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Spatial self-structuring accelerates adaptive speciation in sexual populations

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ABSTRACT

Questions: How does spatial self-structuring influence the waiting time until adaptive speciation in a population with sexual reproduction? Which mechanisms underlie this effect?

Model: Using a spatially explicit individual-based multi-locus model of adaptive speciation, we investigate the evolution of a sexually reproducing population, with different levels of spatial self-structuring induced by different distances of natal dispersal. We examine how the waiting time until speciation is affected by the mobility of individuals, the number of loci determining the phenotype under disruptive selection, and the mating costs for individuals that prefer rare phenotypes.

Conclusions: Spatial self-structuring facilitates the evolution of assortative mating and accelerates adaptive speciation. We identify three mechanisms that are responsible for this effect: (i) spatial self-structuring promotes the evolution of assortativity by providing assortative mating 'for free', as individuals find phenotypically similar mates within their spatial clusters; (ii) it helps assortatively mating individuals with rare phenotypes to find mating partners even when the selected phenotype is determined by a large number of loci, so that strict assortativity is difficult; and (iii) it renders speciation less sensitive to costs of assortative mating, especially for individuals that prefer rare phenotypes.

Keywords: adaptive speciation, assortative mating, frequency-dependent selection, homogeneous habitat, mating cost, multiple loci, spatial self-structuring, waiting time until speciation.

INTRODUCTION

Speciation without geographic isolation has long been surrounded by controversy in evolutionary biology research. For speciation to occur in the presence of gene flow, two essential elements are necessary: ecological diversification and reproductive isolation between extreme phenotypes (e.g. Maynard Smith, 1966). While a number of theoretical studies have shown that these elements can be established as a result of competitive interactions

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between individuals, and this scenario has received much attention in theoretical research (Rosenzweig, 1978; Slatkin, 1979; Udovic, 1980; Felsenstein, 1981; Seger, 1985; Doebeli, 1996; Dieckmann and Doebeli, 1999; Bