, then that seed will germinate and become an adult in the next generation. Lottery competition occurs when more than one seed lands in a cell. In this case, the seed that is going to occupy this cell in the next generation is randomly chosen from all seeds within the cell [You, 2018]. The lottery losing seeds within the cell die and do not survive until the next generation. The next generation begins with those germinated seedlings that have succeeded in acquiring a cell.

4.3 Simulations and analysis

Using computer simulations, we explore case studies differing in the following settings: 1) We consider a fixed and equal pollen radius for hermaphrodites and males and a fixed and equal seed radius for hermaphrodites and females 2) We independently vary the male's pollen radius while holding the hermaphrodite's fixed 3) We independently vary the female's seed radius while holding the hermaphrodite's fixed 4) We consider cells where no seeds can germinate.

For each simulation, we had a torus size of $100 \times 100 = 10000$ cells. Initially, 1666 plants of each genotype AA (hermaphrodites), XX (females) and XY (males) are placed randomly in the field. Females and males were assigned ten units of resources, but different amounts of resources and different investments into pollen and ovules are investigated for hermaphrodites. We considered a focal probability of 0.4 and a pollen factor of 100 in all simulations. This pollen factor defines the number of pollen grains that are as expensive as one seed. The seed radii and pollen radii may differ per case studies. The parameter settings per case study can be found at the beginning of corresponding subsections below.

While the initial population gives rise to a sex ratio of 1/3, 1/3, and 1/3, it is unlikely to be at a steady state in terms of allele frequencies, genotype frequencies, sex ratios, or adult population size. But, the process of pollen flow, ovule fertilization, and seed dispersal will lead to eco-evolutionary dynamics that should in the long run, converge on a steady state. Plants of genotypes AX and AY will naturally evolve within these processes.

For each case study, we explore possible combinations of hermaphroditic pollen and ovule investment. Rather than running a simulation for all possible combinations, we sought boundaries between regions where long term (stationary) sex ratios abruptly changed as a result of the loss or inclusion of a particular sex. These boundaries are visualized by the colors in all following figures. Each symbol in these figures stands for one simulation, and its color shows which sex type(s) prevailed after the considered number of simulation runs.

4.3.1 Effects of varying the hermaphroditic investment into pollen and seeds

The parameter settings for this case study are described in Table 4.3. The pollen radius for both males and hermaphrodites (10 units) was five times larger than the seed radius of females and hermaphrodites (2 units). Males produced 1000 pollen grains, and females produced ten ovules.

For the hermaphrodites, we first consider sex allocations that vary between 0 to 1200 pollen grains and 0 to 12 seeds. With a step size of 0.2 for seeds and 20 for pollen, we explore the state space of pollen investment and ovule investment. The results are shown in Figures 4.2, 4.4 and 4.5. Figure 4.3 shows the results using a step size of 0.02 for seeds and of 2 for pollen.

Figure 4.2 shows what sexes prevailed at the end of 3000 simulation steps upon varying the pollen and ovule allocation of hermaphrodites. The location of each symbol indicates the investment of the hermaphrodites into ovule and pollen production, respectively. On the black line, hermaphrodites neither have an advantage nor a disadvantage in terms of their available resources compared to males and females. The sum of their investments into ovule and pollen production is equal to the resources available for males and females. Thus, on the black line, hermaphrodites allocate ten units of resources where one unit of resources provides for one seed or for 100 pollen grains. Below this black line, hermaphrodites have less resources than males and females – joint production of ovules and pollen is an antagonistic

Initial population size	4998 (1666 of each genotypes AA, XX and XY)
Simulation runs	3000 - 5000
Field size	100 x 100
Interaction probability	0.4
Pollen radius males	10
Pollen radius hermaphrodites	10
Seed radius females	2
Seed radius hermaphrodites	2
Resources (males and females)	10
Pollen factor	100

Table 4.3: Settings used for reference simulations where hermaphrodites have the same pollen radius as males and the same seed radius as females (Figures 4.2, 4.3, 4.4 and 4.5.

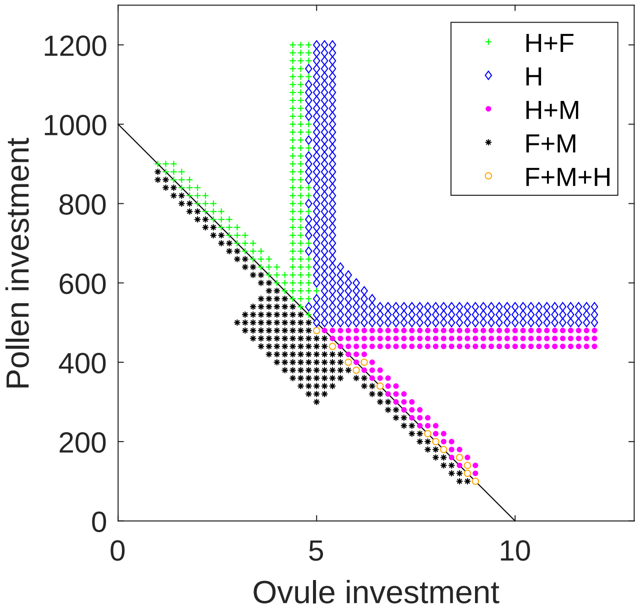


Figure 4.2: Reference results obtained by using the settings described in Table 4.3. The different symbols (and their colors) show what types have prevailed after 3000 simulation steps. The location of the symbols indicate the investment of hermaphrodites into ovule and pollen production.

activity. Above the black line, hermaphrodites have more resources that can be invested in ovules and pollen – joint production is a complementary activity.

Four distinct regions can be observed in Figure 4.2. In the black area, which is entirely below the black line, only males and females survive while hermaphrodites go extinct. In the blue area, only hermaphrodites are present at the end of the simulation. In the green area, hermaphrodites and females prevail. In the magenta area, hermaphrodites and males

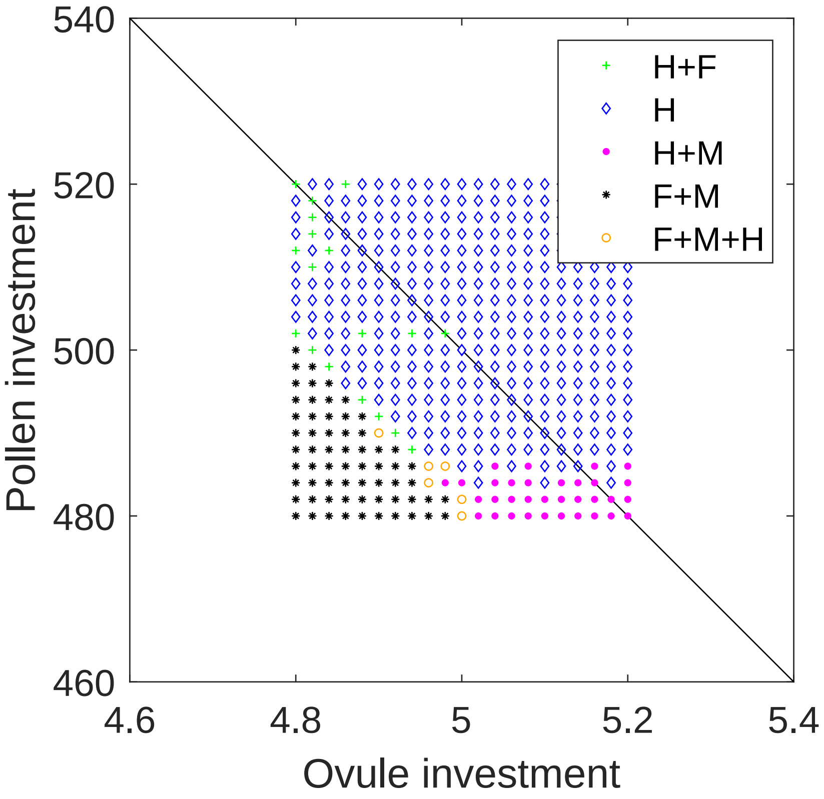


Figure 4.3: Zoomed version of reference results obtained by using the settings described in Table 4.3. The different symbols (and their colors) show what types have prevailed 4000 simulation steps. The location of the symbols indicate the investment of hermaphrodites into ovule and pollen production

survive. However, especially at the border of the magenta and black area, the figure shows some orange circles. For those sex allocations, all three types survive 3000 generations in our simulations.

The major boundaries meet roughly where hermaphrodites invest their resources $50:50$ to pollen and ovules, and have the same total resources ($r = 10$) as males and females. To determine more precisely the boundaries in this critical region, we run experiments at a finer grid by performing 4000 simulation steps at step sizes of 0.02 for ovules and 2 for pollen grains (Figure 4.3 zooms in on the critical region of Figure 4.2). The results show that hermaphrodites do not go extinct until the end of the simulation, even when they have a slight disadvantage regarding the total amount of resources. Qualitatively, the results indicate that a dioecious population can only prevail if hermaphrodites have about 97% or less of the total resources of males and females.

We conjecture that this slight edge of being a hermaphrodite emerges from a form of bet-hedging and/or reduction in competition between siblings. By producing half as much pollen and half as many seeds as males and females, there is a 50% reduction in the likelihood that a seed or pollen grain from the hermaphrodite competes with its sibling within a given cell. Recall that if two seeds from the same plant disperse to the same cell, only one of them can successfully germinate and reach adulthood; similarly, pollen from the same plant may find themselves competing for a limited number of ovules when they land in the same cell.

Thus, we observe a dioecious population (males and females) only when hermaphrodites have less total resources to allocate to pollen and ovule production; this is when joint production of ovules and pollen is an antagonistic activity. In all other cases, hermaphrodites do not go extinct and form a stable part of the population. Above the black straight line, we observe areas where gynodioecious, androdioecious, and hermaphroditic populations prevail. In both Figures 4.2 and 4.3, we see that the horizontal line separating the prevalence of hermaphrodites (above the horizontal line) from that of males and hermaphrodites (below the horizontal line) intersects at about 485 pollen grains (just less than half of the pollen production of a male plant). Similarly, the vertical line separating the prevalence of only hermaphrodites (right of the line) from that of females and hermaphrodites (left of the line) intersects at about 4.85 ovules (just less than half of the ovule production of female plants).

Due to the characteristics of simulation experiments, it is hard to evaluate in advance how many simulation steps are enough to reach a stable population. Often, simulations are very time- and storage-consuming such that a balance between a high number of simulation steps and reasonable waiting time needs to be found. In our simulations, for some combinations of prevailing types, we can be sure that no types will go extinct even when running the simulations much longer. Considering the five different genotypes AA, AX, XX, XY, and AY, we know for sure that in a dioecious population consisting of XX and XY, none of these types will go extinct in the future. For populations consisting of only hermaphrodites (AA and AX or either only AA or only AX), we can conclude that hermaphrodites will never go extinct, but when AX is present in the population, it may still be that females can be observed after more generations. When our simulations show that both hermaphrodites (AA and/or AX) and females (XX) prevail, running more generations may lead to the extinction of females. Accordingly, when hermaphrodites (AA and/or AX) and males (XY and/or AY) stay in the population at the end of our simulations, running more simulation steps may lead to males going extinct. In order to anyway show the robustness of our results, Figure 4.4 shows the frequencies of remaining types at the end of the simulations. Between a dioecious population and all other breeding systems, we observe a jump from a green color indicating that the population consists of 50% females and 50% males to other reddish colors indicating hermaphrodites in the population. The fact that we do not see changing frequencies in the dioecious population supports the well-known fact that in a dioecious population, 50% males and 50% females are the optimal distribution [Fisher, 1930]. Between the area where hermaphrodites survive and the area where hermaphrodites and males survive, there is a smooth transition between the colors. This indicates that from having about 50% males and 50% hermaphrodite in the population (on the right side of the black line at the bottom of Figure 4.4), more and more males are replaced by hermaphrodites by increasing the hermaphrodites' investment into pollen (going up in the Figure). The transitions between the area where hermaphrodites and the area where hermaphrodites and females prevail are similarly smooth. Here, more and more females are replaced by increasing the hermaphrodites' investment into ovules. The smooth transitions between the hermaphroditic and gynodioecious or androdioecious area suggest that different simulation runs for the same hermaphroditic investment do not lead to different types prevailing at the end of the simulation than those observed in Figure 4.5b.

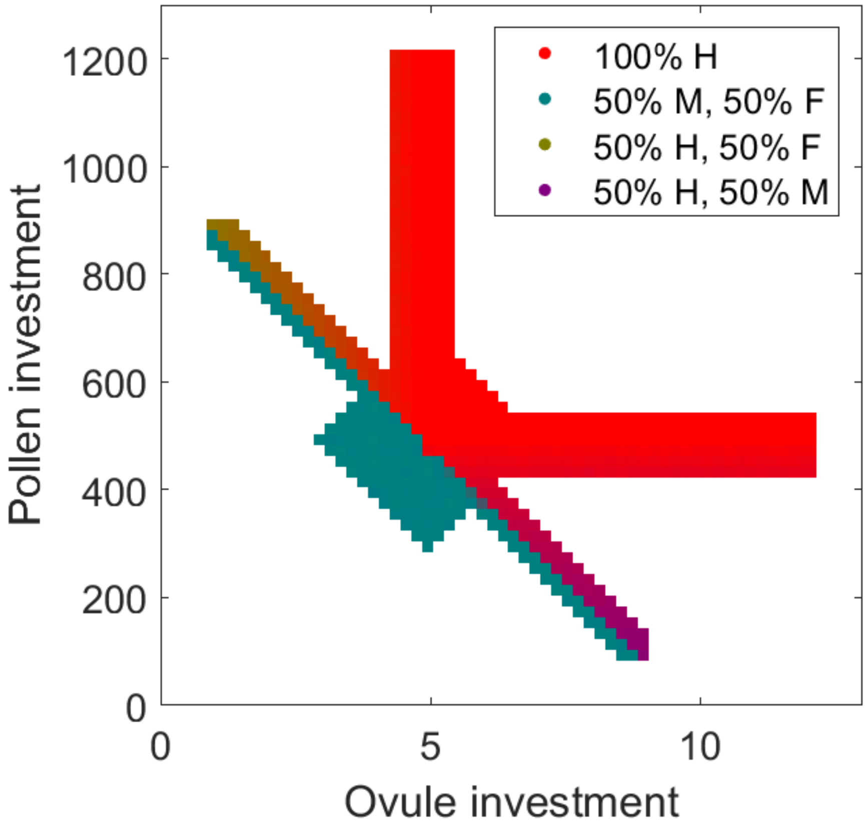
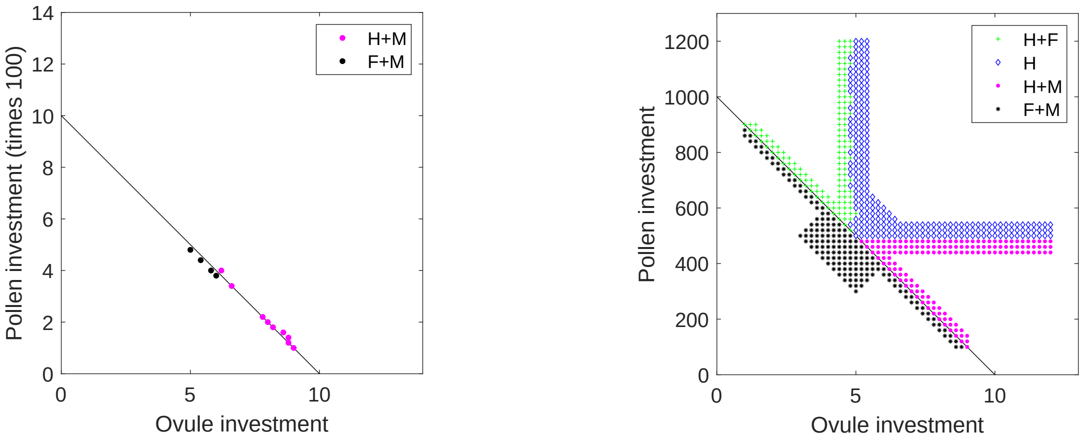


Figure 4.4: Frequencies of prevailing types after 3000 generations. The frequencies were computed from the same simulation results displayed in Figure 4.2.

We furthermore observe in Figure 4.2 that all three types prevail in the population for a few particular sex allocations of the hermaphrodites. However, the simulations were restricted to 3000 generations. To get an intuition on whether all three types will survive in the long run, we did some further experiments on these particular sex allocations with more simulation steps. The results are shown in Figure 4.5a. In all cases where we observed all three types at the end of 3000 simulation steps, at least one type goes extinct after 5000 simulation steps. Figure 4.5b shows a combined presentation of the results obtained after 3000 and after 5000 simulation steps. Thus, the prevalence of three different types was caused by too few simulation runs.

However, there are sharp area borders between the blue (H) and the magenta (M+H) areas. In contrast to that, the borders between the green (H+F) and blue (H) areas do not seem to be as sharp. The reason for this has to do with the genetic system assumed by the model. For sex determination, Y is dominant to A and A is dominant to X. Hence, when hermaphrodites prevail, all male alleles Y will be quickly removed from the population. On



(a) Reference results for 5000 simulation steps

(b) Combined reference results for 3000 and 5000 simulation steps

Figure 4.5: Figure 4.5a shows the reference results with an increased number of simulation steps for those sex allocations of hermaphrodites that led to a prevalence of all three types (F+M+H) in the reference simulations of Figure 4.2. Figure 4.5b shows the reference results for these particular sex allocations for 5000 simulation steps and for all other sex allocations for 3000 simulation steps.

the other hand, removing all X alleles from the population is slower because genotypes of AX will produce hermaphrodites, and as this allele becomes rare, it will mostly occur in the heterozygote state, i.e., in combination with an A allele, protecting it from elimination. Thus, as long as type AX is present in the population, females will not go completely extinct. In the following, we will refer to the point where all four areas meet as the intersection point. Using the parameters of Table 4.3, the intersection point occurs quite close to where the hermaphrodites allocate about 4.85 units of resources to ovules and 4.85 units of resources to pollen production. At this intersection, males and females have ten units of resources, and hermaphrodites have about 9.7 resources.

In the following, we first give a list of the main findings concluded from the simulation results displayed in Figures 4.2, 4.5b and 4.3, before we then compare them to the results of the non-spatial model:

1) If males and females have the same amount of resources as hermaphrodites, then hermaphrodites will prevail, and their best strategy to prevail is to allocate approximately an equal amount of resources to both pollen and seed production because only then, a complete hermaphroditic population prevails. Figure 4.3 shows that when all types have the same amount of resources, hermaphrodites outcompete both males and females (in most of the cases) when their seed allocation is higher than 4.82 and their pollen allocation larger than 486, respectively (blue diamonds on black line in Figure 4.3). For all other simulated allocations under the assumption that hermaphrodites have the same amount of resources as males and females, either males or females additionally stay in the population in addition to hermaphrodites.

2) Figure 4.5b indicates that when hermaphrodites have an equal amount of resources or more resources than males and females, hermaphrodites will remain present in the population. However, in addition, Figure 4.3 shows that hermaphrodites do not need to have more or equal resources available as males and females to stay in the population, but they can also prevail if they have slightly less resources.

3) For a gynodioecious (H+F) system to prevail, two conditions must hold. Hermaphrodites must: 1) have more than, equal amount of, or only slightly less resources than males and females and 2) allocate less than 50 percent of these resources to ovules (Figure 4.3).

4) For an androdioecious (H+M) system to prevail, two conditions must hold. Hermaphrodites must: 1) have more than, equal amount of, or only slightly less resources than males and females and 2) allocate less than 50 percent of these resources to pollen (Figure 4.3).

5) Our simulations never showed a coexistence of all three types (H+F+M) in the long run. Although after 3000 simulation steps, for some hermaphroditic sex allocations, all three types still coexist, we did some further experiments that show that after some more simulation steps, at least one type goes extinct in all our simulations.

Our simulation results suggest that a dioecious population prevails only if males and females can make use of more resources than hermaphrodites. In Figure 4.2, this is the case below the black straight line. This coincides with the findings of Charnov et al. [1976]. However, when zooming in (see Figure 4.3), we can observe that a dioecious population can be invaded by hermaphrodites even if they have slightly less resources than males and females. This may be due to reduced competition between siblings for hermaphrodites: For females, ten siblings are competing with each other for space, while for hermaphrodites, only a reduced number of siblings are competing, as hermaphrodites do not only invest into seeds but also into pollen. In the model of Charnov et al. [1976], competition between siblings would not be observed because of its non-spatial character. While Charnov et al. also suggest that a dioecious population can be invaded by hermaphrodites if these have more resources, the authors do not observe an invasion of hermaphrodites when these have slightly less resources.

We do not observe a coexistence of all three sexes in the population in the long run. Charnov et al. [1976] suggest that this can only happen if hermaphrodites have exactly the same resources available as males and females. In our model, it appears that hermaphrodites have a reproductive advantage over males and females when all types have the same amount of total resources. Due to the finite number of cells in our spatial model, competition for space occurs. Even if hermaphrodites have the same amount of resources as males and females and they split their investment equally in pollen and ovule production, a completely hermaphroditic population prevails.

Furthermore, we also observe that males prevail in the population if hermaphrodites allocate less than about 4.85 units of resources to pollen production, and similarly for females. The four combinations emerging from hermaphrodites investing less than or greater than 4.85 units of resource to pollen or ovules, lead to four distinct regions for the prevalence: dioecy, hermaphrodites only, gynodioecy, or androdioecy.

4.3.2 Impact of pollen and seed radii on the prevalence of sex types

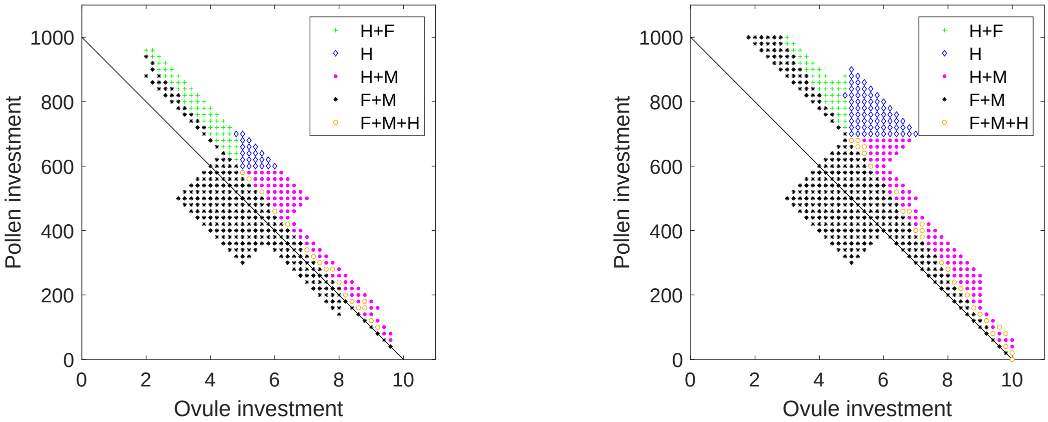
We now continue to investigate the influence of varying the pollen and seed dispersal radii on the prevalence of sex types. We do this by fixing the radii of the hermaphrodites at two for seeds and ten for pollen and then investigating how the boundaries between dioecious (F+M), androdioecious (H+M), gynodioecious (H+F), and hermaphrodite (H) prevalence change if males have a larger pollen radius or females have a bigger seed radius than hermaphrodites.

Figure 4.6 shows the results for an increased pollen radius for male plants to 11 (Figure 4.6a) and 12 (Figure 4.6b) units. All other settings remain as listed in Table 4.3. The horizontal boundary between the prevalence of only hermaphrodites and the prevalence of both hermaphrodites and males shifts upwards from 485 pollen to 590 pollen grains (comparing Figure 4.2 and Figure 4.6a). This moves the intersection point, where all prevalence regions meet, upwards while 4.85 ovules remain at the boundary between a hermaphrodite prevalence (right of the line) and a prevalence of hermaphrodites and females (left of the line). However, the border between a dioecious population surviving (black symbols) and the prevalence of hermaphrodites (all other colored symbols) is skewed: While the black symbols captured large parts of the area above the black line on the upper left, a dioecious population does not seem to get much additional benefit by increasing the male pollen radius compared to an androdioecious population (magenta dots).

The region where a dioecious population prevails is now larger. Especially on the upper left, it extends beyond the black straight line, where all three types have the same total resources. The larger pollen radius of males relative to hermaphrodites gives males an advantage over hermaphrodites. Thus, the black area expands with gains in the green area. The border between the magenta and black areas has not shifted much. The more the hermaphrodites invest into ovules, the lower is the disadvantage compared to the males with increased pollen radius. Therefore, they are not sensitive to reproduction disadvantages caused by a smaller pollen radius compared to their competitors.

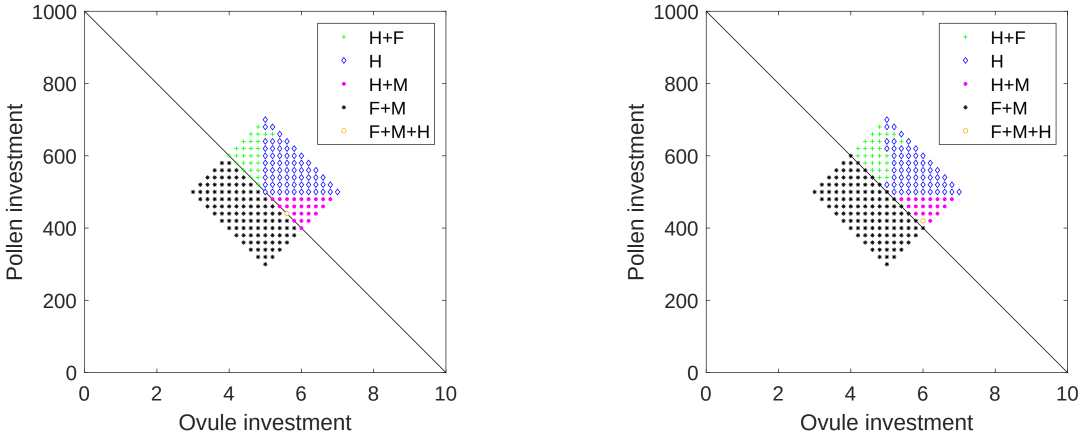
When increasing the pollen radius even further to 12 cells (see Figure 4.6b), the horizontal line between the hermaphroditic (blue) and the androdioecious (magenta) areas shift more to the top. Furthermore, the dioecious (black) area shifts the gynodioecious (green) area even more to the upper right. However, when hermaphrodites invest largely into ovules, due to the same reasons as explained above, no shift of areas can be noticed.

We conjecture that the value of increased pollen radius is two-fold. First, the greater the pollen radius, the less competition between siblings will take place. Second, an increased pollen radius increases the likelihood that a male plant will reach and fertilize all of the ovules of a hermaphrodite or female that otherwise is too far from another hermaphrodite's pollen.



(a) *Male pollen radius of 11 units* (b) *Male pollen radius of 12 units*

Figure 4.6: Sex types that survived after 3000 simulation steps when considering an increased male pollen radius from initially 10 units to 11 and 12 units, respectively. All other settings are as described in Table 4.3.



(a) *Female seed radius of 3 units* (b) *Female seed radius of 6 units*

Figure 4.7: Sex types that survived after 3000 simulation steps when considering an increased female seed radius from initially 2 units to 3 and 6 units, respectively. All other settings as described in Table 4.3.

Increasing the seed radius of females (Figure 4.7a and Figure 4.7b show results for radii of 3 and 6 units, respectively) relative to hermaphrodites (radius of 2) has minimal effects. The intersection point for the prevalence boundaries shifts rightwards to larger ovule numbers. Thus, the region where males and females are the only prevailing types becomes larger. The region where males form part of the prevailing breeding system remains exactly the same because the gain in the region for the male-female prevalence (black area) matches the loss for the androdioecious prevalence (magenta area). The size of the region where females are part of the prevailing breeding system expands with gains in the region of gynodioecy (green area). However, these effects are minimal compared to the effects of increasing the male's pollen radius. Increasing the seed radius should reduce competition between the ovules of females, but it seems that this effect is very small. With a seed radius of 2, 3, and 6 there are 25, 49, and 169 cells, respectively, within a female's seed neighborhood. Hence, most of the seeds dispersing from a female will find themselves in a cell without any sibling seeds. A much higher seed production would likely increase the advantage for the females of having an increased seed radius.

4.3.3 Unsuitable cells

In nature, not all spots are suitable for a plant species to grow. These obstacles include water, rocks, or even other vegetation covers. Therefore, we investigated the influence of cells unsuitable for germination and survival. We define an unsuitable cell as a cell where seeds cannot germinate; it rather acts as a sink where pollen and seeds may land without having any further effects, like growing or competing for space. A seed that disperses to an unsuitable cell dies. For these simulations, we randomly selected 50% of the cells across the landscape and marked them as unsuitable cells. The results are presented in Figure 4.8. Remarkably, the intersection point, where all of the different prevalence boundaries meet, shifted to the left. Thus, the blue (H) area replaced a part of the green (H+F) area. The reason for that is that unsuitable cells increase competition between siblings. As a consequence, hermaphrodites have an advantage over females because they do not use their full resources for the production of ovules, but also for pollen. This pollen is spread far, and thus, for females, the competition between siblings has a bigger influence on the success. Therefore, areas, where hermaphrodites prevail, are larger and areas where females persist in the population are smaller compared to when all cells are suitable (see Figure 4.2).

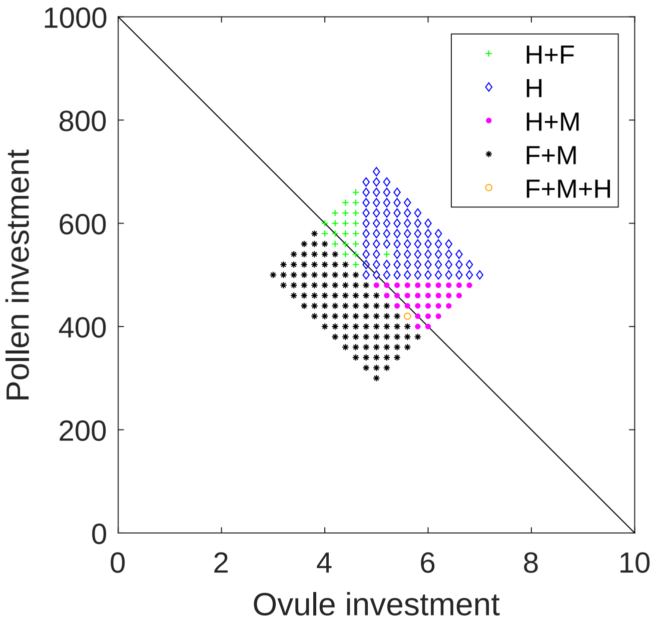


Figure 4.8: Sex types that survived after 3000 simulation steps when considering a field with 50% unsuitable cells.

4.4 Discussion

We here presented a simulation model to investigate the impact of space on the prevalence of breeding systems in a sex allocation model based on a non-spatial model of Charnov et al. [1976]. With this agent-based model, we are well able to investigate spatial aspects like different pollen and seed dispersal distances or obstacles where no seeds can germinate.

One of the key findings is that in all our simulations, we observe that at least one type goes extinct. This holds for all examined sex allocations in all case studies of this chapter. A breeding system consisting of males, females, and hermaphrodites is not stable. In nature, we however can find all breeding systems: Androdioecy on plant level is very rare [Barrett, 1998, De Jong et al., 2008]. However, few examples for species where populations consist of males and hermaphrodites can be found, such as the Japanese ash *Fraxinus lanuginosa* [Ishida and Hiura, 1998] or *Datisca glomerata* [Liston et al., 1990, Wolf et al., 2001]. Compared to androdioecy, gynodioecy is more common. Examples for gynodioecious species are *Thymus vulgaris* (Labiatae) [Tarayre and Thompson, 1997] and the alpine plant *Silene acaulis* (Caryophyllaceae) [Shykoff, 1988]. Furthermore, in nature, we can observe dioecious plant species as well such as the hop *Humulus Japonicus* [Aleksandrov et al., 2011, Grabowska-Joachimiak et al., 2011] or the hemp *Cannabis sativa* [Quimby et al., 1973, Salentijn et al., 2015].

Trioecy can rarely be observed in nature. Albert et al. [2013] define a true trioecious species as species where hermaphrodites producing simultaneously effective pollen and viable seeds, females producing only seeds and males producing effective pollen only co-exist (F+M+H). Although the cactus *Pachycereus pringlei* is considered to be a true trioecious species according to this definition [Fleming et al., 1994], both gynodioecious (F+H) and trioecious populations can be found in Mexico [Fleming et al., 1998], indicating the instability of trioecy. Furthermore, other examples of species can be found where hermaphrodites, females and males co-exist (e.g. *Atriplex canescens* [McArthur et al., 1992], *Spinacea oleracea* [Vitale and Freeman, 1986] and *Thymelaea hirsute* [Dommée et al., 1995]). However, these species consist of males, females, and sequential monoecious hermaphrodites, i.e., hermaphrodites that do not produce pollen and seeds at the same time. Thus, although males, females, and hermaphrodites can be found in the population, the species are not considered as true trioecious species according to the definition by Albert et al. [2013].

The second main finding in this paper is that we observe linear borders between all the areas indicating different breeding systems prevailing. The linearity is caused by the linear set-up of the model: First, in our simulations, we change the hermaphroditic investment into ovules and pollen linearly. Second, we have a uniformly distributed pollen flow not dependent on, e.g., distance or density. Each plant closer to another plant than the pollen radius has an equal chance to fertilize that plant. For future studies, further experiments choosing different pollen flow models can show the impact of the pollen flow model on the prevalence of sex types. As Chapter 5 in this dissertation shows, distance-dependent fertilization probabilities can easily be included in the type of models we consider here. The impact of an increased male pollen radius would be lower with such a distance-dependent pollen flow than with a uniform pollen distribution because with increasing distance to the focal plant, the probability to fertilize ovules decreases. Furthermore, many other extensions to make the pollen flow more realistic are possible, like including wind that more often blows from a certain direction. Assuming a wind-pollinated species and a wind direction biased such that it comes from the East, then, plants on the eastern side of the population will more likely produce pollen than ovules.

The third key finding of this chapter is observed when varying spatial parameters like the male pollen radius and the female seed radius. In our studies, an increased female seed radius only had marginal impacts on the prevalence of types. Considering annual plants and thus no overlapping generations, seeds can also germinate in cells of adult plants from the previous generation. This lowers the competition for space enormously. The total population size after 3000 generations from the simulations visualized in Figure 4.2 varied from 7483 to 9823 plants depending on the sex allocation of the hermaphrodites. The average number of plants in the last simulation step was 8243. This shows that the population, even at the last step, does not cover all cells. Thus the effect of the competition for space may not be that big. For future research, it would be interesting to see the effect of an intensified female competition by for example increasing the interaction fraction or the number of unsuitable cells while simultaneously applying the larger seed dispersal radius for females. Increasing the pollen dispersal radius for males has a higher impact on the prevalence of breeding systems than an increased seed dispersal distance for females. In our model, we consider that a pollen grain costs 100 times less than one seed. Thus, pollen is highly available, and the trees are still able to fertilize all female flowers within their (increased) pollen radius. When increasing the male pollen radius, while keeping the pollen radius for the hermaphrodites fixed, we observe that a dioecious population gains advantage over the gynodioecious population. When hermaphrodites invest a lot into pollen, they are very sensitive to a competitor with an increased pollen radius. On the contrary, when they invest almost all their resources into ovules, increasing the male pollen radius has almost no effect on the prevalence of hermaphrodites. Thus, we observed a skewed line separating the dioecious area from all other areas.

Furthermore, we compare our results to a non-spatial model by Charnov et al. [1976]. Without any asymmetry in the amount of resources or the seed/pollen dispersal distances of the sex types (see Section 4.3.1), we confirm their results: Like Charnov et al. [1976] in their non-spatial model, we observe that hermaphrodites never go extinct if they are in charge of more resources than males and females. Then, either males or females prevail in the population depending on the hermaphroditic allocation to ovules and pollen; the population becomes either gynodioecious or androdioecious. Figure 4.2 indicates that a dioecious population prevails if males and females have more total resources available than hermaphrodites. However, when zooming in on the area where all three sex types have the same total resources and the hermaphrodites split their resources equally to male and female function, we observe that hermaphrodites do not go extinct if they have only slightly less resources than males and females. This is probably due to reduced competition between siblings for hermaphrodites as they need to find space for half as many offspring than females. These effects cannot be noticed in a non-spatial model.

In their paper “Spatial seed and pollen games: dispersal, sex allocation, and the evolution of dioecy”, Fromhage and Kokko [2010] use a game theoretic model to investigate the influence of pollen and seed dispersal on the resulting sex system. Using their model, dioecy evolves if males and females have lower reproduction costs than hermaphrodites or if pollen and seeds disperse far. Our model supports the first observation. However, we did not investigate varying seed and pollen radii for all types. For future work, it would be interesting to examine the influence of increasing pollen and seed dispersal for all sex types rather than for only males or females on the prevalence of types in our model. Furthermore, their model shows that the sex allocation of hermaphrodites is biased towards the sex function that disperses farther. In our simulations, we can observe that the intersection point of all areas moves from (5,500) to (5,600) if we increase the pollen radius of the males. This shows the need of a higher investment into the male function as well.

So far, we did only one simulation run per examined sex allocation. Instead of running every scenario multiple times, we chose to run experiments on more sex allocations. Thus, we increase the robustness of our findings by performing simulations on a very fine grid of hermaphroditic sex allocations. As the sex allocations do not differ that much between simulation runs, we still think that our results are meaningful. Our results showing the frequencies of remaining types support this. Furthermore, we were interested in the breeding system, i.e., the combination of surviving types, after a certain number of simulation steps. Multiple simulations for the same sex allocation would possibly lead to different breeding systems occurring; our results would show probabilities for sex types to prevail rather than a unique breeding system. For future work, this would be an interesting scenario to examine. We furthermore tested the robustness of our results to initial conditions by applying changes to the conditions for our reference case studies. Instead of starting the simulations with only the three genotypes AA, XX and XY, we did some experiments on starting with all five genotypes in the initial population. Additionally, we varied the initial distribution of types in such a way that either only few hermaphrodites (5% AA) or only few males and females (5% XX and 5% XY) are present in the initial population. When starting with all five types, and when starting with only a few hermaphrodites in the initial population, no difference in the prevalence of the sex types can be observed. When starting with only few males and females, and when hermaphrodites have less resources, we could observe in our reference simulations that a dioecious population has a reproductive advantage. Near the threshold, the reproductive success is almost the same for hermaphrodites compared to the success of a dioecious population. Thus, when starting with a low number of males and females, stochasticity will sometimes lead to the extinction of types having a slight reproductive advantage. However, even when starting with a lower number of hermaphrodites or males and females, the main findings (linear borders and prevalence of maximal two types) remain the same, but the borders of the prevalence areas may not be as sharp anymore.

CHAPTER 5

Surplus ovules permit female choice in oak trees

Abstract

Many plants produce surplus ovules that never become fruits. Oak trees produce six ovules per flower, and just one matures to an acorn. Compared to other species, long-distance fertilization in stands of oak trees is much more common. Furthermore, nearby oak trees are often absent as pollen donors. For a wind-pollinated species such as oak, these observations cannot be explained by commonly used pollen flow models, where the probability to fertilize another tree declines with distance between the trees. Here, we extend a two-step lottery model of Craft et al. [2009] to test the hypothesis that oak trees pursue a form of within-flower female choice to increase the diversity of fathers. With our model, we show that producing multiple ovules per flower may allow selection for the rare father, thus increasing the chances that distant trees will be successful fathers. As the number of potential father trees increases, the number of ovules needed for maximizing the diversity of fathers increases as well. However, we show that when considering a certain cost function for ovule production, six ovules per flower achieves a balance between the benefit of diversifying fathers and the costs of producing multiple ovules per flower. Next, assuming that six is the optimal number of ovules within a flower - as it can often be observed in nature - we perform several experiments to investigate the influence of the female choice mechanism on the genetic di-

versity in the stand. For example, we simulate the consequences of a tree's position within a stand and observe that for trees closer to the edge of the stand, the Simpson's diversity index (SDI) is higher than for trees farther away. Finally, we use data from three different field studies to validate the hypothesis that oaks exhibit female choice. Again, we assume that six ovules are optimal and compare the results of the female choice mechanism to a random ovule choice. The studies provide paternal information for a sample of acorns from 10 different individual oaks. We simulate paternity outcomes by using the actual positions of potential pollen donors. Two of the field studies allow for a comparison of the paternal diversity index. For 7 out of the 8 investigated maternal oaks, the actual diversity index of fathers (average paternal diversity index of 15.42) fit the female choice hypothesis (estimated diversity of 14.66) significantly better than a random choice from the six available ovules (estimated diversity of 7.649). A third study allows for a comparison of paternity by distance classes. For both maternal trees, the female choice hypothesis explains the observed fertilization pattern better than random ovule selection.

5.1 Introduction

Many, if not most, plant species produce more ovules per flower than later will become seeds. Examples include various tropical trees [Bawa and Webb, 1984, Ganeshaiah and Shaanker, 1988, Mohana et al., 2001], *Prunus dulcis* (almond tree) [Pimienta and Polito, 1982], *Phaseolus coccineus* (bean) [Rocha and Stephenson, 1991], *Cryptantha ava* [Casper and Wiens, 1981], and oaks [Boavida et al., 1999, Brown and Lloyd Mogensen, 1972]. By way of hypotheses, the overproduction of ovules may be in response to pollen limitation [Kärkkäinen et al., 1999, Stephenson, 1980]. Or, the plant's strategy may be to set some optimal number of seeds per fruit. Offering a larger number of ovules may ensure that this target is met. This could also be the case if a genetic defect or early genetic load, i.e., early occurrence of inviable fertilization products, results in the failed maturation of some of the fertilized ovules [Charlesworth, 1989, Kärkkäinen et al., 1999]. A third possibility is that the plant is bet-hedging. Resource availability following flowering may unexpectedly fluctuate, and the plant may abort some fraction of each flower's fertilized ovules based on resource limitations. In all of these cases, a plant can often achieve the same result by aborting complete flowers rather than single ovules, and such flower abortion occurs among many plant species as well [Hikosaka and Sugiyama, 2004, Marcelis et al., 2004, Stephenson and Winsor, 1986].

Furthermore, these hypotheses only partly explain the observed seed set and fertilization patterns [Charlesworth, 1989]. In self-incompatible perennials, female fertility is lower than in self-incompatible annuals [Wiens, 1984]. This cannot be explained by different pollen availabilities to perennial plants versus annual plants. Other studies show that in many cases, seed-set does not increase if flowers are artificially hand-pollinate [Burd, 1994, Ishii and Sakai, 2000]. The question of why a plant has more ovules per flower than it can or intends to mature becomes even more focused for plants that have multiple ovules per flower but only mature at most one seed. Such is the case for oaks of the genus *Quercus*. The flowers of most oak species have exactly six ovules [Boavida et al., 1999, Brown and Lloyd Mogensen, 1972, Stairs, 1964]. Oaks are wind-pollinated and self-incompatible. Research shows that most if not all of a flower's ovules are fertilized [Borgardt and Nixon, 2003, Craft et al., 2009], but see [Boavida et al., 1999, Lloyd Mogensen, 1975] for contrasting statements. Yet, from these six ovules, only one ovule matures to an acorn.

Craft et al. [2009] proposed that pollinating several ovules while maturing just one, could be a form of female choice. A weighted lottery within the flower could increase the diversity of "dads" that contribute pollen to the maternal function of a given oak tree. They hypothesized a two-step lottery. In the first step, each of the six ovules becomes fertilized. The likelihood of being the father of an ovule is simply a random choice from the pollen grains that arrive at the unfertilized flower. A father that provides twice as much pollen to the flower as another has twice the likelihood of pollinating the ovule, and each ovule becomes pollinated in this manner independent of the other ovules of the flower. In the second step of the lottery, the flower has some choice over the single ovule that will become an acorn. The acorn is formed from that ovule that has no paternal siblings within the flower. If it is not a unique ovule, a random draw from the ovules without paternal siblings selects the surviving ovule. If all ovules have paternal siblings, the surviving ovule is randomly drawn from the ovules with the least number of paternal siblings within the flower. Given the vast amount of pollen produced per oak, such a two-step weighted lottery system increases the odds that more distant oak trees will serve as pollen donors. This happens because winners of the first step are heavily biased towards nearby oak trees. But, pollen of nearby trees becomes selected against during the second-step of the lottery as these trees are the most likely to fertilize multiple ovules within a flower.

The hypothesis of Craft et al. [2009] was inspired by empirical data from Dow and Ashley [1996, 1998]. Using micro-satellites, they showed that acorns of a given oak tree had an over-representation of distant fathers than would be expected from pollen flow. Many acorns were fertilized by fathers far away from the maternal tree. Furthermore, clusters of oak trees in the neighborhood of an oak fertilized remarkably few acorns [Dow and Ashley, 1998]. The distribution of an oak tree's fathers could not be explained by simpler models of pollen flow. Hence, oak trees appear to have some maternal mechanism for preferentially choosing pollen from distant fathers.

Because in the model by Craft et al. [2009], space is only implicitly defined, it cannot be used to validate the female choice hypothesis with real data. Therefore, we here present a spatially explicit model based on the work of Craft et al. [2009]. Their model shows how a two-step lottery could allow an oak tree to increase the diversity of its acorns' fathers by preventing the over-representation of a tree's closest neighbors. We assume that there is a benefit to the individual tree in diversifying the number of fathers among her acorns. A higher diversity of fathers may provide a form of bet-hedging if some fathers are overall more fit than others [Evans et al., 2012, Watson, 1991]. Furthermore, it may reduce competition between siblings by increasing the likelihood that acorns are half- rather than full-siblings [Berglund et al., 1988, Bulmer, 1980]. Or, by maximizing the genetic variability of her acorns, the oak, through her female function, may be bet-hedging in response to environmental contingencies [King and Masel, 2007, Olofsson et al., 2009, Seger and Brockmann, 1987, Simons, 2011]. The fertilization by trees from far away may reduce inbreeding [Hauser and Loeschcke, 1994, O'Connell et al., 2007]. Furthermore, if there is some cost to the plant for increasing the number of ovules, then having six could well provide the optimal balance between ovule number and diversity of fathers. We improve on the model by Craft et al. [2009] in two aspects. First, we model circumstances where there can be any number of oak trees with either spatially implicit or spatially explicit distributions. This becomes essential for comparing model output to actual data. Second, Craft et al. [2009] only considered a single focal tree as the mother, while we allow for more. Oak trees are hermaphrodites well known as non-selfers [Bacilieri et al., 1993, Dow and Ashley, 1996, 1998, Schwarzmann and Gerhold, 1991]. Within a stand of oaks, trees are contributing to acorn production both through female and male function. In our model, we let all trees contribute both pollen and ovules. Our model can track the diversity of fathers for each oak tree within a stand, as well as the diversity of maternal oak trees among the acorns fertilized via pollen by each oak tree. This level of model output further increases the range of predictions that can be tested empirically.

To validate the female choice hypothesis, we use published data sets that explicitly map the coordinates of trees within a stand and the pollen donors among these trees as represented in the acorns. With our model, we can use real coordinates and data to compare the predictions resulting from the model when a flower randomly selects a fertilized ovule versus the two-step weighted lottery. In what follows, we start with a description of our continuous space model. Next, we compare results for spatially implicit (as used by Craft et al. [2009]) and spatially explicit stands of trees. We then compare model predictions with three different published studies [Dow and Ashley, 1998, Pluess et al., 2009, Streiff et al., 1999] to show that the simulations considering female selection in the model explain the data better than random ovule selection.

5.2 The model

Here, we present our spatially explicit model based on the work of Craft et al. [2009]. While we focus on the general description of the model in this section, Sections 5.2.1 and 5.2.2 describe the characteristics of both the spatially implicit and explicit model variants in more detail. We consider a stand of n oak trees that can both receive and produce pollen. Each tree in the model has 10000 flowers and a ovules per flower. In our simulations, we vary the parameter a to see the impact of the number of ovules in a flower on the diversity of fathers within the stand.

The model consists of two lottery steps: In the first step, all ovules within all 10000 flowers of all trees are fertilized by other trees. As oaks are well-known as non-selfers, we do not allow for self-fertilization [Bacilieri et al., 1993, Dow and Ashley, 1996, 1998, Schwarzmann and Gerhold, 1991]. We assume no pollen limitation, and thus, all ovules are fertilized.

The pollen donor for an ovule is determined according to a probability distribution. Each pollen donor i has a probability p_i to fertilize one ovule within a flower. We furthermore assume that all trees within a stand act as pollen donors and that all pollen come from trees within the stand, such that $\sum_i p_i = 1$. In contrast to Craft et al. [2009], who use a density and dispersion dependent probability (see Equation 5.1), we here define a spatially explicit probability p_i to fertilize an ovule within a flower (see Equation 5.2). In the second step of the lottery, one ovule per flower is selected to become an acorn while all others are aborted. The resulting acorn is formed from the ovule fertilized by the father, who fertilized the least number of ovules within that flower. If multiple ovules fulfill this requirement, one ovule among these is chosen randomly to become the acorn. So if there are six ovules in a flower and three are fertilized by father 1, two by father 2 and one by father 3, then only the ovule of father 3 matures to an acorn. All other ovules are aborted. If four ovules are fertilized by father 1, one ovule by father 2 and one by father 3, then either father 2 or 3 will sire the acorn with equal probability. We assume that each ovule chosen to become an acorn for sure matures, i.e., we do not consider germination failure.

This approach favors the rare fathers as trees only become fathers of an acorn if they win the second lottery step. While common fathers most likely fertilize lots of ovules in a flower, i.e., most likely win in the first lottery step, they will lose in the second lottery step. Assuming a probability p_i for father i to fertilize an ovule within a flower, we can conclude that a high p_i will most likely lead to a small probability q_i to be the father of the acorn, i.e., to win the second lottery step. In Appendix A, we derive an explicit formula for q_i dependent on p_i assuming two or three fathers, respectively.

In addition to the above-described ovule selection approach, we furthermore implement the possibility to randomly choose one ovule per flower in order to be able to compare the predictions of the random-choice model with those of the two-step lottery one. In the remainder of the chapter, we will refer to the two models as the female choice and the random choice model.

5.2.1 Spatially implicit model of tree density and dispersion

Craft et al. [2009] consider flowers of a single focal oak tree that can be fertilized by at most n fathers. They order the potential father trees such that father number 1 is the nearest to the maternal tree and father n is the farthest away. As described in the previous section, the model consists of two lottery steps. In the first step, each ovule is fertilized by father i according to the probability p_i defined as:

$$p_i = \frac{\left(\frac{1}{\alpha}\right)^i}{\sum_{j=1}^{n}\left(\frac{1}{\alpha}\right)^j} \tag{5.1}$$

where n is the number of potential fathers and $\alpha > 1$ models the dispersion of father trees around the focal oak tree. If $\alpha = 1$ then all fathers have equal probabilities of fertilizing an ovule. As α increases, the dispersion pattern of fathers becomes broader. With a larger α, the proportional likelihood of fertilizing an ovule declines more rapidly for each successive tree $i = 1, \ldots, n$. In fact, $\alpha = p_i/(p_{i+1})$ is the ratio of success at fertilizing ovules between two sequential trees, i and $i+1$. Hence as α approaches infinity, only the first father fertilizes all of the ovules of the focal oak.

In the second lottery step, the female choice model is applied, i.e., the ovule of the rarest pollen donor in that flower is chosen to become an acorn.

5.2.2 Continuous-space model with pollen dispersal following an inverse square law

In contrast to the model of Craft et al. [2009], we here consider a spatially explicit model. The trees here are distributed on a two-dimensional continuous field. We consider both a torus field with periodic boundary conditions and a square field with discontinuity at the boundaries. In the remainder of the chapter, we will refer to these two spaces as torus and square, respectively. On such a torus, pollen leaving the field on the left side enter the field again on the right side. The same holds for the top and bottom side. No tree experiences any boundary effects. The second scenario imagines woodlots with distinct boundaries. We imagine a square forest. Trees near the boundaries will, on average, be farther away from other trees than trees near the middle.

Also, in this model variant, the two-step lottery is applied. First, all ovules are fertilized. To consider all possible pairwise combinations of pollen flow between trees, we assume that pollen flow follows an inverse square law with distance between any two trees. This assumption will manifest as the so-called leptokurtic distribution of pollen flow from a tree that has been measured empirically for wind-dispersed pollen [Ellstrand, 1992, Levin and Kerster, 1974, Tonsor, 1985]. The probability that tree i pollinates an ovule of tree j with $i \neq j$ is given by:

$$p_{ij} = \frac{\frac{1}{d_{ij}^2}}{\sum\limits_{k \neq j} \frac{1}{d_{kj}^2}} \tag{5.2}$$

where d_{ij} is the distance between trees i and j.

In the second lottery step, the female choice model is applied: Based on the paternal information of the ovules, one ovule per flower is selected to become the acorn. All other ovules are aborted.

In contrast to the model of Craft et al. [2009], in our spatially explicit model, we consider flowers of multiple trees that can be fertilized. Thus, we introduced index j for the tree being fertilized in Formula 5.2. This formula generalizes the notation of Craft et al. in such a way that j can be considered as 0 in their model, with tree $j = 0$ being the unique focal tree that is fertilized.

5.3 Model analysis

In this section, we analyze the relationship between the probability p_i for father i fertilizing an ovule of a certain flower and the probability q_i to be the father selected in that flower. Therefore, we here focus on just one single flower. The ovule selection in the flower is based on the female choice mechanism. Please note that p_i can be determined either by Formula 5.1 (using the spatially implicit model of Craft et al. [2009]) or by Formula 5.2 (using our spatially explicit model).

The within-flower female choice can skew acorn paternity patterns away from what would happen if there was random ovule selection within a flower. Under random ovule choice, the probabilities q_i to be father of the acorn will conform to the probabilities p_i to fertilize an ovule in the flower, because the expected number of ovules fertilized by father i is ap_i with a being the total numbers of ovules in the flower and $q_i = \frac{ap_i}{\sum_k ap_k} = p_i$. And thus it holds that $p_i = q_i$. With female choice, the father nearest to the maternal tree still has the highest probability to win the first lottery step. However, this father is more likely to lose fertilized ovules at the second lottery step, and $p_i > q_i$ for trees close to the focal tree. The situation is reversed for the farthest father. He fertilizes the fewest ovules in the first lottery and sees the fewest discarded ovules in the second: $p_i < q_i$ for distant trees. The second lottery favors more distant fathers at the expense of closer ones.

We can derive explicit expressions for the two-stage lottery when there are two or three potential fathers for a focal oak's flowers. Let p_i be the probability of father i fertilizing this particular ovule. We assume that ovules are only fertilized by other trees within the stand and that all trees in the stand contribute pollen that may fertilize ovules of other trees. Thus, $\sum_i p_i = 1$. Furthermore, let X_i be the number of ovules fertilized in the flower by father i. We then can calculate the probability q_1 of father 1 winning the second lottery (so fertilizing the flower) when considering two fathers in total and six ovules (see Appendix A). This becomes a combinatorial problem. Father 1 only wins the second lottery step for sure if he fertilizes all ovules in that flower, or at least one ovule and at the same time less ovules than father 2. Considering six ovules per flower, this is the case if father 1 fertilizes either one, two, or six ovules. Furthermore, father 1 has a 50% chance to become the father of the acorn, i.e., to win the second lottery step, if he fertilizes the same number of ovules in that flower as father 2. Then, both fathers fertilize three ovules in that flower and the ovule to become an acorn is selected randomly.

Figure 5.1 shows the relationship between p_1 and q_1 considering two possible fathers and six ovules per flower. In the area above the red dotted horizontal line, it holds that q_1, the probability for father 1 to win the second lottery step, is higher than 0.5. While the red dashed line is showing the relationship between p_1 and q_1 for the random choice approach, the blue curve shows the relationship for the female choice model. Considering a random ovule choice (red dashed line), $p_1 = q_1$. The blue curve, resulting from calculations that can be found in Appendix A, shows the non-linearity in the relationship between p_1 and q_1 for the female choice mechanism. From Figure 5.1 we see that there are two possibilities for father 1 to have a larger chance than father 2 to win the second lottery ($q_1 > 0.5$): either $p_1 \in (0.1, 0.5)$ or $p_1 > 0.9$. The first range shows that the rare dad indeed has a higher chance of siring a flower's acorn. However, the rare dad needs to fertilize at least one ovule in that flower. Thus, it needs to hold that $p_1 > 0.1$, because otherwise, father 2 as the common father has a high chance to fertilize all ovules within a flower. For $p_1 > 0.9$, it is very likely that father 1 fertilizes all ovules within that flower and thus also wins the second lottery step. Figure 5.1 furthermore shows that the female choice favors rare fathers as the blue curve lies above the red curve for $p_1 < 0.5$. As mentioned at the beginning of this section, p_1 can be either calculated using Formula 5.1 or Formula 5.2. However, when considering the spatially implicit model of Craft et al. [2009] (i.e. Formula 5.1) and two fathers, it holds that $p_1 > 0.5$. In that case, only the right half of Figure 5.1 needs to be considered.

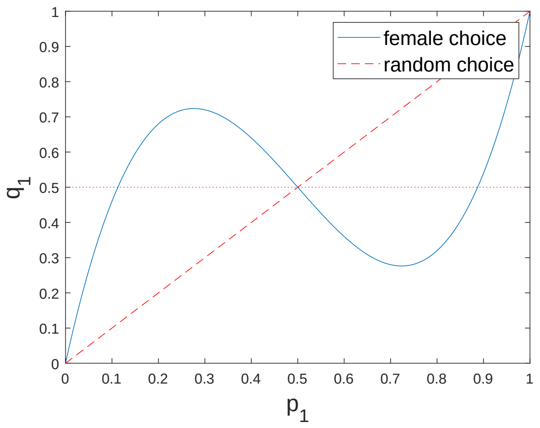


Figure 5.1: Probability q_1 of a father to fertilize the flower dependent on the probability p_1 to fertilize an ovule in that flower considering $a = 6$ ovules and $n = 2$ possible fathers. The blue curve is derived from Formula A.1.

Increasing the number of possible fathers to three fathers makes the calculations more involved. Father 1 will sire the offspring for sure when he fertilizes either all ovules in the flower, or at least fertilizes one ovule but at the same time uniquely the minimal number of ovules in the flower. The following combinations are possible (the number in the brackets indicate, how many ovules are fertilized by the first, second, and third father, respectively): Father 1 either fertilizes six ovules (6,0,0), or one ovule while the other fertilize either none and five ((1,5,0) or (1,0,5)) or two and three ovules ((1,2,3) or (1,3,2)), or two ovules while the others fertilize none and four ovules ((2,0,4) or (2,4,0)). Furthermore, father 1 has a $\frac{1}{3}$ chance to become the father of the acorn, if all three fathers fertilize two ovules ((2,2,2)). If, next to father 1, exactly one other father fertilizes three ovules ((3,3,0) or (3,0,3)), father 1 has a $\frac{1}{2}$ chance to sire the acorn. The calculations can be found in Appendix A.

5.4 Case studies

In the following, we will first present case studies on the influence of the female choice on the diversity in the stand for both the spatially implicit and explicit variant of the model. Therefore, we need a measurement for the paternal diversity to analyze the results of our simulations. For this purpose, we utilize the following interpretation of the Simpson's diversity index (SDI) [Simpson, 1949]:

$$\mathrm{SDI} = \frac{1}{\sum_{i=1}^{n} \hat{q}_i^2} \tag{5.3}$$

where $\hat{q}_i$ is the fraction of flowers fertilized by father i and $\sum_i \hat{q}_i = 1$. Parameter $\hat{q}_i$ is an approximation for the probability q_i of father i winning the two-step lottery in a flower. In Appendix A, we show that calculating q_i explicitly is getting more complicated with increasing number of fathers. In our case studies, we use stand sizes of more than 20 trees. Therefore, we compute $\hat{q}_i$ in our simulations for each of the fathers by tracking the number of flowers each father has fertilized and dividing it by the total number of flowers. Next, we can compute the SDI according to formula 5.3. The SDI lies in the interval $[1, n]$ and thus can be easily interpreted: If all trees are paternal trees of the same number of ovules (i.e., all trees won the second lottery step equally often) then $\mathrm{SDI} = n$, the total number of fathers. $\mathrm{SDI} = 1$ if only a single tree is the paternal tree of all ovules of the focal tree.

5.4.1 Case studies on spatially implicit model

Following Craft et al. [2009], we now consider a single focal oak tree for which each flower can be fertilized by at most n fathers, and we consider the consequences of varying the number of ovules per flower and the dispersion α. We assume that the focal tree produces 10000 flowers, and in each of the flowers, the ovule to become an acorn is chosen according to the female choice model.

All else equal, the SDI will increase with the number of trees. For just one ovule per flower, the SDI will decrease with dispersion parameter α. The relationship between number of ovules and the SDI is more subtle. The SDI tends to increase and then decrease with ovule number, sometimes showing a wave pattern with multiple peaks: For $n = 10$ and $\alpha = 5$, for example, we observe multiple peaks, while for $\alpha = 2$, we only observe a unique maximum of the SDI (see also Figure 5.3 for more examples).

When the number of ovules is 1, then $q_i = p_i$. With two ovules there is no opportunity for female choice directly within a flower, but the nearest tree will lose more fertilized ovules by pollinating both ovules of a flower than the farthest tree (pollen competition between siblings). However, as we do not consider costs for producing pollen or pollen limitation, this effect is not covered by our model. In our model, there is no difference between considering one or two ovules as for two ovules it still holds that $q_i = p_i$. Therefore, we do not observe an increase of the SDI from one to two ovules (see Figures 5.3b and 5.3d). With three ovules, there can now be an active female choice within a flower, and nearer fathers can actually have fertilized ovules discarded by the flower; q_1 and q_n will continue to decline and increase, respectively.

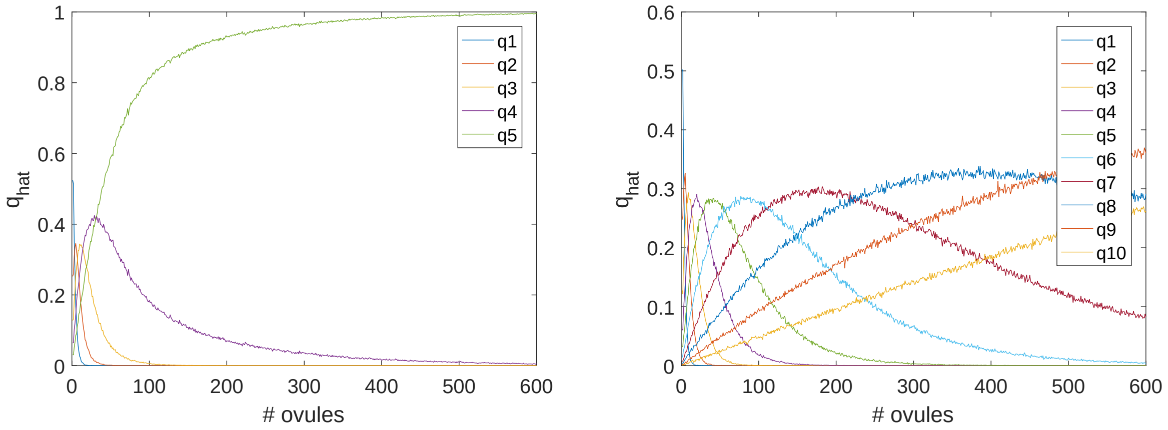
However, as the number of ovules within a flower increases to very large (and unrealistic) numbers, then the farthest tree will be the father of all the acorns, $q_n = 1$, and SDI $= 1$. For an extremely low probability p_n for the farthest father to fertilize ovules of the focal maternal tree, the number of ovules needs to be extremely large to ensure that this father fertilizes almost surely one ovule per flower. For $\alpha = 2$ and $n = 5$ it already follows that for the farthest father, $p_n \approx 0.032$. Increasing the number of fathers to 20, leads to $p_n \approx 10^{-6}$. Thus, the number of ovules to ensure that this father almost surely fertilizes at least one ovule per flower needs to be extremely large.

The SDI for different numbers of fathers ($n =$ 5, 10 and 20), dispersions ($\alpha =$ 2 and 5) and ovules per flower ($1, \ldots, 1000$) are presented in Figure 5.3. The results of our simulations show that the SDI reaches a maximum at about 6 and 25 ovules per flower, respectively, for a relatively dense distribution of trees ($\alpha = 2$) and for $n = 5$ versus $n = 10$ fathers (see also Figures 5.3a and 5.3b). With $n = 20$, the SDI reaches a maximum at about 20 ovules per flower and does not decrease much beyond that. With a small number of fathers ($n = 5$), the SDI decreases rapidly with the number of ovules as the nearest trees begin to father fewer acorns than the farthest trees: $q_1 < q_5$ as the number of ovules increases.

With a higher number of ovules, there is a sliding window where at first q_1 is highest, then q_2, then q_3 and so on, until q_n is the greatest and converges to $q_n = 1$ as the number of ovules per flower approaches infinity. With a small number of father trees ($n = 5$) and a small dispersion parameter ($\alpha = 2$), this sliding window moves quickly with increasing ovule numbers. Figure 5.2 illustrates this process. It shows how the fraction of fertilized flowers evolves for each father with increasing number of ovules. We considered up to 600 ovules to visualize the sliding window effect that can be noticed especially in Figure 5.2b.

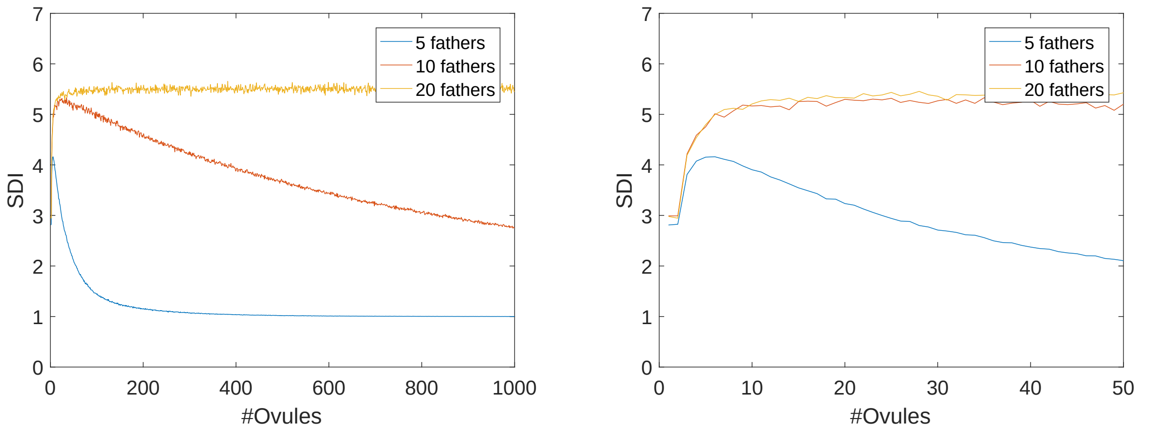
As the dispersion parameter increases ($\alpha = 5$), the sliding window narrows and favors higher numbers of ovules to maximize the SDI (see Figures 5.3c and 5.3d). The simulated data show multiple local maxima for the SDI at about 5, 30, 130, and 700 ovules per flower. This holds for each of the investigated numbers of fathers. In all simulations, the maximum SDI achievable by varying the number of ovules per flower declines with the dispersion parameter α. Interestingly, the situation with the greatest spread of trees (higher α) produces the lowest SDI, yet has the most to gain in SDI with female choice and multiple ovules.

In all cases, the diversity of fathers present in a focal tree's acorns can be maximized by choosing a certain number of ovules larger than 3. In many cases having the 6 ovules typical of *Quercus* [Boavida et al., 1999, Brown and Lloyd Mogensen, 1972, Stairs, 1964] produces a large increase in SDI relative to just one, two or three ovules per flower (see Figures 5.3b and 5.3d). Sometimes a much greater number of ovules produce the highest SDI as in the case of ten fathers in the stand and 25 ovules per flower (see red curve in Figure 5.3b). But, such large numbers of ovules must entail a cost that presumably becomes prohibitive. Adding a cost for ovule production would decrease the optimal number of ovules.

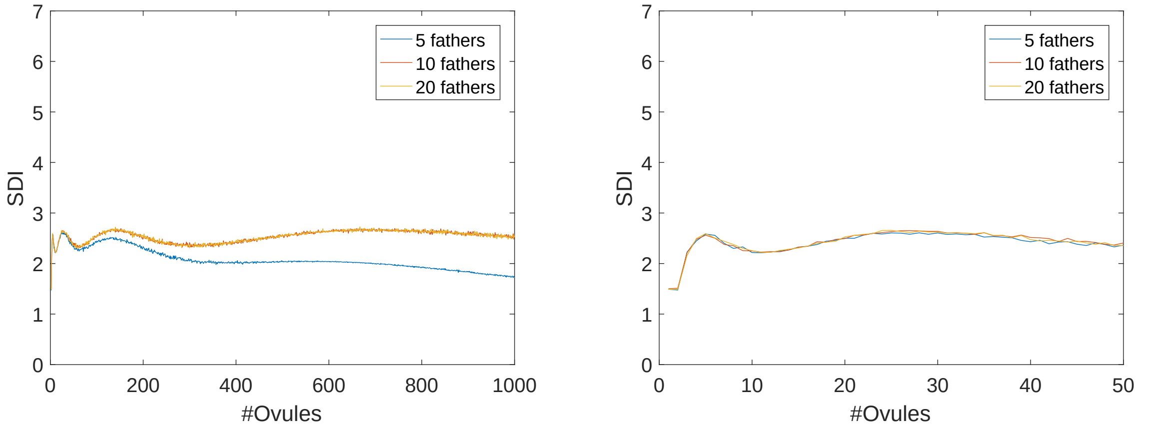


(a) Simulated $\hat{q}$ for five fathers *(b) Simulated $\hat{q}$ for ten fathers*

Figure 5.2: Simulated $\hat{q}$ for $n = 5$ and $n = 10$ fathers and varying ovules per flower. In both simulations, $\alpha = 2$.



(a) SDI for $\alpha = 2$ for 1...1000 ovules *(b) SDI for $\alpha = 2$ for 1...50 ovules (zoomed)*



(c) SDI for $\alpha = 5$ for 1...1000 ovules *(d) SDI for $\alpha = 5$ for 1...50 ovules (zoomed)*

Figure 5.3: Simulated SDI for 5, 10 and 20 fathers using the spatially implicit model with different values for α

5.4.2 Case studies on spatially explicit continuous-space model

We can use the spatially explicit model to consider stands of oaks distributed on a two-dimensional continuous space. Since oaks are non-selfing hermaphrodites, we can track male success, diversity of trees pertaining to a focal oak's male success, as well as our original measure of SDI for each trees' acorns. For each simulation, we consider the number of trees and their locations fixed. We give each tree exactly 10000 flowers, and the number of ovules per flower will be the same in all trees.

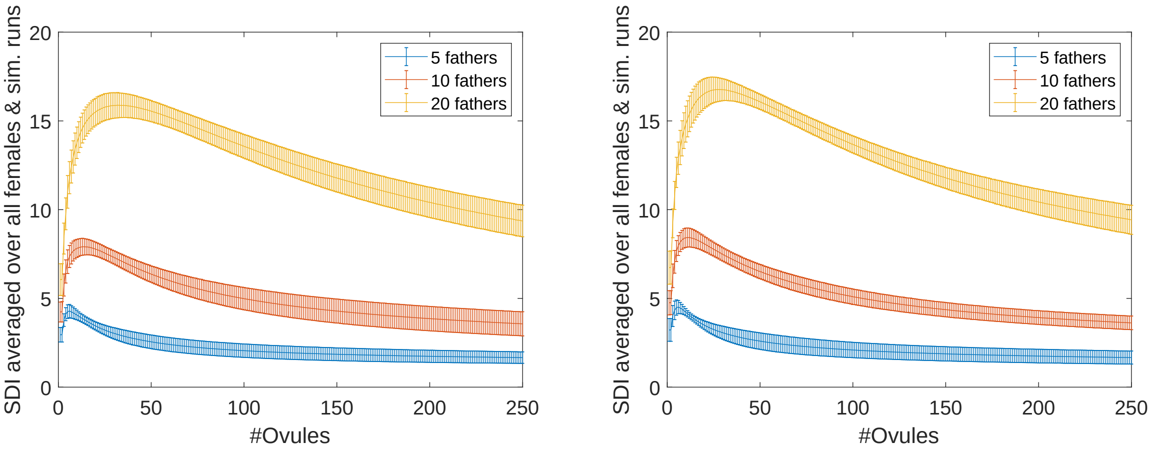
We again examine the effects of having multiple ovules and the two-stage lottery of female choice within a flower. During the simulations, we keep track of the number of acorns each father has fertilized. With these values, we are able to compute the SDI according to Equation 5.3 for each of the trees in the stand. For a given simulation, we then take the average of these SDI values to get a mean measure for the diversity of fathers of a tree's acorns. Additionally, we can also compute the diversity of maternal trees among the acorns sired by a given tree in the stand.

For our simulations, we chose a field of size 10 by 10 units, though the spatial units are not important as Equation 5.2 remains invariant to scale. For each simulation, we randomly place a certain number of trees into the stand. For comparison to the spatially implicit model, we chose 6, 11, and 21 trees as this equates to 5, 10, and 20 potential fathers for each tree. The random placement of trees creates additional sources of stochasticity compared to the previous model. With explicit placement of trees, each tree can now have a unique distribution of distances from other trees. Thus, each tree of the stand may have a separate SDI of fathers for its acorns. To account for this, we will average the SDI across the trees of a simulation. With random placement of trees, the matrix of distances between trees will vary from run to run of the simulation. Thus, we ran 20 simulations with different initial tree placements to measure the mean and variability.

Simpson diversity index for different number of fathers

Female choice via multiple ovules and the two-step lottery can greatly increase a tree's SDI of fathers compared to a random ovule choice. Figure 5.4 shows how the average SDI for forest stands with 5, 10, and 20 fathers depends on the number of ovules per flower. The SDI values are averaged over 20 simulation runs and over all trees in the stand (6, 11, and 21) and are presented as $(\mu - s, \mu + s)$ where μ is the mean and s the standard deviation. In all cases, the SDI increases rapidly with the number of ovules up to a global maximum, after which the SDI decreases slowly. Regardless of the number of possible fathers, the maximum SDI is at about 80% of the number of possible fathers. Doubling the number of potential fathers essentially doubles the maximum SDI. However, the maximum SDI occurs at a larger number of ovules per flower as the number of fathers increases. The results are similar whether we assume a torus or a square field. The boundary-less torus reaches a slightly higher maximum SDI, and this maximum is reached with slightly fewer ovules (Figure 5.4). As would be expected, the variance among trees in SDI is smaller for the torus than for a square field.

The results obtained with the continuous-space models (for torus and square) are very similar to the spatially implicit model if one assumes a fairly dense stand with a dispersion parameter $\alpha = 2$ (see Figure 5.3a). For all of these cases, we observe a single maximum of the SDI at a value well below 50 ovules per flower. It seems that the random placement of trees on a continuous landscape creates a dispersion where a tree's consecutive nearest neighbors have a ratio of about $\alpha = 2$ as the simulated results are very similar.



(a) Average SDI for a square field

(b) Average SDI for a torus

Figure 5.4: SDI for 5, 10 and 20 fathers. Values are averaged over 20 simulation runs and over all trees in the stand

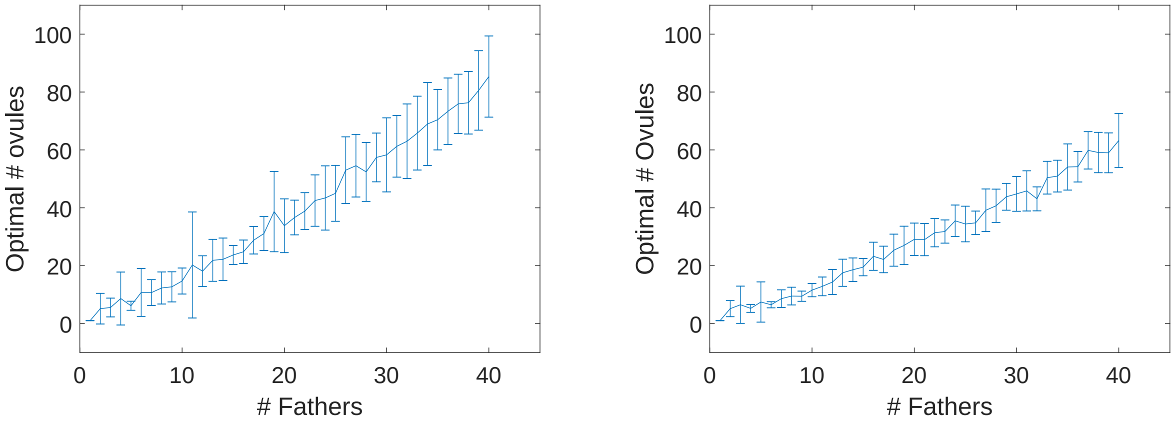
Optimal number of ovules per flower

For each space (torus and square) and for the different number of trees in the stand (2, ..., 41), the values for the SDI maximizing number of ovules per flower are presented as $(\mu - s, \mu + s)$ where μ is the mean and s the standard deviation of 20 simulation runs (Figure 5.5). As the number of trees in the stand increases, the optimal number of ovules for maximizing a tree's SDI of fathers increases almost linearly (Figures 5.5a and 5.5b). This rate of increase is smaller for the stand modeled on a torus than for the stand modeled on a square. For example, to maximize the SDI in an oak stand with 30 possible fathers (31 trees), the flowers would need to have 58 and 43 ovules for the square and the torus, respectively. Trees near the border achieve a smaller SDI (see case studies about the preferable position for a tree in a stand). On a torus, no tree experiences such border effects, and thus, the SDI is higher for a torus. Furthermore, the variance in the optimal number of ovules per run of the simulation is higher for the square than for the torus.

There presumably is a cost to producing multiple ovules per flower. An unlimited number of ovules per flower is unrealistic. Figures 5.5c and 5.5d show the results when considering linear costs for the production of ovules. In this case, we define the cost of ovules in units of SDI. As proposed by Craft et al. [2009], we reduce the SDI by 0.2 units for each ovule produced resulting in the following formula for the SDI in case of a ovules per flower:

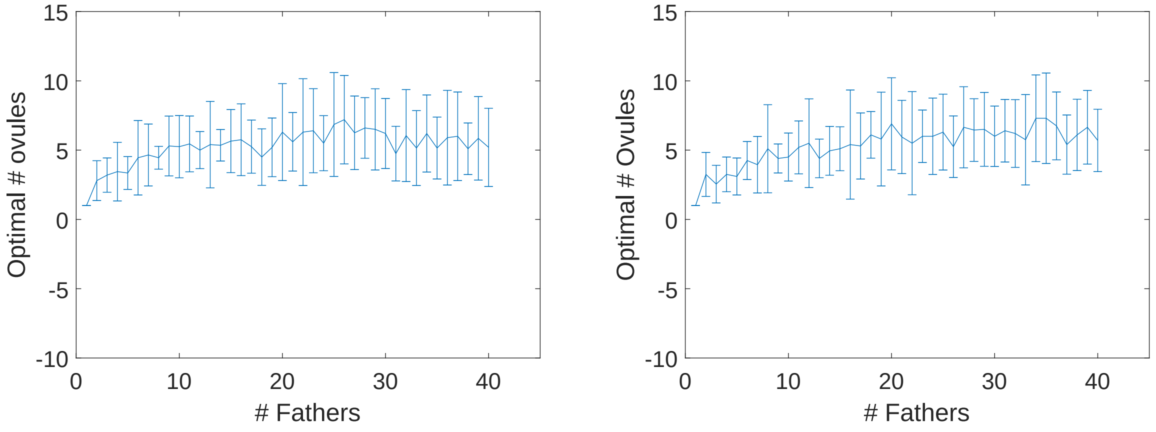
$$\mathrm{SDI}_{\mathrm{costs}} = \mathrm{SDI} - 0.2 \cdot a$$

Assuming these costs for ovule production, the optimal number of ovules increases with the number of trees in the stand and converges on about five to six ovules per flower (see Figures 5.5c and 5.5d). While the cost and benefits of multiple ovules in terms of diversifying fathers are not known, the simulations in the previous section already showed that having six ovules results in an increased SDI relative to having just one.



(a) Square field without costs

(b) Torus without costs



(c) Square field with costs

(d) Torus with costs

Figure 5.5: Optimal number of ovules per flower for different numbers of fathers either on a square or a torus field. Figures 5.5a and 5.5b do not include costs for ovule production, while Figures 5.5c and 5.5d consider costs per ovule of 0.02 times the number of considered fathers.

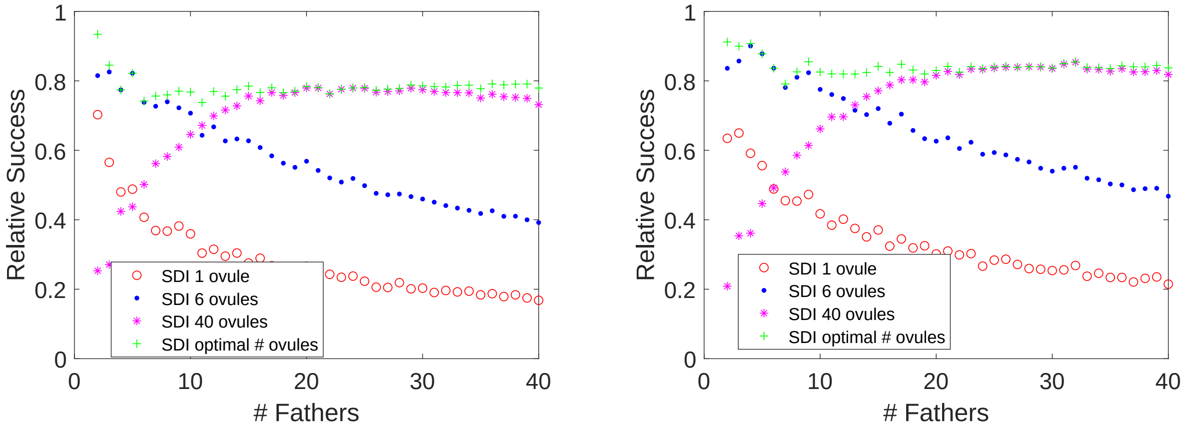
Success of stand in relation to the maximal possible SDI

A stand with a large number of trees can achieve a much higher SDI than a stand with a low number of trees. Therefore, to compare the success of stands with different numbers of trees, we define the relative success s_r by

$$s_r = \frac{\mathrm{SDI}}{n}. \tag{5.4}$$

It is the fraction of the average SDI measured in the stand of trees with a certain number of ovules per flower, relative to the maximum possible SDI, which equals the total number of fathers, n. We consider all combinations of different numbers of possible fathers in the stand (1,. . . ,40), with and without stand boundaries (square versus torus), and four different numbers of ovules per flower (1, 6, 40, or the optimal number for that particular number of fathers). This choice is motivated as follows: Oaks are well-known to have six ovules. A random ovule selection in the 6-ovule scenario gives exactly the same results as a female choice selection in the 1-ovule scenario. This implies that the female choice set up generalizes on the random choice set up. Furthermore, we present two extreme cases, namely considering 40 and the optimal number of ovules per flower. We ran 20 simulations of each combination of number of ovules and fathers to obtain the mean and the variance of relative success, s_r (Figure 5.6). Each simulation re-randomizes the initial position of trees in the stand.

Regardless of the number of ovules, relative success will always start at 100% when there is just one possible father. With just one ovule (no female choice), the relative success declines rapidly to around 20% with 40 possible fathers. By definition, relative success is always highest when the number of ovules is optimal for maximizing SDI, given the number of fathers. It declines from 100% and then flattens out at about 80% once the number of fathers has increased past 4. Producing 40 ovules generates worse results in terms of relative success than just one ovule for stands with fewer than five fathers. The relative success then rises rapidly with the number of fathers until it also approaches about 80% once there are more than 15-20 fathers. The actual value of six ovules per flower is always superior to producing just one, but lower than the SDI of 40 ovules for a large number of fathers. However, the relative success of 6 ovules declines steadily with the number of fathers. With 40 fathers, relative success with 6 ovules per flower is between 40-50%, substantially higher than for just one ovule. In all cases, the torus generates a slightly higher relative success than the square stand of trees.



(a) Relative success for a square field *(b) Relative success for a torus*

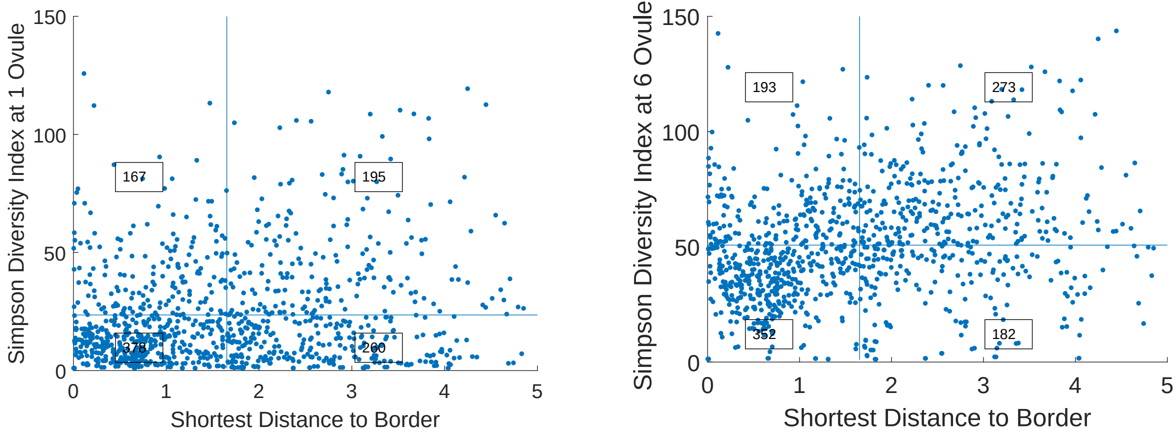
Figure 5.6: Success of stand in relation to the maximal possible SDI. The optimal number of ovules is the one maximizing SDI and varies per number of fathers.

Preferable position for a tree in a stand

When considering the square field of oaks with fixed boundaries, there may be differences between trees near the boundary and those more in the interior of the stand. A tree near the boundary may experience a greater dispersion of nearest neighbors than one in the middle. Hence we may expect trees in the center of the stand to have a higher SDI than those near the edge.

To examine this edge effect, we created a simulated stand of 1000 trees, each of the trees having 10000 flowers. We evaluated each tree's acorns SDI of fathers under the assumption of one and six ovules per flower, respectively. These two ovule numbers compare a random ovule selection with what might be observed in nature. We then plotted each tree's SDI versus its shortest distance to a boundary (Figure 5.7). There, a vertical line and horizontal line show the mean distance to the border and mean SDI, respectively. Since we compare the same stand of trees, the mean distance to the border remains the same, whether there are one or six ovules per flower. With one ovule, the mean SDI (23.56) is less than half of the SDI for six ovules (50.73). At the high end of SDIs, the top 1% of oaks achieve mean SDIs of 113.55 and 130.99 for one and six ovules, respectively. Though, with just one ovule, the lowest 10% of oaks have SDIs less than 2, whereas for six ovules, the maximum SDI in that class is still 11.5.

We used a χ^2-test on the counts in each of the four quadrants formed by the vertical and horizontal median lines (Figure 5.7) to determine whether there is a positive or negative association between distance to the edge and SDI. Both one ovule ($\chi^2 = 16.0$, $p < 0.01$) and six ovules ($\chi^2 = 16.2$, $p < 0.001$) produce a positive association between distance to the edge and SDI, and this effect is much stronger when oaks can exert female choice (six ovules per flower) versus when they cannot (one ovule per flower). This suggests that the effective dispersion of nearest neighbors away from the focal tree is higher for those close to the edge than those on the interior.



(a) SDI at 1 ovule per flower dependent on the shortest distance to the border

(b) SDI at 6 ovules per flower dependent on the shortest distance to the border

Figure 5.7: SDI for 1000 trees dependent on the shortest distance to the border

5.5 Comparing the predictions of one ovule versus six ovules female choice with empirical data

Three published field studies by Dow and Ashley [1998], Pluess et al. [2009] and Streiff et al. [1999] measured paternity patterns in oak trees in relation to the explicit spatial positions of the trees. We can use these studies to compare the predictions between producing just a single ovule versus six ovules female choice. For generating predictions we used the two-dimensional distance between trees in a stand and the square field rather than the torus.

With the first two studies by Dow and Ashley [1998] and Pluess et al. [2009], we test whether a model with female ovule selection can better explain the observed SDI, while with the last study by Streiff et al. [1999], due to the characteristics of the provided data there, we focus on the fertilization patterns with respect to the distances of the trees.

5.5.1 Field study of bur oak in Illinois, USA [Dow and Ashley, 1998]

Dow and Ashley [1998] used microsatellites to examine paternity in a stand of oaks (*Quercus* macrocarpa). They present spatial data from three different maternal trees (3E, 17M, and 33W) and their pollen donors. Figure 5.8 shows the three focal trees and the distribution of other oak trees in the stand. From these spatial data, we extracted for each of these three maternal trees, how many of the surrounding trees have fertilized a particular number of acorns (see Table 5.1). In this table, the first entry shows that for maternal tree 3E, eight trees have successfully fertilized exactly one of the ovules leading to an acorn. The other entries can be read accordingly. The last columns present the resulting number of seeds where the father could be assigned and the SDI computed for each of the three maternal trees (see Equation 5.3).

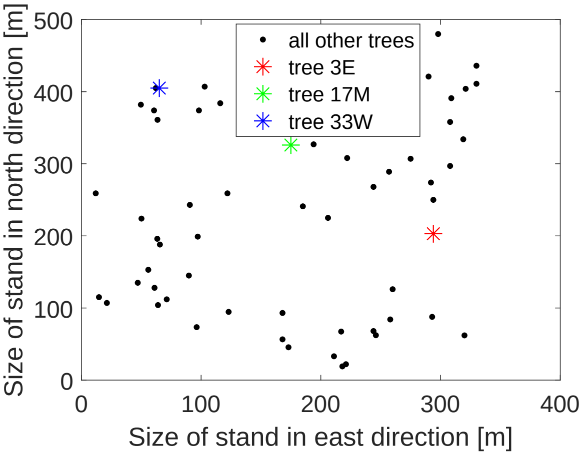


Figure 5.8: Locations of a stand of bur oaks in northern Illinois. The picture is adapted from Dow and Ashley [1998].

	1	2	3	4	5	6	7	8	9	# seeds	SDI
3E	8	4	4	1	2	1	1	0	0	55	14.336
17M	7	3	4	1	1	0	0	0	0	34	12.042
33W	10	1	3	2	0	0	0	0	1	38	9.377

Table 5.1: Extracted values from spatial data from a field study conducted by Dow and Ashley [1998].

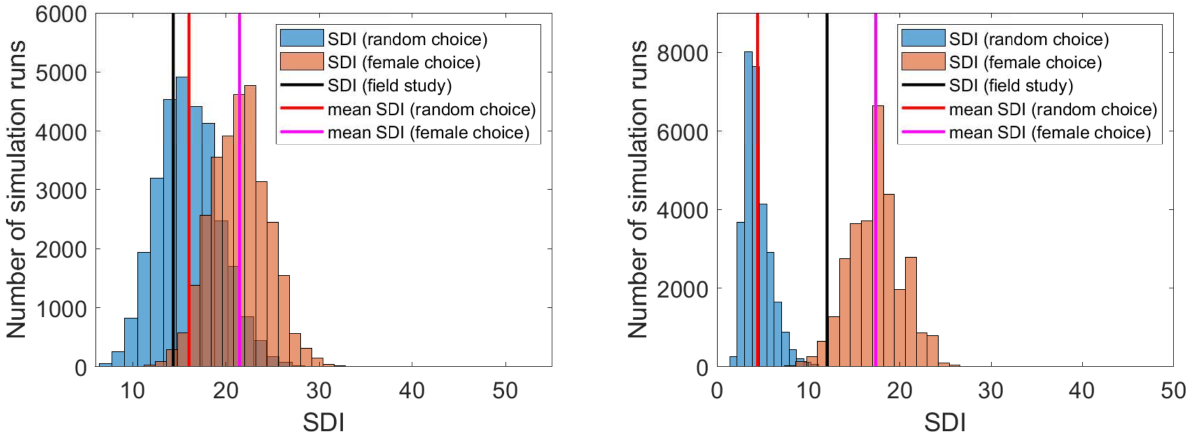
For each maternal tree, we ran 30000 simulations. Each simulation considered the spatially explicit distribution of all possible fathers. These fathers then fertilized the ovules of a flower. Instead of considering trees with 10000 flowers each, here we adjusted the flower number such that it corresponds to the actual number of acorns sampled for a given maternal tree. We then calculated the paternal Simpson diversity index (SDI), assuming female choice from the ovules of a flower (two-stage lottery) versus random choice from the fertilized ovules of a flower. Figure 5.9 shows the histograms of the paternal Simpson diversity index (SDI) of 30000 simulation runs. The orange histograms present the values considering one ovule (without female choice) and the blue histograms the values considering six ovules (with female choice) per flower.

For all three maternal oaks, the SDI for female choice is higher than for random ovule selection. For tree 3E, the actual SDI lies very close to the mean of the SDI under random ovule selection, though it lies within the range of possibilities for female choice. For the remaining two maternal oaks (17M and 33W), the actual SDI coincides better with the simulation results for female choice than for random choice. For these two trees, the actual SDI is beyond any of the 30000 values generated by random choice.

For tree 33W, we have made a judgment call and adjustment: Dow and Ashley [1998] show a separate bur oak extremely close to the maternal tree. If we include this tree as a potential father, then it overwhelms the fertilization of ovules even to the point of often fertilizing all six ovules. This generates simulated SDIs of 1.6828 and 1.0938 for female choice and random choice, respectively, both well below the actual SDI of 9.377 (see Figure 5.9). If we eliminate this father under the assumption that it may be a split trunk of the same maternal tree, then the simulated SDIs accord much better with the actual one, and the female choice model continues to provide a better estimate (see Figure 5.9d).

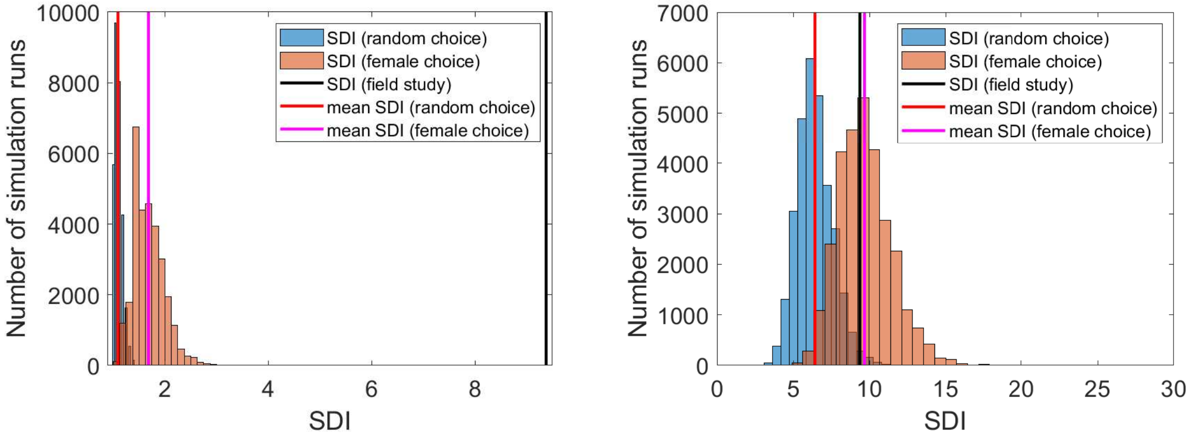
5.5.2 Field study of *Quercus* lobata Née in the Sedgwick Reserve, USA [Pluess et al., 2009]

Pluess et al. [2009] measured paternity in a *Quercus* lobata stand. They present spatial data on five different maternal trees and their pollen donors within 250m distance (see Figure 5.10). The maternal tree is located in the center marked with a red star. In order to compare these results with results obtained by simulations with our continuous-space



(a) Tree 3E

(b) Tree 17M



(c) Tree 33W

(d) Tree 33W - adjusted settings

Figure 5.9: SDI histogram of 30000 simulation runs for each of the trees 3E, 17M, 33W and adjusted settings for tree 33W from the field studies by Dow and Ashley [1998].

model, we can compute the SDI for each of the five maternal trees. Pluess et al. [2009] do not provide exact numbers of offspring for each of the paternal trees. Rather, they present paternity based on fathers at different distance intervals (see first column "Offspring data from field studies" in Table 5.2). Therefore, we used the middle distance of each interval for our computations (see column "Converted number offspring" in Table 5.2). Considering these assumptions, the number of seeds under investigation varied from 82 to 108 for each maternal tree (see row "Number of Seeds"). The resulting SDIs are shown in row "SDI".

We applied the same technique for simulating the five maternal trees as described in Section 5.5.1. Figure 5.11 shows the histograms for the SDI of 30000 simulations each when using the exact tree locations of the field study. For each maternal tree, we considered as many flowers in our simulations as empirically investigated acorns (see Table 5.2, row "Number Seeds"). The orange histograms contain the SDIs assuming random choice of ovules and

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[1] The authors of Pluess et al. [2009] visualize by rings of different sizes how many acorns of each maternal tree have been fertilized by each surrounding tree. The numbers presented in this table are the categories for different ring sizes. The smallest ring around a tree shows that this tree has fertilized 0-1 acorns of the maternal tree.

Offspring data from field studies[1]	Number offspring used as input for SDI calculations	Tree 32	Tree 35	Tree 165	Tree 844	Tree 889
0-1	1	22	22	10	19	11
1-2	2	4	0	5	0	2
2-4	3	7	6	11	4	8
4-10	7	3	4	4	3	7
>10	10	1	2	2	4	2
Number Seeds		82	88	101	92	108
SDI		19.3218	16.4068	19.4305	14.0598	18.3975

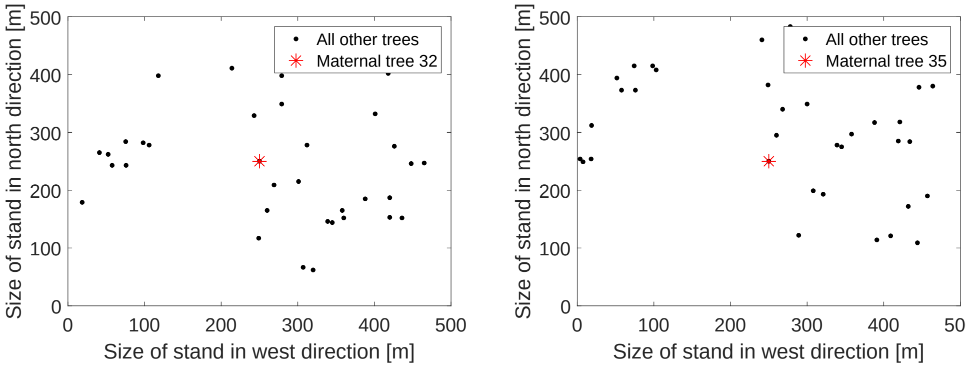
Table 5.2: Extracted values from spatial data from a field study conducted by Pluess et al. [2009]

the blue histograms the SDIs considering female choice from the six ovules of a flower. For all five cases, the simulated SDIs are higher for female choice than for random ovule selection. For all cases, the actual SDI conforms more closely to female choice than random ovule choice. In two cases, the actual SDI is close to the simulated mean for female choice (one higher and one lower). In the other three cases, the actual SDIs are considerably higher and in the upper tail of the distributions for female choice and far outside any of the simulated values when there is random choice.

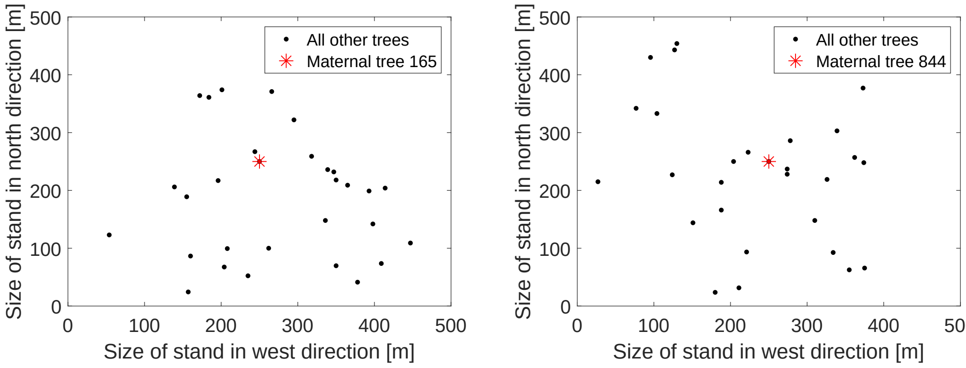
5.5.3 Field Study of *Quercus* petraea and *Quercus* robur in the northwest of France [Streiff et al., 1999]

Streiff et al. [1999] examined the spatial distribution of paternal trees in an oak stand in France. Tree locations are displayed in Figures 5.12a and 5.12c. The rings surrounding the maternal trees indicate the distance classes. The other trees are considered in the simulations as well, i.e., they can act as pollen donors as well. However, in the results, we only present distance classes from $0-20$ m to $100-120$ m. The authors compared potential and actual paternal trees in relation to their distance to maternal trees within a mixed oak stand of *Quercus robur* and *Quercus patraea*. Potential trees are those trees that could have sired acorns of a focal maternal tree, while actual paternal trees successfully fertilized acorns of the focal tree. They present the data for two different maternal trees (tree B and tree E) and the surrounding male trees. Figures 5.12b and 5.12d show the frequencies of potential (blue bars) and pollinating (red bars) paternal trees for six different distance classes from maternal trees B and E, respectively.

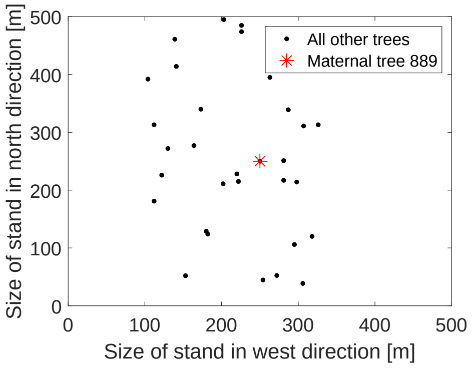
The distribution of potential fathers (blue bars in Figure 5.12) for maternal tree E increases with distance. This is to be expected for an evenly or randomly distributed stand of trees since the area covered by a distance ring will increase with distance. In contrast to that



(a) Tree 32 *(b) Tree 35*



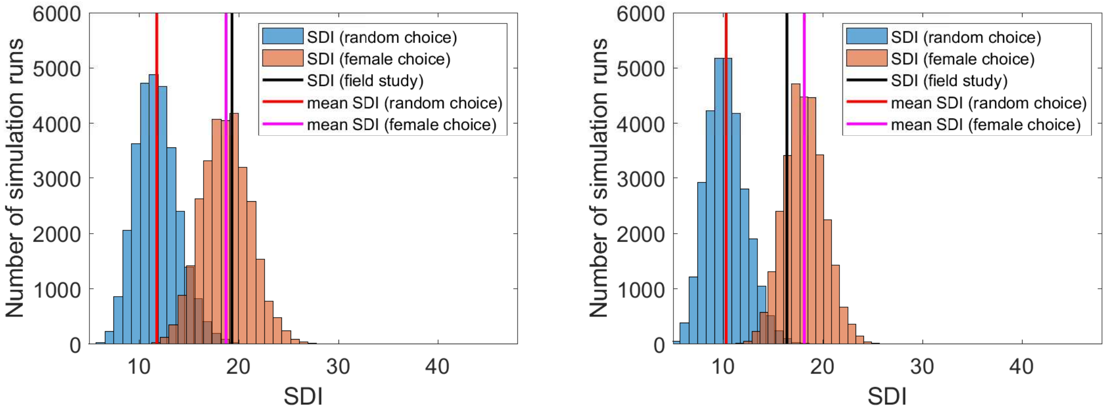
(c) Tree 165 *(d) Tree 844*



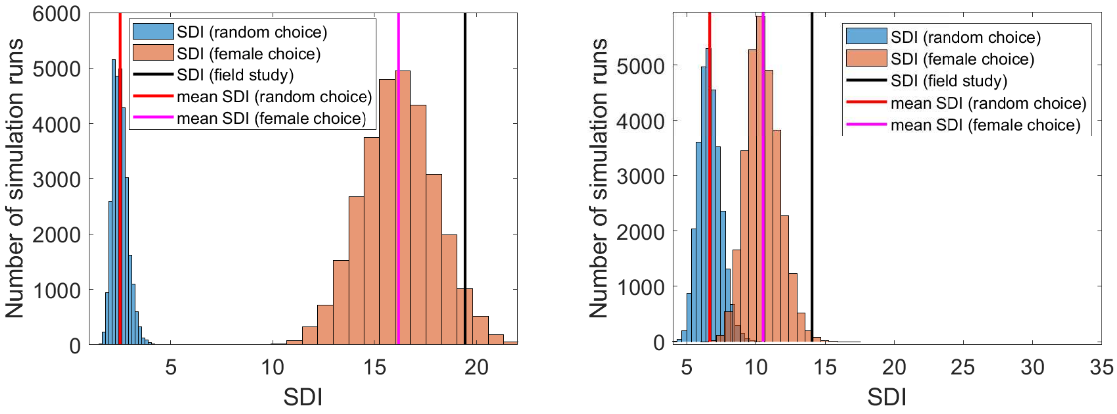
(e) Tree 889

Figure 5.10: Locations for maternal trees 32, 35, 165, 844 and 889 and the surrounding trees. The pictures are adapted from Pluess et al. [2009].

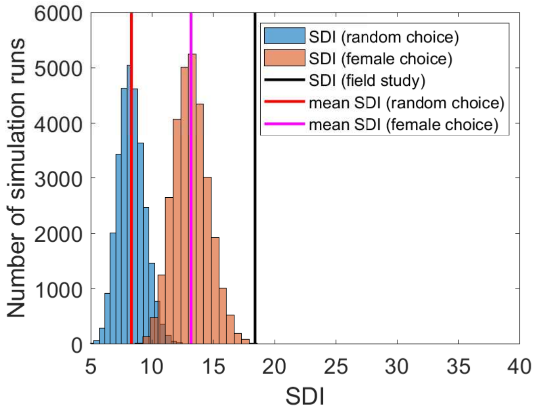
expectation, we see a skewed distribution of trees surrounding maternal tree B. With a maximum at the 50m category, we observe a steady decline in tree numbers at 70m, 90m, and 110m. This happens because tree B exists within a clump of trees that thins with distance. For both trees, B and E, nearby trees are the likeliest fathers, though distant trees are well represented among the acorns (red bars in Figure 5.12).



(a) Tree 32 *(b) Tree 35*



(c) Tree 165 *(d) Tree 844*

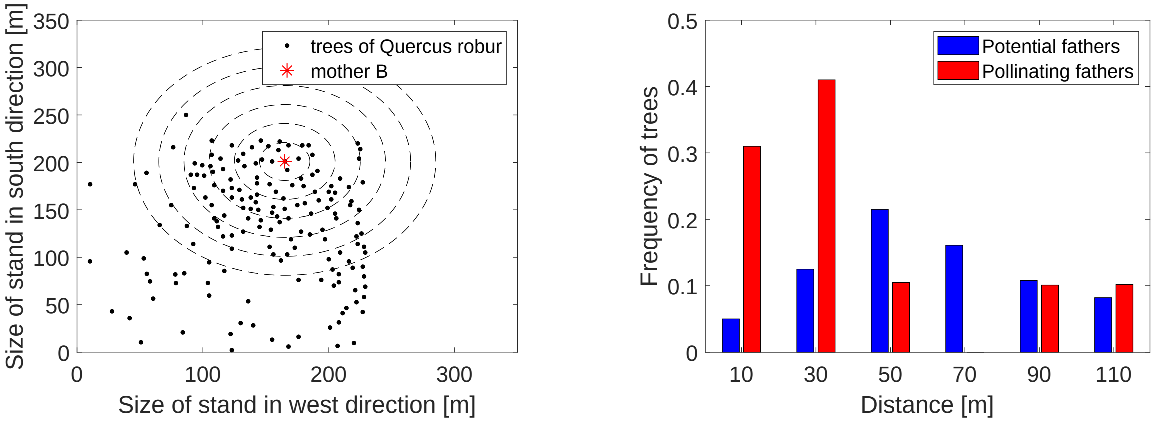


(e) Tree 889

Figure 5.11: SDI histogram of 30000 simulation runs for each of the trees 32, 35, 165, 844 and 889 from the field studies by Pluess et al. [2009].

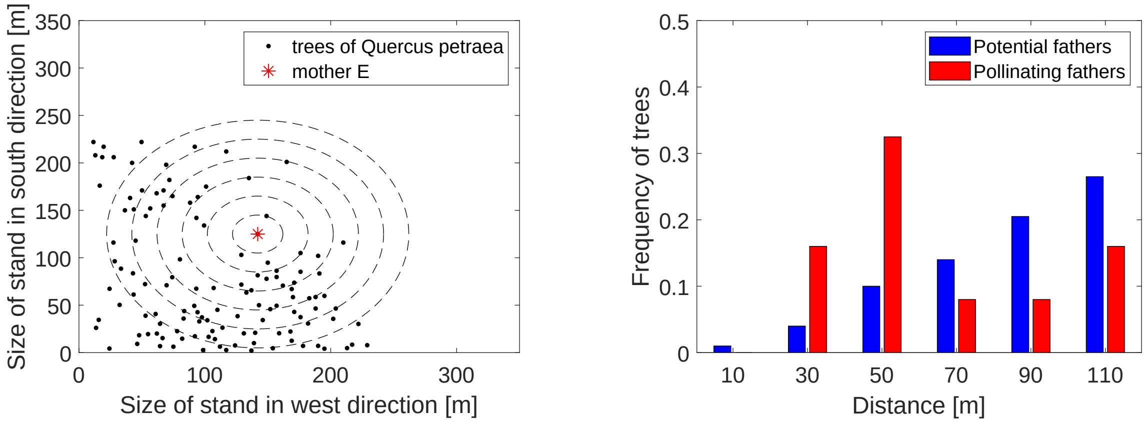
Figure 5.13 shows the simulation results using the locations of the oak trees examined by Streiff et al. [1999] as inputs for our continuous-space model. We performed 30000 simulation runs and considered 21 flowers for maternal tree B and 20 flowers for maternal tree E. This coincides with the number of acorns tested for paternity.

In the previous two studies (see Section 5.5.1 and 5.5.2), we were able to compute the SDI from the data obtained in the field studies. Here, they present paternal information binned



(a) Locations for maternal tree B and surrounding trees

(b) Potential and pollinating male parents for maternal tree B



(c) Locations for maternal tree E and surrounding trees

(d) Potential and pollinating male parents for maternal tree E

Figure 5.12: Figures 5.12a and 5.12c show the locations of oak trees. The rings surrounding the maternal trees indicate the distance classes. Figures 5.12b and 5.12d show a comparison of potential (blue bars) and pollinating (red bars) male parent distributions dependent on the distance to maternal tree B and maternal tree E. Both the locations and results are taken from Streiff et al. *[1999]. While only showing the results for six distance classes, the authors included also the outside trees in their studies.*

into distance categories in relation to the maternal trees. Thus, we focus our analysis on the distance-dependent fertilization pattern (see Figures 5.12b and 5.12d).

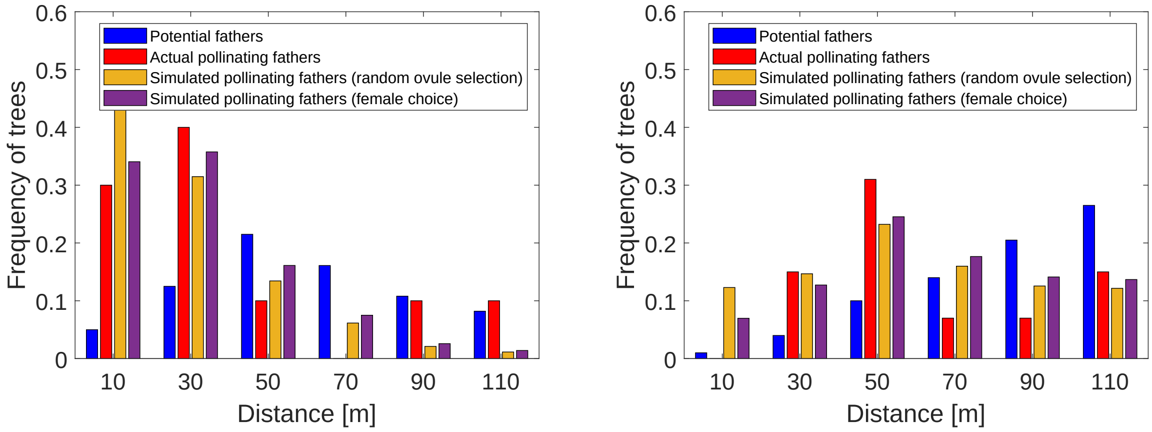
In Figures 5.13a and 5.13b, the blue bars indicate the potential fathers and the red bars the actual pollinating fathers from the field studies, whereas the yellow and magenta bars show the simulation results considering random ovule selection and female choice, respectively. As expected, the female choice model increases the frequency of more distant paternal trees as compared to random choice. In order to evaluate whether the female choice hypothesis better explains the fertilization patterns of the field study than a model with a random ovule selection, we compare the errors associated with these simulations and the actual data. For each of the six distance classes, we compute the average number of trees that have fertilized flowers of the maternal tree. This results in frequencies of fertilizing trees per distance class. This simulation data can be compared to the data of pollinating fathers (red bars in Figures 5.12b and 5.12d): We use the squared differences of the simulated frequencies x_{sim} and real frequencies x_{real} of the pollinating fathers as the error measure. For both maternal trees (Figure 5.13a and 5.13b), the sum of errors over all distance classes is lower for the female choice model (Tree B: 0.0257; Tree E: 0.0262) than for the random ovule selection model (Tree B: 0.0449; Tree E: 0.0332). Thus, for both maternal trees, the female choice hypothesis explains the underlying fertilization patterns better than a random ovule selection.

In Figures 5.13c and 5.13d, the blue histograms show the mean distances of successful fathers to the maternal tree from 30000 simulations with random ovule choice. The orange histograms show the distances when considering a female choice. The red line indicates the estimated mean distance of the fertilizing trees from the field study. We approximated it by taking the middle of the distance classes as an estimate for the distance for all trees within this class. For our simulations, we considered all trees, i.e., also trees with a position outside of the six distance rings. For both maternal trees, the random choice simulations yielded the smallest mean distance. The female choice model simulations yielded intermediate mean distance values, and the actual data had the highest mean distance values. For Tree B, both random choice and female choice substantially underestimate the actual mean, while the difference to the real data is worse for the random choice model. For Tree E, the actual value lies closest to the mean for the female choice model. Therefore, the female choice model provides a better fit to the actual data.

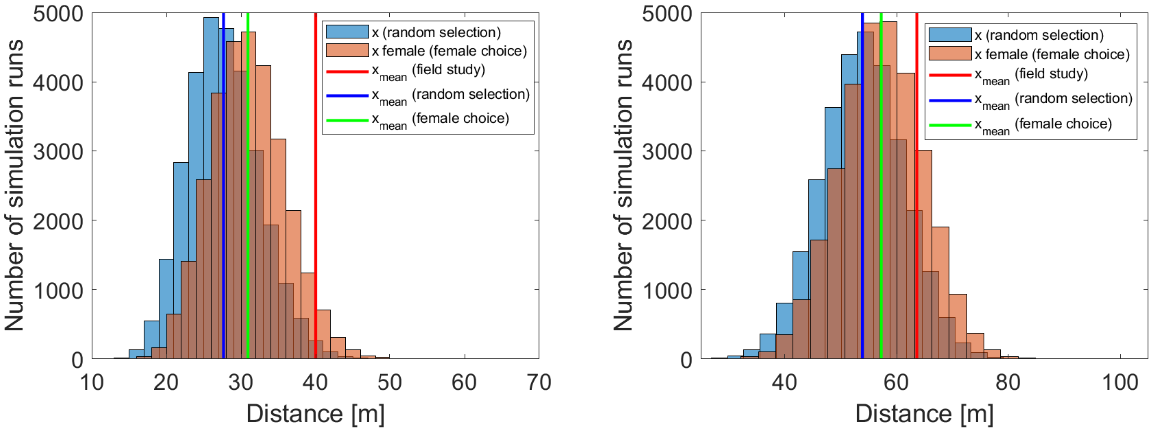
5.6 Discussion

Craft et al. [2009] hypothesized that oaks produce multiple ovules per flower as a means for the individual tree to diversify the number of fathers across its acorns. We found modeling and empirical support for this hypothesis. For wind-pollinated species like oaks, the challenge is to discourage nearby pollen donors and encourage more distant ones. Like in Craft et al. [2009], our model shows how this can be achieved through a two-step lottery. The second step of the lottery can happen if a plant, like oaks, fertilizes multiple ovules per flower yet matures just one seed per flower. Even if ovule fertilization occurs randomly with respect to pollen flow (which favors nearby paternal trees), a tree can give an edge to rare pollen donors by maturing a flower's acorn from the ovules of a flower that have the fewest fathers. A nearby pollen donor sees its contribution discarded when it fertilizes two or more ovules of a flower. Step one of the lottery strongly favors the nearest paternal trees. Step two favors the more distant pollen donors.

For this flowering strategy to work, the plant must produce three or more ovules per flower. The optimal number of ovules per flower to maximize the diversity of paternal oaks among a tree's acorns depends strongly on the number and dispersion of oaks within and between forest patches. In our simulated oak stands, this optimal number can range from as little as 5 to well over 100; and it tends to increase with the number of potential fathers and the



(a) Maternal tree B *(b) Maternal tree E*



(c) Maternal tree B *(d) Maternal tree E*

Figure 5.13: Comparison of data obtained from field studies by Streiff et al. [1999] to data obtained from simulations for both maternal tree B and maternal tree E. Figures (a) and (b) show the frequency of paternal trees that have fertilized flowers of the maternal tree dependent on their distance classes. Figures (c) and (d) show the distance histograms of fertilizing paternal trees.

steepness of the decline in pollen flow with successively more distant paternal trees. However, as the production of ovules is associated with costs, 100 ovules are not very realistic. For most species of oak, six ovules per flower are characteristic. While more ovules per flower would generally be optimal for diversifying fathers, having six achieves large increases in diversity relative to having just one. Six may be adaptive when the benefits of diversifying fathers are balanced against the cost of producing and discarding multiple ovules within a flower [Sutherland and Delph, 1984].

Ten trees from three separate studies provided information on the paternity of their acorns [Dow and Ashley, 1998, Pluess et al., 2009, Streiff et al., 1999]. From these studies, we evaluated the distribution and diversity of fathers. We compared empirical results to our model of female choice (with six ovules per flower), and to random choice where fathers of acorns occur in proportion to their pollen contribution. In all cases, random choice predicted a lower diversity of fathers than within-flower female choice. For nine trees, the data more closely fit the predictions of female choice and, in only one case, fit better the predictions of random choice. For the nine cases, the female choice model either closely fits the actual data (6 times) or underestimated the true diversity of fathers (3 times). The model will underestimate the diversity of fathers if there are potential pollen donors that were not measured, and that occurred beyond the boundaries of the study.

A number of factors not considered in the present version of our model would likely skew, diminish, or amplify the diversity of pollen donors to a given oak tree. One factor we did consider was a tree's position within a stand. The model predicts that a more centrally located oak will have a higher diversity index of fathers among its acorns than an oak nearer to the boundary of the forest. Other important factors influencing pollen flow and hence paternity (whether random or through the female-choice two-step lottery) include topography such as mountains, rivers, ravines, and spatial variation in elevation. Wind speed, prevailing wind directions, and wind gusts or eddies will distort pollen flow in ways that may create more or less mixing of pollen donors. Including different formulations for pollen flow would expand the utility of the model, though current data may not yet permit model validation for these additional features. A variety of studies showing leptokurtic pollen flow for wind-pollinated plants provide a valid starting point [Gleaves, 1973, Tonsor, 1985].

Our model considered the trees as dots on the landscape. Actual trees occupy space with varied and often expansive canopies. Such trees can vary in their pollen production. A smaller or less robust tree producing less pollen will have less success in fertilizing ovules regardless of its position relative to a focal tree. While it has a lower likelihood of fertilizing multiple ovules of a given flower (and hence being discarded), it also has a lower chance of even fertilizing one ovule of a flower, particularly when the focal tree is far away. Nevertheless, the within-flower two-step lottery will result in less of its fertilized ovules being discarded than those of a robust tree producing much more pollen. Thus, producing more pollen may not always be advantageous for a tree (unless this tree fertilizes all ovules).

Proximity to different sides of a neighbor's canopy should matter. One would expect the pollen of a southward neighbor to contribute disproportionately to the south rather than the north side of a focal tree [Free, 1962]. While highly likely, data on this point is sparse, and data for paternity in oaks has not yet been localized to position on the maternal tree. If nearby pollen donors spatially clump their pollen onto different regions of a recipient tree, then our model of female choice would further enhance the diversity of fathers based on distance. To see this, imagine four trees all close and equally distant to a maternal tree. Assume that they only differ in their orientation to the tree. If these trees contribute pollen randomly across the focal tree, they would mutually favor each other relative to more distant trees. This is because they would reduce the odds of one of their own fertilizing two or more ovules of a flower. Thus, less of their pollen would be discarded during the second step of the lottery. The focal oak would be less effective at discarding the ovules pollinated by nearby trees. On the other hand, if each of these four neighbors concentrate its pollen on the most proximal region of the focal tree, then many more flowers would have multiple ovules fertilized by the same tree. With a high probability, these would be discarded, as they most likely lose the second lottery step. Aspects of this could be modeled and investigated by giving each tree's canopy spatial dimensions and letting pollen flow correspond to directionality and proximity. For instance, a focal tree's canopy could be divided into quarters (or smaller slices). Then, the pollen flow from a given tree could be distributed non-randomly depending on the quarter it comes from.

Other empirical studies have examined the diversity of fathers in self-incompatible plants and how various mechanisms could enhance such diversity. Lankinen and Madjidian [2011] for example found that delayed stigma receptivity in the species *Collinsia heterophylla* results in a higher paternal diversity.

Others have modeled and proposed ways for plants to exhibit female choice. Melser and Klinkhamer [2001] experimentally tested the hypothesis that females of the species *Cynoglossum officinale* choose to abort low-quality offspring. They investigated the effects of artificially removing ovules and the effects of adding nutrients. They found that offspring survival was lower with random ovule abortion (by hand) than when the plant aborted ovules. As expected, adding nutrients increased offspring survival. This result might also be influenced by positive correlations between seed mass, added nutrients, and seed survival. Furthermore, Sakai [2007] modeled the hypothesis that females choose certain fertilized ovules to create seeds of uniform size. By producing surplus ovules, females can choose ovules that absorb a similar amount of resources.

Our model requires some sort of self/non-self recognition among fertilized ovules of a flower. The flower must recognize full-siblings (same father) relative to half-siblings (different fathers). To our knowledge, there have not been studies done looking at the distribution of full- and half-siblings within the fertilized ovules of an oak. We propose that fertilization is random with respect to pollen accrual to the flower. Yet, other mechanisms exist for preventing successful fertilization of ovules by pollen based on mating types or histone compatibility. Mechanisms ensuring self-incompatibility genetically prevent fertilization from the plant itself or from closely related plants [Bedinger et al., 2017, Goldraij et al., 2006, Nasrallah, 2002]. These systems can further be distinguished between gametophytic and sporophytic systems. In the first case, the growth of the pollen tube towards the ovary is blocked while in the latter case, the pollen tube growth is blocked on the surface of the stigma [Vervaeke et al., 2001]. Moreover, pre-fertilization barriers might prevent fertilization from different species. In several tulip species, Van Creij et al. [1997] identified different forms of barriers that occurred at various developmental phases. Barriers to fertilization could include failure of pollen germination, pollen tube growth, and pollen tube penetration of ovules [Van Creij et al., 1997]. These pre- and post-fertilizing mechanisms have been more often described for short-lived plant species than for long-lived species like oak trees [Yacine and Bouras, 1997]. Hagman et al. [1975] showed how species of *Quercus* use a gametophytic control of pollen tube growth to prevent selfing. Furthermore, Boavida et al. [2001] investigated post-pollination mechanisms in the species *Quercus suber*. Their study examined pollen-pistil interactions in order to gain insights into intra- and interspecific crosses.

Oaks are not alone in having multiple ovules per flower while maturing just one. In species of *Symphoricarpos* and *Cornus* only one out of multiple ovules mature [Wiens et al., 1987]. Moreover, in *Erodium cieutarium*, only one ovule per schizocarp develops into a seed [Wiens et al., 1987]. We can observe a similar behavior in the species *Pongamia pinnata*, which matures only one of the two seeds in most of the pods [Arathi et al., 1999]. Though with just two seeds, some sort of between flower selection would be required to improve paternal diversity.

Our model can be extended and made more realistic. Such extensions could be used to predict the distribution and diversity of fathers for a focal plant's seeds. While the model shows promise, it needs and invites empirical tests of its assumptions, hypotheses, and predictions. For instance, natural and controlled pollination experiments with oaks in the field could vary the pollen mix of fathers (either by distance or by hand pollination) to subsets of flowers of focal individuals. One could then measure a father's success from this mix in fertilizing ovules of a flower, and in siring acorns. Such experiments could answer the question of whether fathers contributing less pollen gain a proportional advantage at either the ovule stage or, as predicted, at the acorn stage.

CHAPTER 6

Game theory of pollution: national policies and their international effects

Abstract

This chapter presents a game-theoretical model of pollution control, where the countries of the European Union (EU) as of 2017 control their own pollution, while the environmental effects of policies do not stop at country borders. In this non-cooperative differential game, countries as players minimize the present value of their own costs defined as a linear combination of pollution costs and costs of environmentally friendly policies. The state vector of the system consists of the pollution stock per country. A player's time-varying decision is her investment into clean policies, while her expected costs also include pollution caused by her neighbors. Three variants of this game are analyzed: (1) a Nash game in which each player chooses her investment into clean policies such that her expected costs are minimal, (2) a game in which the players imitate the investments into clean policies of their neighbors without taking the neighbor's success concerning their costs into account and (3) a game in which each player imitates her neighbors' investments into clean policies only if this behavior seems to bring a profit. In each of these scenarios, it is shown under which conditions the countries have incentives to act environmentally friendly. The results of these games can be used to understand and design effective environmental policies.

6.1 Introduction

Current worldwide environmental policy goals aim at lowering emissions in the air in order to fight global warming [Schandl et al., 2016]. These policies include energy generation via renewable energy sources (RES) and various mechanisms to clean the air. For example, the European Union (EU) is striving to achieve 20% of energy generated from RES by 2020 and to reach a minimum of 27% of renewable generated energy by 2030, while aiming to reduce greenhouse gas emissions by at least 40% by 2030 compared to their level in 1990 [European Commission, 2013, Ferreira et al., 2017]. Objectives for 2050 are even more challenging, with a reduction of the carbon emissions by 80–95% [European Commission, 2011]. All around the world (e.g., in China [Ming et al., 2013], Japan [Esteban and Portugal-Pereira, 2014], New Zealand [Mason et al., 2013], United States of America [Eyer and Corey, 2010, Rastler, 2010] and Turkey [Dursun and Alboyaci, 2010]) countries turn to energy generation via RES.

However, some countries are more committed to green policies than other ones, and the behavior of each country may influence the pollution of other countries. For example, each country's air policies contribute to the quality of the air of its neighbors [Lelieveld et al., 2002, Nkuiya, 2015, Stohl et al., 2002]. In the last decades, countries therefore detected the need to cooperate in order to fight global warming. There are many joint policies aiming at the reduction of greenhouse emissions, e.g., the Kyoto Protocol [United Nations, 1998] or The United Nations Framework Convention on Climate Change [United Nations, 1992].

Besides joint policies, every country has its own interests and standards regarding its more or less green policies. Of course, the government of each country keeps in mind its own costs and tries to avoid policies harming its economy. This may give rise to conflicting objectives and behavior among different countries. In discussions among different countries belonging to the same geographical regions, some countries like the Scandinavian ones or Germany act as leaders trying to impose the emission reduction strategies on other countries that are less prone to the green policies [Andresen and Agrawala, 2002, Jänicke, 2005, Liefferink and Andersen, 1998]. In some countries, such as the United States of America, there are nation-wide policies taking into account the geographical characteristics of the country, such as the fact that downwind states suffer from cross-border pollution by upwind states and need to be protected [United States Environmental Protection Agency, 2011].

There are many different strategies to achieve emission reduction. While some countries are mainly focusing on punishment of emission via taxes [Bruvoll and Larsen, 2004], other countries provide funding for low-emission technologies or approaches, such as implementing solar plants. After many discussions about the impact of taxes on emissions [Bruvoll and Larsen, 2004], there is evidence that this impact is positive [Wier et al., 2005]. On top of the national incentives, the European Union offers *super-credits* for car manufacturers to produce low-carbon vehicles [European Parliament and Council of the European Union, 2014]. Furthermore, quite some countries implemented low-emission zones [Boogaard et al., 2012, Ellison et al., 2013] or driving restrictions [Davis, 2008] in big cities to at least lower pollution locally.

Fighting global warming involves both global and national policies. On the one hand, countries need to cooperate and, on the other hand, they often do not want to lose independence in their environmental choices.

Much research focuses on the influence of local pollution on the global or local environment of a country [Akimoto, 2003, Lelieveld et al., 2002]. Additionally, some researchers model and analyze the role of cooperative country associations fighting against global warming (e.g., [Breton et al., 2010, Dockner and Van Long, 1993, Jørgensen and Zaccour, 2001, Long, 1992]). However, in those associations, punishment from an external source often plays a role [Harford, 1978]. Krass et al. [2013], for example, address the ability to force firms to invest in emission-reducing technologies and produce their goods in a more environmentally friendly way. They use a two-player Stackelberg model to find the optimal level of emission punishment to maximize welfare. One of their main conclusions is that taxes may have a positive effect but have to be used carefully since extremely high taxes can have the opposite effect. In contrast to this pollution reduction forced by an external source, Barrett [1994] models self-enforcement of international environmental agreements. Additionally, Nkuiya [2012], Nkuiya et al. [2015] and Miller and Nkuiya [2016] investigate voluntary participation in climate treaties, also including the possibility of a sudden regime shift using both cooperative and non-cooperative game theory. Moreover, Lazkano et al. [2016] study how adaptations of costs influence the decision of developed and developing countries to join international agreements. Furthermore, there is much research done about the influence of dominant players on the pollution behavior of weaker players. Garrab and Breton [2016], for example, examine two different groups of players, namely signatories and defectors. In their model, signatories punish defectors with higher pollution costs. Their main focus lies on the comparison of Nash and Stackelberg information structures and their influence on the pollution policies of the players.

In this chapter, a game-theoretical approach is adopted to model and understand interactions among EU countries and their subsequent choices of investment into green policies. Different EU countries are individual players in the game. The players pursue different strategies to invest in green policies. First, each player has a cost function to be minimized with respect to its choice of investment into green policy. Such costs may include the development costs for pollution reduction technologies or costs for cleaning the environment [Amann et al., 2011]. Second, the investment into environmentally friendly policies is influenced by the neighbors of a country - a country may imitate the behavior of its neighbors. While the choice to behave environmentally friendly will decrease the pollution stock of the country, it is expected to be costly. These costs are proportional to the pollution stock in the country. However, pollution increases the costs of a country as well.

Turnock et al. [2016] estimated that air pollution reducing technologies caused an economic benefit of 232 billion US dollars due to the prevention of premature deaths annually in the EU. Thus, aside from the property value reduction and health costs, countries should be penalized and rewarded for increases and decreases in pollution, respectively. It is assumed that this penalty/benefit for pollution flow can be regulated by the EU.

The first part of the chapter focuses on optimal time-varying investment decisions per country when a country minimizes the present value of its own costs. This includes an analysis of what happens if the costs/benefit for pollution flow per country are increased. Additionally, two different types of imitation behavior as possible strategies of the countries involved are considered. Imitation has had a central role in evolutionary game theory, focusing on the properties of the attractors of the underlying dynamical games [Apesteguia et al., 2007, Björnerstedt and Weibull, 1994, Selten and Ostmann, 2000]. A direct to the existing results in the field are made. Subsequently, the outcomes of all three game variants are compared, and the observed phenomena are mapped to the challenges in implementing green policies worldwide.

The remainder of the chapter is composed as follows: In Section 6.2 the basic model assumptions and a short description for each of the variants of the models are presented. Next, a short stability analysis is provided. In Section 6.3, different case studies about all variants of the model are shown. The chapter ends with the discussion of the results and directions for future work in Section 6.4.

6.2 The model(s)

In this section, the modeling framework for the pollution game is introduced.

6.2.1 Basics for all variants

Let us assume that $\mathcal{N}$ is the set of EU countries, where country $i \in \mathcal{N}$ has a pollution stock $x_i(t)$ at time $t \in [0,T]$ with $T > 0$ a fixed and known time to address. The pollution stock x_i changes according to the differential equation

$$\dot{x}_i = (1 - u_i(t))\, x_i(t) + \sum_{j \in \mathcal{N}^i \setminus \{i\}} (\psi_{ji}(1 - u_j(t))\, x_j(t)) - u_i(t) x_i(t), \tag{6.1}$$

where $\mathcal{N}^i \subset \mathcal{N}$ is the neighborhood of country i, i.e., country i itself and all countries neighboring with it. The neighborhood of a country is defined by the connections in a network of countries (see Figure 6.1 as an example). The initial pollution stock $x_i(0) > 0$ is fixed and known a priori to all countries, $\psi_{ji} \in [0,1]$ is the rate at which country j pollutes the environment of country i. Values of ψ_{ji} can be arranged in an adjacency matrix of a network in which countries that are polluting each other are connected ($\psi_{ji} > 0$).

Control $u_i \in [0,1]$ can be interpreted as the investment of country i into environmentally friendly (clean) policies. If $u_i = 0$, country i is not investing into the clean policies while, if $u_i = 1$, country i is spending its maximal effort into the investment. For example, a country can invest a lot into renewable energy or confine itself to coal-fired power stations. Please note that in our model, the investment into clean policies influences the current investments of the other countries as well. There exist other models, in which u_i is interpreted as a pollution abatement level for country i, and in these models, each country's costs depend only on its own abatement level [Barrett, 1994].

The last term, $u_i(t)x_i(t)$, can be seen as the reduction of the pollution stock due to investments into clean policies. Each country i has pollution costs defined as

$$c_i(t) = e_i\left(\beta \dot{x}_i(t)\right) + \lambda_i u_i(t), \tag{6.2}$$

where $e_i\left(\beta \dot{x}_i(t)\right)$ with $\beta \geq 1$ can be interpreted as the environmental costs that are caused by the pollution flow and $\lambda_i u_i(t)$ defines the costs for clean policies. These costs for clean policies can vary per country. Constant $\beta \geq 1$ denotes a factor defined by an external party (e.g., European Commission) as a rate of punishment for the pollution stock. In Section 6.2.2 different versions of the model based on the way how the investment u_i into clean policy is defined are presented:

1. Nash game: Country i minimizes pollution costs (6.2) with respect to its investment $u_i(t)$ at each time $t \in [0,T]$, where other countries are assumed to do the same (Section 6.2.2).
2. Countries imitate the behavior of their neighbors independently of the neighbors' costs (Section 6.2.2).
3. Countries imitate the investments of their neighbors dependent on the neighbors' costs such that more profitable neighbors influence a country in a stronger way.

To give function e_i from (6.2) a more specific form, let us define it as

$$e_i(t) = \exp\left(\beta \dot{x}_i(t)\right) - 1. \tag{6.3}$$

In this case, the environmental costs e_i grow exponentially with the pollution flow $\dot{x}_i$. Increasing parameter β increases the impact of the current pollution flow on the costs. The last term of Function (6.3) ensures that the costs are zero when no pollution flow takes place.

Thus, in our model, the individual costs for each player are given by

$$\begin{aligned} c_i(t) &= \exp\left(\beta \dot{x}_i(t)\right) - 1 + \lambda_i u_i(t) \\ &= \exp\left(\beta\left((1-u_i(t))\,x_i(t) + \sum_{j\in\mathcal{N}^i\setminus\{i\}} \left(\psi_{ji}(1-u_j(t))\,x_j(t)\right) - u_i(t)x_i(t)\right)\right) - 1 + \lambda_i u_i(t). \end{aligned} \tag{6.4}$$

6.2.2 Different variants of the model

Nash game: optimizing individual costs

In this variant of the model each player minimizes her individual costs at time $t \in [0,T]$ defined in (6.2), i.e., the optimal strategy u_i^* minimizes the costs (6.4) for each $i \in \mathcal{N}$. The strategies u^* therefore form a Nash equilibrium of the game at each time $t \in [0,T]$.

Basic imitation behavior

In contrast to the model described in Section 6.2.2, one can also think of countries that are influencing other countries' behavior. Considering the pollution stock defined by Equation (6.1), country i is now no longer optimizing its own costs but rather imitating the average of investments into clean policies of all its neighbors. Please note that countries can thus be influenced by multiple countries at once.

A country i's decision u_i is influenced by each neighbor in the same way. For this basic imitation approach, the change of investment u_i of player i is defined as

$$\dot{u}_i = -\frac{1}{|\mathcal{N}^i|} \sum_{j \in \mathcal{N}^i} (u_i(t) - u_j(t)). \tag{6.5}$$

More advanced imitation behavior

This variant of the model assumes that countries with a successful investment have bigger impact on the decision of other countries. Here *successful* means that the pollution costs of a country are low. Similar to the consensus protocol described by Ren et al. [2005] or Olfati-Saber et al. [2007], the change of investment u_i of player i is defined as

$$\dot{u}_i = -\frac{1}{|\mathcal{N}^i|} \sum_{j \in \mathcal{N}^i} S_{ij}(t)(u_i(t) - u_j(t)) \tag{6.6}$$

with $S_{ij}(t)$ being the sigmoid function $S_{ij}(t) = \frac{1}{1+\exp(c_i(t)-c_j(t))}$.

A country is therefore more influenced by countries that have lower costs than by countries paying much for their (less environmentally friendly) behavior.

6.2.3 Stability analysis

This section briefly discusses the linear stability properties of the system defined by differential Equation (6.1).

Nash game

Equilibria of Equation (6.1) must satisfy

$$\dot{x}_i = 0,$$

which gives us

$$x_i^*(t) = \frac{\sum\limits_{j \in \mathcal{N}^i \setminus \{i\}} \Big(\psi_{ji} (1 - u_j^*(t))\, x_j^*(t) \Big)}{2\, u_i^*(t) - 1} \tag{6.7}$$

where x_j^*, u_i^*, and u_j^* are the equilibrium pollution of country j, the optimal clean investment strategy for country i, and the optimal clean investment strategy for country j. The derivative of the right-hand side of the Equation (6.1) with respect to x_i is $1-2u_i$. This means that the equilibrium given by (6.7) is an attractor for $u_i^* < 0.5$ and a repeller for $u_i^* > 0.5$. This implies that if u_i^* is small for each $i \in \mathcal{N}$, there is a single attractor x_i^*. If the values for u_i^* are all bigger than 0.5, then there is a single repeller. Therefore, in case of the strategy u_i^* of country i minimizing costs (6.4), our interest is whether or not u_i^* gets (and stays) under 0.5. This analysis however gives us a good idea only about the situation with all countries being in the same neighborhood and might not help us much in case of some players belonging to more neighborhoods.

Imitation game

For both imitation behavior cases, where strategies of the players are given by (6.5) and (6.6), respectively, strategy u_i^* is in attracting equilibrium if $u_i^* = u_j^*$ for each $j \in \mathcal{N}^i \setminus \{i\}$. This means that if all countries were within the same neighborhood, one would expect their optimal strategies asymptotically converge to each other. The attracting equilibria coincide with the results on imitation in evolutionary games [Ranjbar-Sahraei et al., 2014a,b].

6.3 Simulations

6.3.1 Implementation

The models from Section 6.2.2 were implemented numerically. The software to find optimal investments is developed using Eclipse IDE for Java Developers, Version Neon.3, Release (4.6.3) with execution environment JavaSE-1.8 provided by Eclipse Foundation Inc. (Ottawa, Canada).

Depending on the selected model, a computation step in our simulation is defined by the following sub-procedures.

- Nash game: When each country wants to minimize the present value of its own costs, the simulation starts with initial values for the pollution stock x_0. Then, a fixed point approach is used to compute u_i^* for each country such that the costs c_i become minimal for each country $i \in \mathcal{N}$. The optimization itself is done by a software implementation called jcobyla [Gustafsson, 2012]. For some specific scenarios, u^* can be computed analytically. However, especially for larger problems, u^* cannot be found analytically that easily. The software implementation is based on Powell's numerical optimization implementation for constrained problems with unknown derivatives of the objective function [Powell, 1994]. The next computation step includes the computation of pollution x^*, with discretization of the differential Equation (6.1) via a fourth-order Runge-Kutta approach with step size 0.01.

- Imitation game: Considering that the countries imitate other countries' behavior, a computation step starts with values for x_i^* and u_i^* from the Nash game for the initial phase. Using those values, the investment into clean policies can be computed by applying either Formula (6.5) or (6.6). Again a fourth-order Runge-Kutta approach is used to compute the pollution stock. The next computation steps continue until the defined number of total computation steps corresponding to time T is reached.

6.3.2 Simulation settings

In all case studies, the network is based on the geographical structure of the EU. The 28 member countries of the EU are the players of the game. A country i is polluting the environment of country j if i and j share a geographical border. Those borders also include maritime borders [Charney et al., 2011]. An overview of all neighbor relations is provided in Table 6.1. Thus, influencing among countries is bi-directional, i.e., if country i can pollute the environment of country j, country j can also pollute the environment of country i. In this case, we assume that $\psi_{ji} = \psi_{ij} > 0$. The resulting network is shown in Figure 6.1. It does not include phenomena like the fact that downwind states suffer much more from the pollution by upwind states than in the opposite direction. However, our simulation software offers the possibility to choose any symmetric as well as asymmetric values for ψ_{ij}.

All numerical studies start with an initial pollution stock x_0 based on values of carbon dioxide emissions from 2010 [Marland et al., 2016]. These values are in the unit of Mt. Due to the scalability of our model, we do not specify a fixed time unit. In the remainder of the chapter, λ_i is considered to be fixed to 4 for all countries as this value seems to be rather realistic and, also, due to a limited availability of better data. In the future, we would like to find and use more appropriate data in order to model the influence of λ_i in a more realistic way. However, the influence of this parameter is anyway limited due to the much bigger impact of term $\exp(\beta x_i)$ on the cost function.

6.3.3 Optimizing individual costs

Without any force of a joint administration like the European Commission, each country wants to minimize its individual costs. In our model, those costs are influenced by the geographical neighbors in such a way that neighbors pollute the country's environment, and the country has to pay for this (see (6.4)). Apart from that, the neighbors do not influence the costs of another country.

The results show that there is a strong increase of the pollution stock compared to the initial values. All values start in the range of about 0 Mt to 832 Mt and end with a pollution of 2000 Mt. However, after the initial phase, both the pollution stock x and the countries' investment u into environmentally friendly policies converge to the equilibrium values. This behavior is shown in Figure 6.2a. It is remarkable that the pollution stock x_i for all countries converges to the same value while there is no consensus in the underlying

Country	**Neighbors**
Sweden	Germany, Poland, Lithuania, Latvia, Estonia, Finland, Denmark
UK	Ireland, France, Spain, Germany, Netherlands, Belgium, Denmark
Ireland	UK
France	UK, Spain, Germany, Belgium, Luxembourg,Italy
Spain	UK, France, Portugal, Italy
Portugal	Spain
Germany	Sweden, UK, France, Netherlands, Belgium, Luxembourg, Poland, Czech Republic, Austria, Denmark
Netherlands	UK, Germany, Belgium
Belgium	UK, France, Germany, Netherlands, Luxembourg
Luxembourg	France, Germany, Belgium
Italy	France, Spain, Austria, Slovenia, Croatia, Greece, Malta
Poland	Sweden, Germany, Czech Republic, Slovakia, Lithuania, Denmark
Czech Republic	Germany, Poland, Austria, Slovakia
Austria	Germany, Italy Czech Republic, Slovakia, Hungary, Slovenia
Slovakia	Poland, Czech Republic, Austria, Hungary
Hungary	Austria, Slovakia, Slovenia, Croatia, Romania
Slovenia	Italy, Austria, Hungary, Croatia
Croatia	Italy, Hungary, Slovenia,
Greece	Italy, Bulgaria, Cyprus
Romania	Hungary, Bulgaria
Lithuania	Sweden, Poland, Latvia
Latvia	Sweden, Lithuania, Estonia
Estonia	Sweden, Latvia, Finland
Finland	Sweden, Estonia
Bulgaria	Greece, Romania
Malta	Italy
Cyprus	Greece
Denmark	Sweden, UK, Germany, Poland

Table 6.1: Overview of Neighbors of all Countries.

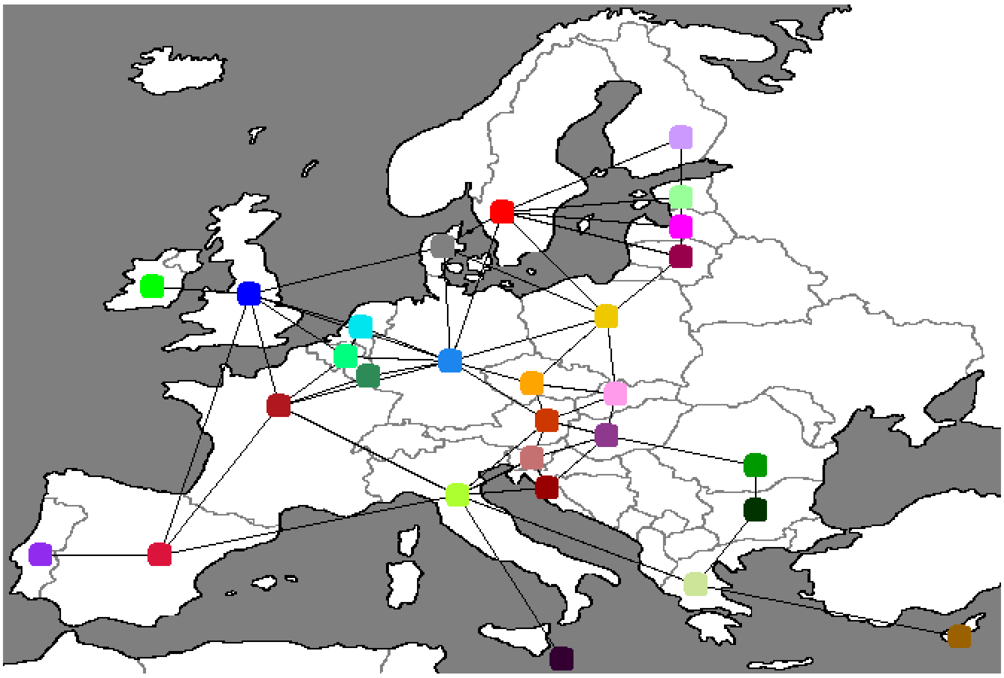


Figure 6.1: European Union Network Based on its Geographical Structure.

investments u, which coincides to the equilibrium from Section 6.2.3. An overview of the different investments into green policies of the countries is shown in Figure 6.2b.

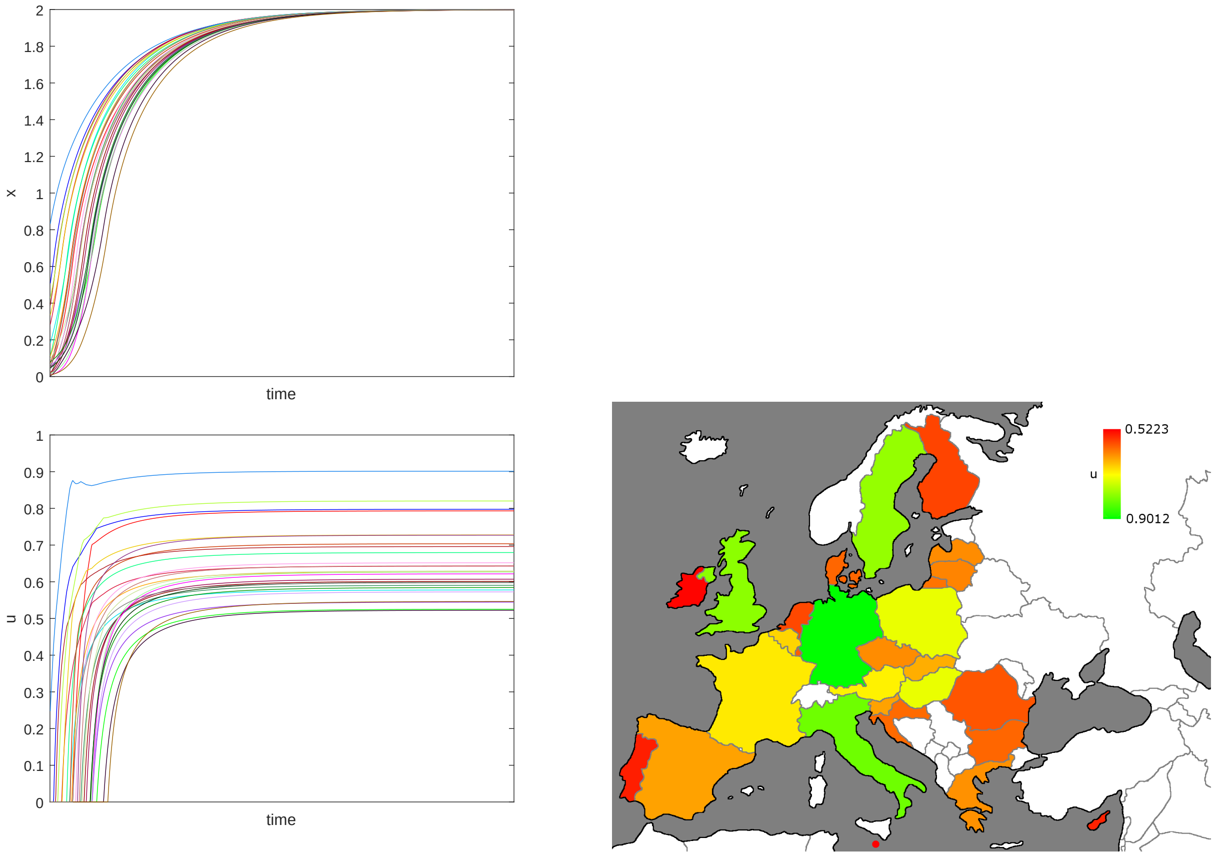
Furthermore, earlier or later, the countries start acting more environmentally friendly. The more neighbors a country has, the higher the chance is that it starts fighting pollution earlier since all neighbors are additionally polluting its environment and increasing the costs. Germany, the country with the highest number of neighbors (see Table 6.1), acts most environmentally friendly.

Influence of the external control parameter β on pollution costs

When the countries' investments into environmentally friendly policies only depend on their own costs, it can be observed that the pollution stock increases a lot until it reaches a saturation point. In order to lower this pollution increase, an external administration (e.g., European Commission) can punish pollution flow by increasing the corresponding costs. $\beta > 1$ models this punishment by influencing the costs for pollution (also see (6.2)). The punishing party then becomes a leader in a Stackelberg game, while the countries as followers minimize their pollution costs. The leader wants to find an optimal β^* that minimizes the total sum $\zeta_\beta(T) = \sum\limits_{i \in \mathcal{N}} x_i(T)$ of all pollution stocks $x_i(T)$ at time T when equilibrium values of x_i's are reached:

$$\beta^* = \arg\min_{\beta \in B} \sum_{i \in \mathcal{N}} x_i(T), \tag{6.8}$$

where the compact set $B \subset (1, \infty)$ of feasible policies is known a priori. The EU countries acting as the followers in the game choose their strategies u_i minimizing their costs (6.4).



(a) (b)

Figure 6.2: Pollution stock x and investment u into environmentally friendly policies for each player. (**a**) *Pollution stock x and investment u into environmentally friendly policies for each player without any external control on pollution costs ($\beta = 1$);* (**b**) *Overview of the Investments into Green Policies. Red color denotes a low investment into green policies, green color a large investment.*

Their strategy is the best response to the leader's choice (6.8), while the leader can take this best response into account in advance. The dynamics of the system in this game is given by (6.1).

The sum of all pollution stocks at equilibrium is decreasing with increasing β. This behavior is displayed in Figure 6.3. Thus, the leader should choose $\beta > 1$ sufficiently large in order to decrease the overall pollution up to a satisfactory level.

The simulation results, displayed in Figure 6.4, show that it is indeed possible to lower the pollution stock while the remaining behavior like the consensus in pollution does not change. Compared to the case without punishment (Figure 6.2a), already a weak external punishment (Figure 6.4a) can halve the pollution $x_i(T)$ which all approach the attractor x_i^* given by (6.7). A strong punishment can force countries to behave more ecologically friendly than in the initial situation. For larger values of β, the pollution stocks $x_i(T)$ for all countries i and so the sum of all pollution stocks $\zeta_\beta(T)$ even converge to zero (see Figure 6.3).

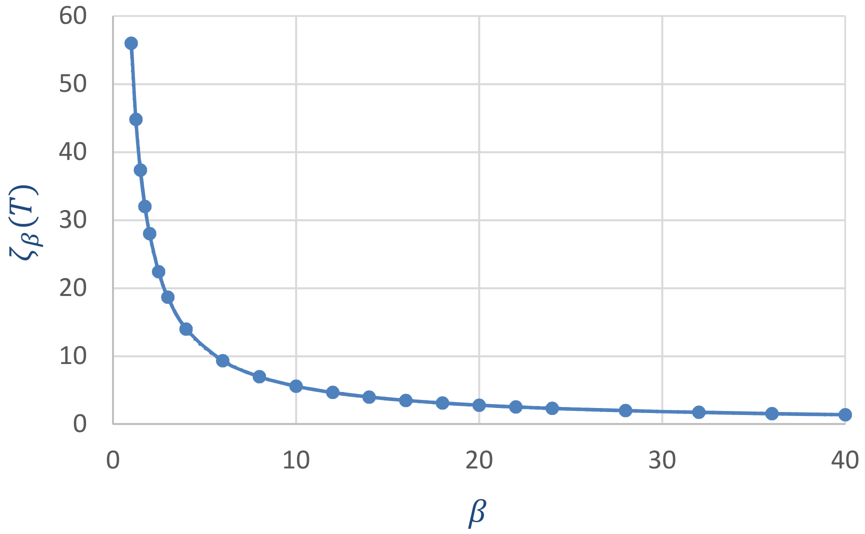
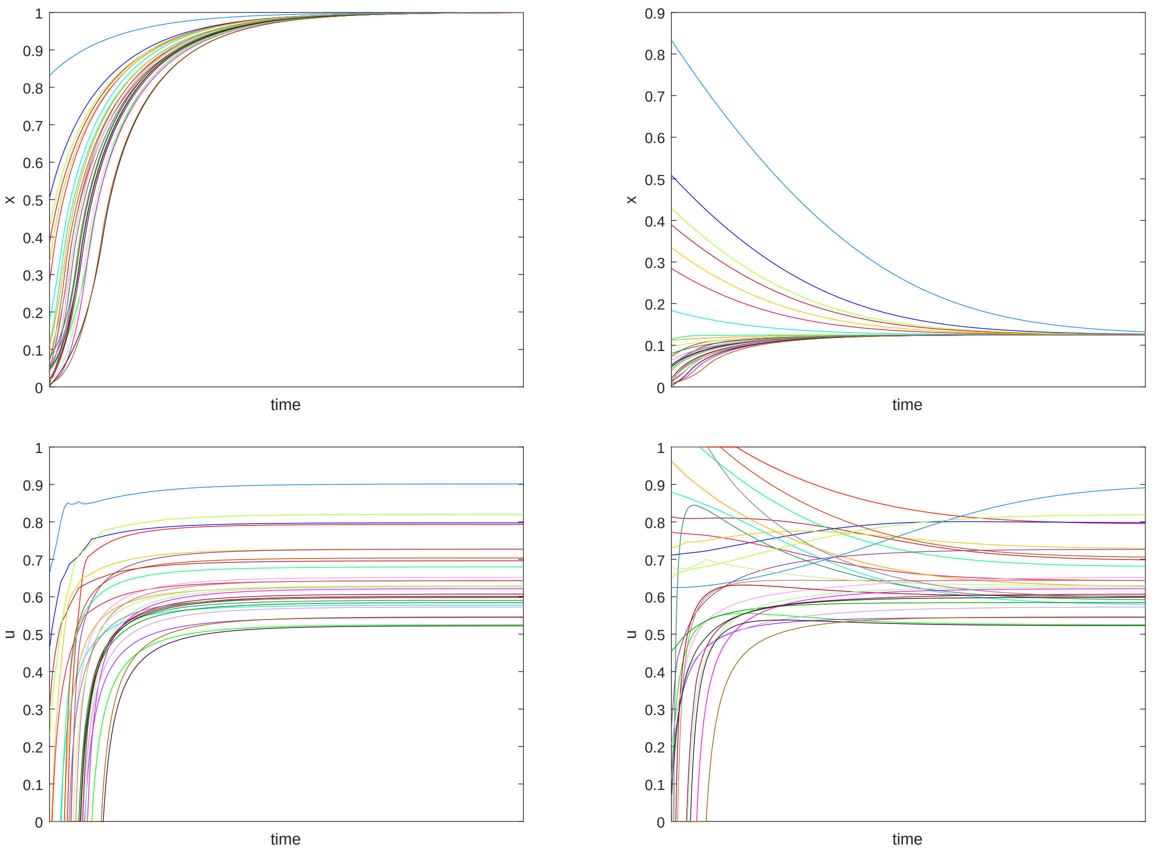


Figure 6.3: Dependency of the sum of pollution stocks $x_i(T)$ on β.

6.3.4 Imitation behavior

In Section 6.3.3, an external administration needs to punish the countries very much in order to reduce the pollution stock to a moderate level. This strong penalty from an external force leads to a loss of independence regarding individual environmental choices. Therefore, this section investigates whether an imitation behavior of countries can also reduce the pollution stock. In this case, we do not consider such a strong influence from an external administration. In the following, we distinguish between a basic imitation according to (6.5) and a more advanced imitation according to (6.6).

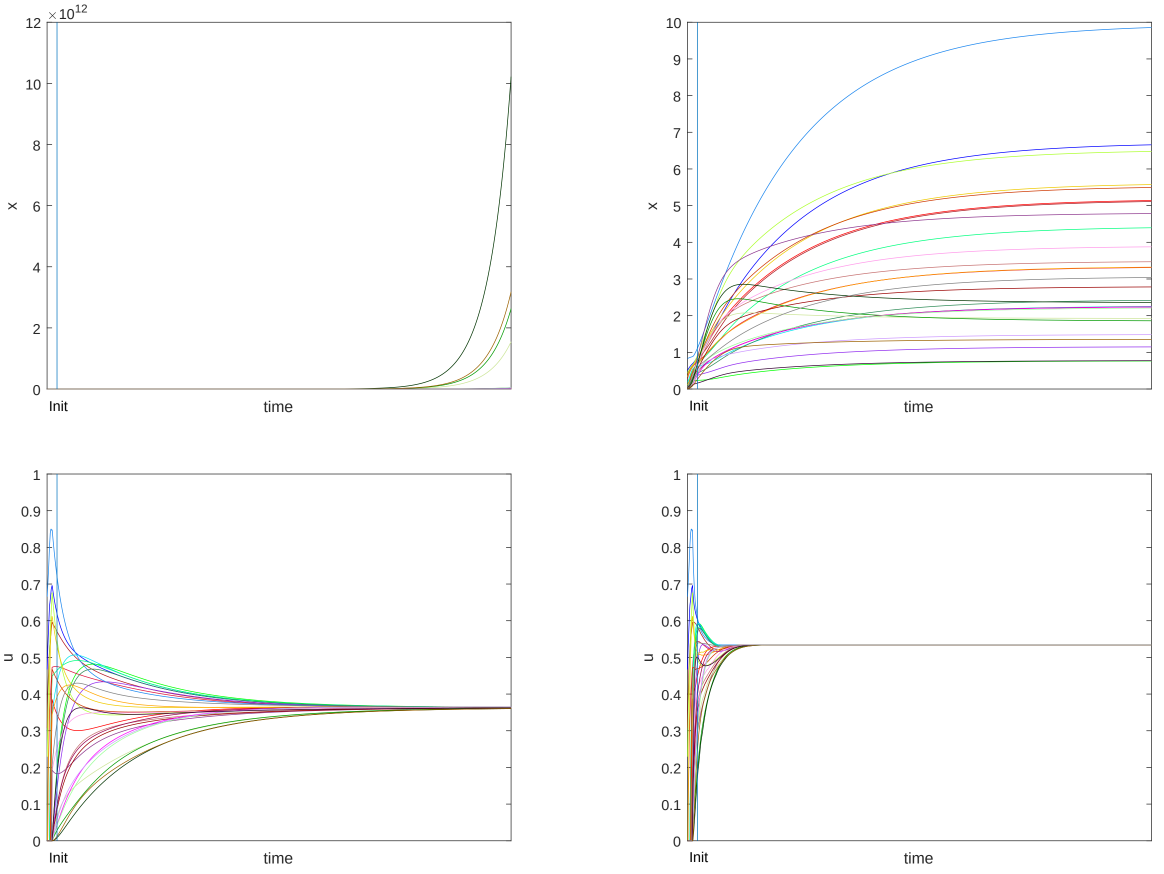
In both cases, we observe that the players agree on their investment into environmentally friendly policies, but they converge to different pollution stocks $x_i(T)$. This is due to the fact that in our model, all countries of the EU are connected and imitate each other in terms of



(a) *(b)*

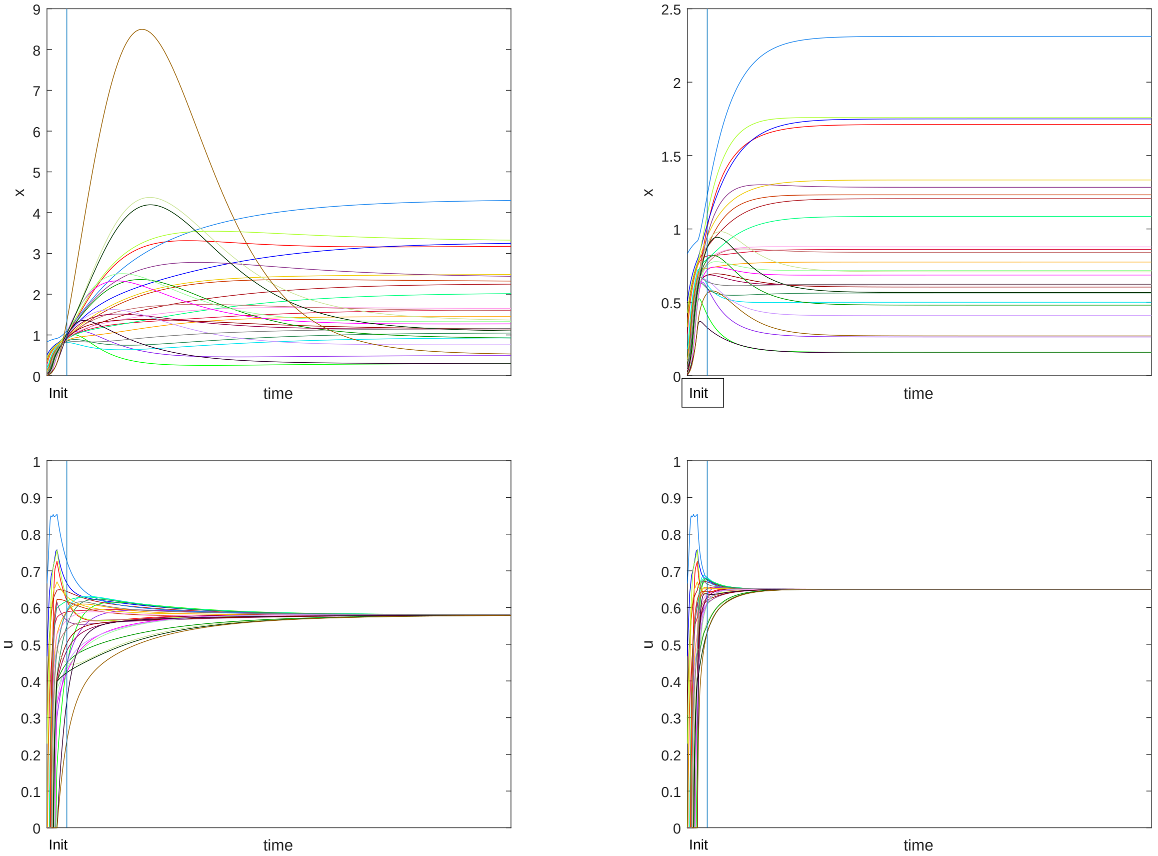
Figure 6.4: Pollution stock x and investment u into environmentally friendly policies for each player with an either weak or strong external control on pollution costs. (**a**) *Weak external control of pollution costs ($\beta = 2$);* (**b**) *Strong external control of pollution costs ($\beta = 16$).*

their investment u. This result is not very surprising as similar results by Ranjbar-Sahraei et al. [2014a,b] show. Comparing Figures 6.5a and 6.6a, we can see that this coinciding investment differs for different starting values for u. The results of Figure 6.5 are obtained when considering a short initial phase in which each country minimizes its own costs. Afterwards, they start with imitating the neighbors' investment strategies according to (6.5) or (6.6). In contrast to this, the results displayed in Figure 6.6 are obtained after a long initial phase. Compared to the short initial phase, we consider here twice as much time in which the countries minimize their own costs. Of course, the investment into clean policies determines the pollution stock as well. For a consensus on a non-environmentally friendly behavior, the pollution stock may even increase exponentially. The more advanced imitation behavior is more robust against the initial conditions. In both cases, see Figures 6.5b and 6.6b, we do not notice an exponential growth but rather a convergence of the pollution stock towards different values $x_i(T)$ per country. Again, the countries differ in the amount of pollution they produce. Furthermore, when the countries perform a more advanced imitation behavior, they converge to a lower amount of pollution stock (see Figure 6.6).



(a) *(b)*

Figure 6.5: Pollution stock x and investment u into environmentally friendly policies for each player with both a basic and more advanced imitation behavior with a ***short*** *initial phase in which all players minimize their individual costs. All results are obtained with the same initial conditions, such as the initial values for $x_i(0)$.* (**a**) *Basic imitation behavior after a short initial phase;* (**b**) *More advanced imitation behavior after a short initial phase.*



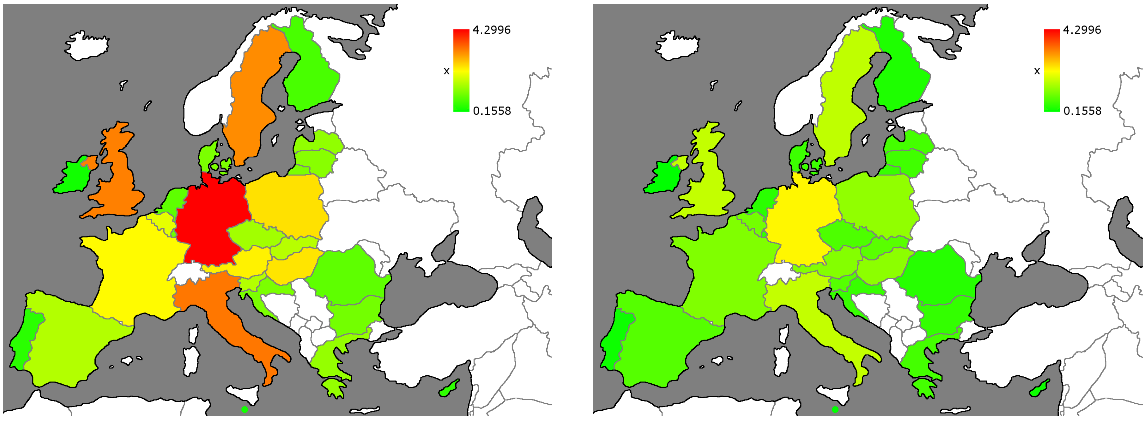
(a) *(b)*

Figure 6.6: Pollution stock x and investment u into environmentally friendly policies for each player with both a basic and more advanced imitation behavior with a ***long*** *initial phase in which all players minimize their individual costs. All results are obtained with the same initial conditions, such as the initial values for $x_i(0)$.* (**a**) *Basic imitation behavior after a long initial phase;* (**b**) *More advanced imitation behavior after a long initial phase.*

6.4 Discussion

In this chapter, we introduce different variants of a game-theoretical model in order to give a starting point for understanding the pollution behavior of the EU countries. This is important since then, one can find feasible ways how to control and improve the pollution behavior of countries. Our case studies demonstrate that the pollution stock can indeed be reduced by the influence of an external force that increases the costs for pollution. However, this scenario is not very realistic, since the countries would lose their independence of decision. We believe that no country would accept such a high intervention from an external party. However, if each country acts only according to its own interests, thus minimizing its individual costs, the pollution stock increases a lot before it starts to saturate.

With basic imitation, we observe that the increase of pollution can be reduced depending on the initial conditions. The basic imitation approach, where a country is influenced equally strong by each of its direct neighbors, is very susceptible to the initial conditions. Starting with large values for u may end up in an exponential pollution growth. Using the same initial conditions for the more advanced imitation approach, where a country is more influenced by neighbors that pay less for applying their strategy, the pollution stock is not growing exponentially. Additionally, with the same initial phase, the pollution can be reduced remarkably by applying a more advanced imitation behavior instead of a basic imitation behavior. Figure 6.7 shows the differences in the remaining pollution stock between the two imitation strategies.



(a) (b)

Figure 6.7: Overview of pollution stock for each country in relation to all other countries. Red color denotes a high amount of pollution, green color indicates a low amount of pollution. (**a**) *Final pollution stock $x_i(T)$ per country for a basic imitation behavior after a long initial phase;* (**b**) *Final pollution stock $x_i(T)$ per country for a more advanced imitation after a long initial phase.*

Thus, we could show that there are incentives possible to make all EU countries act environmentally friendly. Additionally, by choosing a different network in the form of an adjacency matrix, not only countries of the EU can be modeled but rather all the countries in the world. The presented case studies only consider a network of 28 countries, but it can easily be extended. There is no other modification of the model necessary. Our numerical software can also handle different network structures. For example, we can add or remove countries or even consider a completely different association of countries. Furthermore, the initial conditions like the initial pollution values can easily be modified. Thus, the simulations can be updated by using most accurate available data.

This chapter only considers three different variants of the model. It would be interesting to see what happens if the countries do not minimize their own costs but jointly minimize global costs consisting of the sum of all individual costs. Then, all countries would have one common goal instead of only addressing their own welfare. In this case, we can evaluate both the individual pollution per country as well as the global pollution. Additionally, with a feasible measurement of the political power of countries, we could also model a stronger influence of those countries that have more political impact. Not only this is difficult to include due to missing data but other details of the model as well: For example, one can think of an asymmetric adjacency matrix because of common wind directions. However, the simulation software can easily handle these extensions.

CHAPTER 7

Conclusions and discussion

In this thesis, we presented several problem settings and their models. Although all models are agent-based models, they differ a lot in their properties. In this chapter, we answer the research questions raised in Chapter 1, explain what type of models we used to find answers and discuss our model limitations. Future perspectives for the models used in this thesis are given at the end of the chapter.

Chapter 3:

Problem context

In Chapter 3, we examined how the mean viability (directly related to the fitness of individuals) of sexual and asexual populations develop genetically, either in fixed or in changing environments. In this chapter, we used a non-spatial simulation model where sexual and asexual populations evolve in discrete-time generations without any spatial restrictions on the interactions. We considered haploid individuals and mutation-free interactions. During the simulations, the genetics of the individuals present in the population were stored at every time step. This allowed for an analysis of the viability dynamics based on the genetic development of the populations. Thus, we were able to compare how viability dynamics of sexual and asexual populations evolve over time in fixed environments. We furthermore explored the trade-off between viability optimization, i.e., specializing on a certain genotype, and robustness of the population's growth rate against sudden environmental shocks. An environmental shock was simulated by randomly choosing new genotype viability values at a predefined moment in time (called the shock generation).

Research question 1

What are the differences in the mean viability development of sexual populations compared to asexual populations in fixed environments?

Answer to research question 1

We expected to observe that sexual populations maintain a greater genetic diversity within their population than asexual ones. However, we discovered that both types of populations end up with a single genotypic population in the long run. Still, the processes differ considerably in the way they reach a genetically optimized population. While asexual populations very quickly develop towards the best genotype in terms of mean viability available within their initial population, sexual populations undergo three phases: 1) a random walk phase, in which they do not increase their mean viability much but rather explore the genotype space that is available, 2) an increase phase, in which the mean viability increases and deleterious genotypes are eliminated, and 3) a plateau phase, that occurs after specializing on one genotype and, in which their mean viability does not increase anymore. The lengths of the phases vary with properties of the populations, e.g., with their genome size and diversity. However, in any case, this specialization on a genotype takes much longer for sexual populations to occur than for asexual populations. We also observed that in the long run, sexual populations will most likely achieve a higher mean viability than asexual ones.

Research question 2

How can a population be more robust against environmental shocks?

Answer to research question 2

An asexual population can only survive after an environmental shock if either, by coincidence, the genotype that the population has specialized on still performs well after the shock, or if the population has not specialized on a genotype yet and still contains a genotype that performs well after the shock. For a sexual population, our results showed that at the very beginning of our simulations, sexual species are still robust against environmental shocks, while they have not yet specialized much on a genotype. Thus, they have not been increasing their mean viability by much yet. After some more generations, however, they have specialized to a narrow set of successful genotypes and are far less able to adjust to environmental shocks. Thus, a sudden disaster has the least impact on the development of the population if it happens very early on in the process. When we considered recurring disasters, for a sexual population to thrive, it has to increase its mean viability between two disasters, but still needs to maintain robustness against sudden environmental shocks. We showed that the best moment for a population to face this trade-off, is during the increase phase that follows right after the learning phase.

Impact of model assumptions on results and possible future work extensions

The aim of the study in this Chapter was not to model a specific species in a specific environment but rather to get a better understanding of the general processes of sexual and asexual reproduction. Therefore, in order to examine the influence of parameters on the mean viability development, we kept the model simple. For example, we did not consider any mutations in our model. By mutating, asexual populations may create genotypes that are not present in the initial population. With mutation included, asexual populations could become more competitive when compared to sexual populations also in the long run, and be more robust to sudden environmental shocks. Populations that do not recombine monotonically increase the number of mutations because a newborn individual always has at least as many mutations as its parent individual [Muller, 1964]. This mechanism is known as Muller's ratchet. When assuming that advantageous mutations can be neglected, asexual populations become weaker over time. Sexual reproduction, on the contrary, can be seen as a genetic repair, because a newborn individual may, due to the recombination of its parent individuals, bear less mutations than its parents [Maynard Smith, 1978]. Due to the absence of mutations, phenomena such as the sexual DNA repair mechanisms cannot be observed in our model outcomes. For future work, it would be interesting to examine, how advantageous or deleterious mutations influence our findings. Furthermore, we did not distinguish between male and female individuals among the agents. Thus, individuals reproducing sexually can mate with any other individual in the population. By extending our model in that sense, the viability development of sexual populations is expected to slow down, i.e., they would evolve slower to a population bearing only a single genotype. However, we do not expect results in the long run to change, as long as offspring numbers are adapted such that sexual and asexual populations remain comparable in terms of absolute population size.

In contrast to all other models in this thesis, we utilized a non-spatial model in Chapter 3. This is because we wanted to avoid potential effects of spatial limitations on population size (or spatial impact on viability) to confound our findings with regard to sexual and asexual reproduction mechanisms as such. If we introduced space limitations for the populations, especially asexual populations, could not grow as fast as they did in our model. But as sexual populations increase slower than asexual ones, they would be restricted by spatial constraints only at a later stage. Thus, it is expected that the process of sorting out deleterious genotypes would only be marginally influenced by limited space. We do not think that space limitations would qualitatively influence the main findings in Chapter 3, as the viability development of the populations would slow down, but not change much in its characteristics. Introducing limitations in the interaction distance would only affect sexual populations because asexual individuals in our model do not interact with other individuals. Without introducing additional space limitations or a distinction between males and females, we do not expect that a limited interaction distance would have a big impact on the viability development of the sexual population. The population may form clusters, which can become extremely dense without a space limitation and thus do not restrict the population growth.

The environmental shocks arrive at certain generations. In our model, there is no relation between a genotype's viability before and after a shock. As a consequence, very successful genotypes before the shock may immediately go extinct after the shock. Of course, many different scenarios can be considered, which deviate on this point. One possibility would be to study a continually changing environment (with the populations still evolving at discrete steps). In such a scenario, the environmental changes will influence the population dynamics in a much smoother way. Then, there would be far less abrupt changes to genotypic properties of the populations.

Furthermore, we used a control mechanism for population sizes, implemented by randomly removing half of the population if the population size exceeds a certain threshold. Although we think that this population size "normalization" does not affect the population dynamics qualitatively, future research could examine population size controls that are more realistic. This could for example be achieved by introducing a death probability for at the end of each time step, or by having the population size negatively impact the growth rates.

Chapter 4:

Problem context

Charnov et al. [1976] already showed that the prevalence of the different sex types (males, females, and hermaphrodites) depends on the sex allocation of hermaphrodites within the population. However, Charnov's model and its extensions did not take into account any spatial effects. In order to examine how spatial effects influence the prevalence of the three sex types, we implemented a discrete-space model of plant reproduction. The plants in our model were annual plants, i.e., they died after one generation. Thus, we did not consider overlapping generations. Within that one year, each plant had the chance to reproduce. However, the pollen flow from a plant was restricted to a certain area such that it could not fertilize plants outside it. Furthermore, seeds could only be placed at nearby distances from the maternal plants. As such, the germination was limited by the available discrete space within that seed area. This competition for space was even increased when introducing special infertile areas, where no seeds could germinate. We used simulations to track the frequencies of the three different sex types and examined which ones went extinct.

Research question

How do spatial effects, such as competition for space or varying pollen dispersal distances, influence the prevalence of males, females, and hermaphrodites within a plant population?

Answer to the research question

When considering spatial aspects, such as individual positioning and pollen and seed dispersal distances, choosing them equally for all types, our simulations showed that a dioecious (M+F) population only prevailed if males and females had more total resources than hermaphrodites. Even more so, also when hermaphrodites had a slight disadvantage in terms of total resources, it still resulted in males and females going extinct. When having the same amount of resources, an exclusively hermaphroditic population prevailed under the assumption that the hermaphrodites split their resources approximately equal to male and female function. When the hermaphrodites invested more into female function, pure females were outcompeted, and the population developed into an androdioecious (H+M) one, while when the hermaphrodites invested more into male function, it developed into a gynodioecious (H+F) population. When hermaphrodites were able to use more resources than males and females, they never went extinct. When introducing a larger pollen radius for males, the previously observed conditions for the prevalence of breeding systems shifted: a dioecious population could prevail even when hermaphrodites had a higher amount of resources. Remarkably, the influence of the larger male pollen radius on the prevalence of hermaphrodites in the population was much higher when hermaphrodites invest more into ovules than into pollen. In our simulations, the influence of a higher female seed radius was only marginal. When introducing cells where no seeds could germinate, then the conditions shifted such that hermaphrodites could prevail even when they had less resources than males and females. There, the difference between the amount of resources could be bigger than before, and still hermaphrodites prevailed.

Impact of model assumptions on results and possible future work extensions

In our model, plants were assumed to be annual plants, i.e., they die after one year. Considering perennials instead would lead to a higher competition for space because the adult plants would occupy space that in our model could be used by newborn plants. Probably, this would favor hermaphrodites as they invest both in seeds nearby and in pollen far away, such that they reduce space competition between siblings.

In our model, plants nearby a focal plant had the same probability to fertilize it as far away plants. Pollen flow models in which the probability to fertilize another plant decreases with distance of the plants would be more realistic, but also more complex to model. In such a case, the impact of an increased male pollen radius on the prevalence of sex types would be lower, as plants far away would have a smaller probability to fertilize a plant and gain less. One example of a pollen flow model taking into account the distance between pollinator and plant to be fertilized can be found in Chapter 5 of this thesis.

In Chapter 4, we used a discrete-space model to examine the impact of various spatial parameters on the prevalence of types. A continuous-space model where the density of plants is not restricted is expected to favor female over hermaphroditic plants. Compared to hermaphrodites, females in a discrete space promote a higher competition for space between their offspring as they invest their complete resources into seeds. Without any density restriction, competition for space would not take place.

While here we focus on the prevalence of types after a predefined number of simulation runs, it would be interesting for future work to examine the transient dynamics as well. Especially, for hermaphroditic sex allocations close to a border between the blue (H) area and the green (H+F) area or the magenta (H+M) area, it may be that certain spatial structuring within the population leads to a faster extinction of the underrepresented types. The analysis of the transient dynamics of these border cases may increase the reliability of our results further, as we may be able to identify how spatial structures corresponding to these dynamics change in time.

Chapter 5:

Problem context

It is well-known that oak trees produce six ovules per flower, usually have all of them fertilized, but only mature one of them to an acorn. Furthermore, commonly used pollen-flow models cannot explain that in oaks, nearby trees are more often absent as pollen donors, while far away trees more often serve as pollen donors than in other species. Therefore, here we examined the hypothesis that oak trees exercise a female ovule choice. We implemented the female choice mechanism as a two-step lottery model and used real data of three published studies to validate whether the female choice model fits the data better than the commonly assumed random ovule choice. In the first lottery step of our model, all ovules in a flower are fertilized by pollen from other trees, and in the second lottery step, the female choice mechanism is applied. Here, the oak chooses that ovule in a flower that has been fertilized by a father having fertilized the least number of ovules in that flower. The oak trees are placed in a two-dimensional continuous space. In our model, we can distinguish between a field with and without periodic boundary conditions. The pollen flow is modeled by an inverse square law, i.e., the distance of a paternal tree to a focal tree has an inverted quadratic influence on the probability to fertilize an ovule of that tree. The genetic diversity within the stand is measured by the Simpson diversity index (SDI) during our simulations.

Research question

Can the female choice hypothesis in oak trees explain the observed fertilization patterns of these trees?

Answer to the research question

Our simulations showed that the female choice model explains the available data better than a common hypothesis that oak trees choose the ovule, which becomes an acorn at random. We used data from three published field studies on oak tree reproduction to validate our model. These field studies provided paternal information of acorns from ten different maternal trees. Data for eight out of these ten maternal trees (from two of the published studies) allowed for a comparison of the SDI assuming a female choice to assuming a random ovule choice mechanism. In most of the cases (seven out of eight), the female choice mechanism explained the observed SDI better than a random ovule choice. Due to the characteristics of the third study, data for the two remaining maternal trees (from the third published study) allowed for a comparison of paternity by distance classes. Here, for both maternal trees, the female choice hypothesis also explained the observed fertilization patterns better than a random ovule choice.

Impact of model assumptions on results and possible future work extensions

With our simulations, we showed that a female choice mechanism is more likely present in oaks than a random ovule choice. However, there may still be other hypotheses that explain the data even better.

In our study, time was not modeled explicitly. Clearly, our static model can be extended to a time-variant population model where birth and death processes of oak trees are examined. To obtain such a dynamic model, we would need to add seed germination and space competition processes in our model. In continuous space, competition for space can for example be modeled by introducing a minimum distance between trees and seeds. If the distance between two seeds, or between a seed and a tree, falls below that minimum distance, then a seed would not be able to germinate. Similarly, one could also introduce a density limit for seeds within a certain area. If this limit is exceeded, a seed could not germinate.

We validated the female choice hypothesis by field studies involving ten maternal trees. In order to obtain a more reliable validation, data from more trees is needed. Furthermore, the data we used did not contain geographical details like influence of wind directions or obstacles such as rivers or rocks. It would be interesting to see how a certain wind direction influences the fertilization patterns. It may well be that up-wind trees are more likely to fertilize ovules of a certain tree than others even when having the same distance. Including such data would make our model more realistic. We expect that the female choice hypothesis might then fit the data even better. However, such detailed data is not available yet, currently making validation for the model very difficult. For future research, it would also be interesting to restrict the amount of pollen a tree can produce. We here assumed that each tree has an unlimited amount of pollen. When restricting the pollen amount, it would be more difficult to fertilize many ovules within one flower. On the one hand, trees that have fertilized many ovules within one flower would most likely lose the second lottery step, and on the other hand, they would lose possibilities to gain chances in other lotteries.

Chapter 6:

Problem context

Chapter 6 examined the air pollution behavior of all countries[1] in the European Union (EU) and the air pollution development in all these countries. We modeled this as a discrete-space continuous-time game where the players are the countries of the EU that want to minimize their costs. These countries can choose how environmentally friendly they produce their goods. However, their decision on the pollution level does not only influence their own air pollution, but also the pollution of the neighboring countries. The neighbors of a country are defined by means of a network of countries (a graph) corresponding to the geography of the EU. In that network, countries that pollute each other are connected. Each connection is unweighted and bidirectional. The pollution stock in our model changes in continuous time

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[1] As of 2020, the UK left the EU, but was part of the EU during the time of the study.

according to a differential equation. We examined three different strategies of the countries: 1) minimization of their own costs, 2) mimicking the behavior of all neighboring countries by applying an average of their pollution strategies (basic mimicking), and 3) mimicking the behavior of neighboring countries only if this behavior is more profitable (smart mimicking).

Research question

What are potential effective policies that would lead to a more environmentally friendly goods production throughout the European Union?

Answer to the research question

Three variants of the game were examined and gave insights in the pollution behavior of EU countries and the development of pollution within Europe. We showed that with a strong regulatory influence of the EU administration that introduces fees for pollution, the overall pollution in the EU can be reduced. However, as countries are sovereign, it would be difficult to enforce such high fees for pollution in the EU. Therefore, other more realistic policies have to be designed with the aim of lowering air pollution in Europe. With a basic mimicking approach as a strategy for the countries, the increase of pollution was very sensitive to the initial pollution levels of the countries. For some pollution levels, we even observed an exponential increase of pollution. However, with the smart mimicking approach, the pollution stabilized. The level of pollution stock on which the approach stabilizes, depends on the initial pollution conditions of the countries. We can conclude that, from the three examined policies, introducing large fees for pollution would be best for lowering pollution in Europe. However, this would have a major impact regarding economic competition with non-EU countries. From the remaining two policies, the smart mimicking approach is best. It can further be improved by incentives in research about cheap techniques to reduce the pollution of factories.

Impact of model assumptions on results and possible future work extensions

One major advantage of our pollution model is that it can be applied to many other scenarios as well. Only the adjacency matrix of the network needs to be changed in order to model another composition of countries. Thus, for future research, other regions or even the pollution of the whole world could easily be modeled in a similar fashion. However, in our model, the influence of a country's pollution on a neighboring country was always bi-directional, i.e., if two countries share a (sea or land) border, they both influence each others' air. This approach did not take into account, e.g., wind directions or country sizes, that may increase the likelihood that a country is polluting the down-wind countries, while the down-wind countries have a low probability to pollute up-wind countries. It would be interesting to see what influence such extensions of our model have on the pollution, and the pollution behavior of countries as the down-wind countries should be the countries that have the largest interest that the pollution is reduced. By making the network directed and weighted, we could model more realistic scenarios. The weights could then also take into account the distance of the source of pollution in a country to another country. Until now, the influence of a country's pollution on the pollution stock of another country depends only on the pollution behavior of the country and whether both countries share a border. Besides making the influence of a country's pollution on the pollution of other countries more realistic, we could furthermore investigate more realistic decision scenarios of the countries regarding their environmentally friendly incentives in addition to our three investigated variants of the model. We could, e.g., examine how the pollution behavior of the countries would develop if they wanted to minimize the global costs for pollution rather than only their individual costs.

Future research directions far away

The models of Chapters 3 to 5 focused on reproduction mechanisms. While Chapter 3 examined the mean viability dynamics of sexually and asexually populations, Chapter 5 investigated phenomena in the reproduction of oak trees. We applied the same form of modeling to both very general problem settings as well as to a very specific one. In Chapter 3, we kept the model as simple as possible to get insights into the general processes in sexual and asexual reproduction rather than modeling a specific species. By contrast, in Chapter 5, we examined oak trees as a concrete example of hermaphroditic plants and made a realistic model for oak reproduction. For future studies, the models used in this thesis can be used to examine various other reproduction mechanisms not only in plants but also in animals. Then, the interaction between the individuals needs to be interpreted in a different way: The pollen radius would no longer set the area in which pollen is spread, but the area in which animals look for mating partners. The seed radius would be transferred into a region where the offspring will settle. Death processes would have to be aligned with the lifetime of concrete species. However, the most important part, the exchange of good strategies by exchanging genes, stays the same. Chapter 4 presented a model where males, females, and simultaneous hermaphrodites interact and compete for space. For future research, it would be interesting to examine also sequential hermaphrodites as they often occur in animals like fish for example. These may change from one sex to the other during their lifetime. This extension would even increase the variety of reproduction mechanisms that can be investigated by means of the type of models used in this thesis.

Reproduction mechanisms can also be interpreted more generally as the exchange of good ideas. While Chapters 3 to 5 examined the exchange of good ideas in the context of reproduction, Chapter 6 investigated the spreading of good ideas in the context of pollution control. This already shows that the type of models used in Chapters 3 to 5 not only can be applied to reproduction but also to quite different problem settings like pollution control.

Furthermore, the reproduction models of this thesis can not only be used to describe certain phenomenons, e.g., the dynamics of populations driven by natural selection (as it is done in Chapters 3-5 in this thesis) but can also be used to solve optimization problems. By spreading the good ideas, the population fitness improves and evolves towards an optimum. This optimization process can be used to find optima in other problem settings as well. Evolutionary algorithms have already been applied successfully to all kinds of combinatorial optimization problems [Reeves, 2000]. Genetic algorithms - one example of evolutionary algorithms - use reproduction operators such as crossover, mutation, and selection to address optimization or search problems [Davis, 1991, Holland, 1992, Weile and Michielssen, 1997]. Usually, in genetic algorithms, fitness is defined as the value of the objective function in the optimization problem. Due to natural selection, less fit individuals are sorted out, and the population improves towards an optimal population. This optimal solution then gives information on the solution of the optimization problem. Imagine for example a simple logistic problem, where a delivery truck has to find the best route for several destinations. When using evolutionary optimization, a population of random routes has to be initialized. By mutating the routes and selecting for the time-efficient routes, the population evolves until it approaches a solution to the optimization problem. When using evolutionary algorithms for optimization, we need to take into account that they may approach a local optimum rather than a global one [Larrañaga et al., 1999, Rocha and Neves, 1999]. For a population consisting of rational individuals, we would expect that they evolve towards the global optimum, while a population driven by natural selection usually ends up in a local optimum. The model presented in Chapter 3 can directly be used for finding solutions to optimization problems. There, the population evolves towards a locally optimal population consisting of only one genotype. However, we could not predict in advance towards which locally optimal genotype a sexual population evolves.

This thesis shows that there is a huge variety of problems that can be addressed using the types of agent-based models used here. While we applied these models to various reproduction mechanisms and pollution control problems, the variety does not stop there.

For example, there is already a lot of work done in cancer modeling by using spatially-explicit agent-based models [Kather et al., 2017, Wang et al., 2007, You et al., 2017]. Heterogeneity in a tumor is now well accepted as relevant to its development: Various types of cancer cells that differ in their consumption of resources and their proliferation interact within the tumor. This interaction plays a huge role especially in metastatic cancers where resistant tumor cells can (so far) only be controlled by the help of non-resistant cells that compete with them for space and other resources. In this context, metastatic cancer cannot be cured, i.e., eliminated completely, but only controlled. A recent study by Zhang et al. [2017] at the Moffitt Cancer Center in Florida shows that with adaptive treatments taking this knowledge into account, the life expectancy of patients can be prolonged significantly.

As already shown in Chapter 6 of this thesis, the types of models used here do not necessarily include death and birth processes. While the example of tumor modeling includes these processes, there are also many spatially-explicit agent-based models, where good ideas are not spread by giving birth to individuals that (partly) apply these ideas, but rather by transferring them to individuals of the same generation. Furthermore, it may also well be that the ideas that are spread out over the population are deleterious rather than beneficial. Imagine for example the spread of contagious diseases. These diseases can be transferred by local interactions of individuals. Here, spatially-explicit agent-based models are used to model the dynamics of disease spreading [Parker and Epstein, 2011, Perez and Dragicevic, 2009]. With increasing computational power and possibilities to store a huge amount of data, more and more details such as real-life data defining the behavior of agents can be added to these models [Frias-Martinez et al., 2011].

Thus, to conclude, agent-based models, where beneficial or deleterious ideas are spread over heterogeneous populations, can be considered as a powerful way to examine complex phenomena and scenarios in all kinds of different research fields.

Summary

This thesis examines various real-world phenomena by means of models and simulations. All these phenomena are modeled by an agent-based approach, using quite different model properties in each case. The modeling approaches differ per chapter, varying from static to discrete-time and continuous-time models and from non-spatial to discrete-space and continuous-space ones. We use a non-spatial discrete-time model to compare sexual and asexual reproduction in general (Chapter 3), a discrete-space discrete-time model to examine the influence of explicit spatial aspects like positions of plants and distance restricted pollen/seed dispersal on the prevalence of sex types in annual plants (Chapter 4), a continuous-space discrete-time model to test the hypothesis that oak trees exercise a female ovule choice to increase the genetic diversity in a stand (Chapter 5) and a discrete-space continuous-time pollution model to investigate conditions under which the EU countries have incentives to produce their goods environmentally friendly (Chapter 6).

In Chapter 3, we compare sexual and asexual reproduction in stable and unstable environments. Although in the literature sexual reproduction is considered more costly, for example due to needing two individuals for reproduction, our simulations show that sexual reproduction can anyway be more successful in terms of the population fitness, even in a stable environment. Moreover, we observe that all sexual populations pass a learning phase before they are able to increase their fitness and that they do not increase the genetic diversity in populations (as often assumed) but specialize on a single genotype, just like with asexual reproduction. By tracking the genetics of the individuals during our simulations, we can examine the underlying mechanisms that lead to the observations in more detail. Furthermore, our simulations show that, if the environment suddenly changes, the populations face a trade-off between being robust against such changes and fitness improvement due to specialization.

Populations of plants appear in different compositions of males, females, and hermaphrodites. It is well-known that the sex allocation of hermaphrodites influences the prevalence of the different types. In Chapter 4, we examine the influence of explicit spatial aspects like positions of plants or distance restricted pollen/seed dispersal on the prevalence of the sex types. Our simulations show that a dioecious breeding system (only males and females in the population) prevails only when males and females can use more resources than hermaphrodites. In all other cases, hermaphrodites do not go extinct. Depending on the amount of resources available to hermaphrodites and on their sex allocation, either females or males may stay in the population as well, leading to an androdioecious or gynodioecious breeding system. Additionally, we investigate the influence of a type-dependent pollen dispersal on the prevalence of sex types. If males can distribute their pollen farther than hermaphrodites, then it is more likely that only males and females survive than with equal pollen distribution distances. Furthermore, the chances for males to survive increase, and thus, androdioecious populations become more likely than gynodioecious populations.

Oak trees are one example for hermaphroditic plants, i.e., they produce both pollen and ovules. Remarkably, oaks produce six ovules in a flower, but only one becomes an acorn even though all ovules within the flower are fertilized. Moreover, compared to other tree species, long-distance fertilization in stands of oaks is more common, while short-distance fertilization is more rare. In Chapter 5, we examine the hypothesis that oaks exercise a female choice of ovules in a flower to increase the genetic diversity, using a two-step lottery model. Next to showing that this female choice mechanism indeed increases the genetic diversity, we show that this mechanism explains the data of published field studies on oak reproduction better than if one of the ovules is chosen randomly.

In Chapter 6, we model EU countries maximizing their own benefits by choosing more or less environmentally friendly ways of producing goods. This is to understand how such decisions are made and to analyze what would be the best stimuli to lead the countries to more environmentally friendly policies. The EU countries control their own air pollution but, by doing so, influence the air pollution of neighboring countries. We analyze three variants of this model: 1) each country chooses its investment into clean policies such that the expected costs are minimal, 2) each country imitates the investment of neighboring countries no matter whether they are successful (basic mimicking) and 3) each country imitates the investment of neighboring countries only when they seem to bring a profit (smart mimicking). For each of the considered variants, we show that the pollution can indeed be reduced by the influence of an external government exposing high costs for pollution. Without such an influence and when all countries only have their own benefits in mind, the pollution stock increases a lot before saturation. While the basic mimicking variant is very sensitive to initial conditions, the smart mimicking variant is a very promising approach for pollution reduction.

Overall, we demonstrate how simulation models can be used for describing, understanding, and predicting the behavior of real-world systems.

Addendum: Valorization

In the manual of Maastricht University on how to write a valorization chapter, it is said that "Knowledge valorization involves the process of creating societal and/or economic value from scientific knowledge". I strongly believe that the scientific knowledge of my content chapters (Chapters 3-6) can be the basis for societal and/or economic value.

Chapter 3 shows that for sexually reproducing populations, there is a trade-off between optimizing the population fitness and being robust against environmental changes. In particular, we show that if a population is too much specialized, it cannot respond well to changes of the environment. This problem occurs in day-to-day life all the time. Many people in their career have to decide at some point whether to specialize more in one direction or to achieve a wider range of knowledge. While a specialized worker may be indispensable, he might lose his complete expertise if the production system in the company is changed. However, the trade-off can also be noticed from the company's point of view: If they hire people that are very good at producing a certain good, then the company will be very successful in the production of that good. If, however, some development in terms of modifications of the good is needed, these workers might not perform that well anymore, and the company loses its supremacy. Thus, the original problem can be translated to very many situations of day-to-day life where a trade-off between specialization and generalization can be noticed. Our findings can be used to better evaluate the advantages and risks of being too specialized in all situations. For example, biodiversity of plants helps to adapt to climate change [Mijatović et al., 2013]. However, agriculture destroys the biodiversity and thus promotes climate change [McLaughlin and Mineau, 1995]. Thus, we need more understanding about the advantages of biodiversity and how to protect it.

Chapters 4 and 5 examine plant reproduction strategies. Some newspapers say that until 2050, in order to feed the human population, the world has to produce twice as much food as compared to today without using more resources like space or water. Even if these numbers are not correct, it is obvious that more and more food is required to feed the growing number of humans in the world. Plants are needed both as food for humans and as food for other animals. Thus, increasing, e.g., the biomass of plants without using more resources, may solve a big part of the problem. In order to be able to modify genetic structures or plant growing processes, it is essential to understand how these mechanisms work in plants. Furthermore, it may be that nature shows us ways to improve artificially produced goods. One example of such a good is the lotus wand paint, where the plant *Nelumbus* was the inspiration for a water-repellent surface. When understanding mechanisms of plants, this understanding may be useful in order to invent new tools as well.

Chapter 6 directly addresses a big societal and economic problem, namely air pollution. There, we investigate how national policies of the European Union (EU) countries influence the air pollution over Europe. With our model and the simulation results, we give insights into how countries can be forced to produce their goods environmentally more friendly while also keeping their national needs in mind. This model can easily be extended to any set of countries and can, as such, serve as a basis for understanding the mechanisms behind pollution problems.

Additionally to these concrete problem contexts, the models used in this thesis can be applied to many other scenarios. After implementing the framework, only small changes, e.g., in defining other interactions among the agents, may be enough to apply the model to scenarios in all kinds of different domains. These domains include, e.g., tumor growth, asset pricing, migration, and disease spreading.

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APPENDIX A

Supplement of Chapter 5

Let p_i be the probability of father i fertilizing a fixed focal tree j. We are only interested in which surrounding tree is fertilizing ovules of the focal tree j and thus, we assume that only the focal tree j is fertilized and that all other trees in the stand do not fertilize each other. Furthermore, let X_i be the number of ovules fertilized in the flower by father i and let $a \geq 3$ be the number of ovules in a flower. We assume that the number of fertilized ovules, $\sum_i X_i$, is always equal to the total number a of ovules in a flower and $X_1 \neq 0$. Furthermore, we assume that $\sum_i p_i = 1$.

We then can calculate the probability q_1 of father 1 winning the two step lottery (so really fertilizing the flower) when considering two fertilizing fathers in total and six ovules per flower:

$$\begin{aligned} q_1 =& P(X_1 = 6) + P(X_1 < X_2) + 0.5 \cdot P(X_1 = X_2 = 3) \\ =& p_1^6 + \binom{6}{1} p_1 p_2^5 + \binom{6}{2} p_1^2 p_2^4 + 0.5 \binom{6}{3} p_1^3 p_2^3 \\ =& p_1^6 + \binom{6}{1} p_1 (1-p_1)^5 + \binom{6}{2} p_1^2 (1-p_1)^4 + 0.5 \binom{6}{3} p_1^3 (1-p_1)^3 \end{aligned} \tag{A.1}$$

In Figure 5.1, we display q_1 as a function of p_1 based on this formula.

Let $\delta_k(b)$ be 1 if b is divisible by k, and 0 otherwise. When considering $a \in \mathbb{N}$ ovules per flower, the probability q_1 for father 1 to fertilize the flower becomes:

$$
\begin{aligned}
q_1 =& P(X_1 = a) + P(X_1 < X_2) + \frac{1}{2} \cdot P(X_1 = \frac{a}{2}) \cdot \delta_2(a) \\
=& p_1^a + \sum_{k=1}^{\lfloor \frac{a-1}{2} \rfloor} \binom{a}{k} \cdot p_1^k p_2^{a-k} + \frac{1}{2} \cdot \binom{a}{k} \cdot p_1^{\frac{a}{2}} p_2^{\frac{a}{2}} \cdot \delta_2(a)
\end{aligned}
$$

Increasing the number of possible fathers to three fathers ($i \in \{1,2,3\}$), makes the calculation for six ovules per flower slightly more complicated:

$$
\begin{aligned}
q_1 =& P(X_1 = 6) + 1/3 \cdot P(X_1 = X_2 = X_3 = 2) \\
&+ 1/2 \cdot [P(0 < X_1, X_1 = X_2, X_1 \neq X_3) + P(0 < X_1, X_1 = X_3, X_1 \neq X_2)] \\
&+ P(0 < X_1, X_1 < X_2, X_1 < X_3) + P(0 < X_1, X_1 < X_2, X_3 = 0) \\
&+ P(0 < X_1, X_1 < X_3, X_2 = 0) \\
=& p_1^6 + \frac{1}{3} \cdot p_1^2 p_2^2 p_3^2 \cdot \frac{6!}{2!2!2!} \\
&+ \frac{1}{2} \cdot \left[(p_1^3 p_2^3 \cdot \frac{6!}{3!3!} + p_1 p_2 p_3^4 \cdot \frac{6!}{1!1!4!} + p_1^3 p_3^3 \cdot \frac{6!}{3!3!} + p_1 p_2^4 p_3 \frac{6!}{1!4!1!} \right] \\
&+ \frac{6!}{1!2!3!} \cdot p_1 p_2^2 p_3^3 + \frac{6!}{1!2!3!} \cdot p_1 p_2^3 p_3^2 + \frac{6!}{2!4!} \cdot p_1^2 p_2^4 + \frac{6!}{1!5!} \cdot p_1 p_2^5 + \frac{6!}{2!4!} \cdot p_1^2 p_3^4 + \frac{6!}{1!5!} \cdot p_1 p_3^5
\end{aligned}
$$

For a ovules per flower and still considering three possible fathers, we obtain the following:

$$
\begin{aligned}
q_1 =& P(X_1 = a) + \frac{1}{3} \cdot P(X_1 = X_2 = X_3 = \frac{a}{3}) \\
&+ \frac{1}{2} \cdot \left[P(X_1 = X_2 = \frac{a}{2}, X_3 = 0) + P(X_1 = X_3 = \frac{a}{2}, X_2 = 0) \right] \\
&+ \frac{1}{2} \cdot [P(0 < X_1, X_1 = X_2, X_1 < X_3) + P(0 < X_1, X_1 = X_3, X_1 < X_2)] \\
&+ P(0 < X_1, X_1 < X_2, X_1 < X_3) + P(0 < X_1, X_1 < X_2, X_3 = 0) \\
&+ P(0 < X_1, X_1 < X_3, X_2 = 0) \\
=& p_1^a + \frac{1}{3} \cdot p_1^{\frac{a}{3}} p_2^{\frac{a}{3}} p_3^{\frac{a}{3}} \cdot \frac{a!}{\lfloor \frac{a}{3} \rfloor ! \lfloor \frac{a}{3} \rfloor ! \lfloor \frac{a}{3} \rfloor !} \cdot \delta_3(a) \\
&+ \frac{1}{2} \cdot \left[p_1^{\frac{a}{2}} p_2^{\frac{a}{2}} \cdot \frac{a!}{\lfloor \frac{a}{2} \rfloor ! \lfloor \frac{a}{2} \rfloor !} + p_1^{\frac{a}{2}} p_3^{\frac{a}{2}} \cdot \frac{a!}{\lfloor \frac{a}{2} \rfloor ! \lfloor \frac{a}{2} \rfloor !} \right] \cdot \delta_2(a) \\
&+ \frac{1}{2} \left[\sum\nolimits_{k=1}^{\lfloor \frac{a-1}{3} \rfloor} p_1^k p_2^k p_3^{a-2k} \cdot \frac{a!}{k!k!(a-2k)!} + \sum\nolimits_{k=1}^{\lfloor \frac{a-1}{3} \rfloor} p_1^k p_2^{a-2k} p_3^k \cdot \frac{a!}{k!k!(a-2k)!} \right] \\
&+ \sum\nolimits_{j=1}^{\lfloor \frac{a-2}{3} \rfloor} \sum\nolimits_{k=j+1}^{a-2j-1} p_1^j p_2^k p_3^{a-j-k} \cdot \frac{a!}{j!k!(a-j-k)!} \\
&+ \sum\nolimits_{j=1}^{\lfloor \frac{a-1}{2} \rfloor} p_1^j p_3^{a-j} \cdot \frac{a!}{j!(a-j)!} \\
&+ \sum\nolimits_{j=1}^{\lfloor \frac{a-1}{2} \rfloor} p_1^j p_2^{a-j} \cdot \frac{a!}{j!(a-j)!}
\end{aligned}
$$

These examples show that it is possible to determine the probability of a father to fertilize a flower dependent on the locations of the trees as these define the probabilities to fertilize an ovule. Furthermore, it shows that the formula becomes more complicated when increasing the number of fathers and/or the number of ovules.

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About the author

Katharina Schüller was born on April 27, 1988 in Sittard in the Netherlands. Although she was born across the border, she grew up in Germany. From 2009 to 2012 she did dual Bachelor studies. Simultaneously to being trained as a software developer at the Chair and Institute of Industrial Engineering and Ergonomics (RWTH Aachen University), she studied Scientific Programming at FH Aachen University of Applied Sciences. In 2014 she graduated with cum laude from Maastricht University with a master's degree in Operations Research.

In the same year, she started doing her PhD at the Department of Data Science and Knowledge Engineering at Maastricht University. Since then she has carried out her research in agent-based modeling of complex dynamical systems in various applications such as reproduction methods, plant mating, and pollution control. Besides her research, she was involved in several activities at the department: she was the PhD coordinator of the department, she was involved in the department's research evaluation 2016 and in the organization of female events. During her PhD she established various international collaborations resulting in research visits like a 1-month stay at the Moffitt Cancer Center, Tampa, and a shorter visit to Hebrew University of Jerusalem. She presented her work at several conferences, workshops, and events.

Publications and Presentations

Articles

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Presentations

"Surplus Ovules Permit Female Choice in Oak Trees", talk at the workshop *4C Modelling*, July 2019, Vaals, the Netherlands

“Simulations of Various Game Theoretic Models”, poster presentation at the workshop *Understanding Cancer Through Evolutionary Game Theory*, January 2018, Lorentz Center, Leiden, the Netherlands

“The (dis)advantage of sex”, talk at the *23rd Mathematical Modelling Competition Maastricht*, January 2017, Maastricht University, the Netherlands

“The Selfish Gene and the Advantage of Sex”, *DKE Seminar*, November 2016, Maastricht University, the Netherlands

“The Selfish Alleles and the Advantage of Sex”, talk at the *Parcours of Art and Science Festival*, September 2016, Maastricht, the Netherlands

“The Selfish Alleles and the Advantage of Sex”, talk at the *5th World Congress of the Game Theory Society*, July 2016, Maastricht, the Netherlands

“Evolutionary Simulations”, poster presentation at the workshop *Game Theory and Evolutionary Biology: Exploring Novel Links*, April 2016, Lorentz Center, Leiden, the Netherlands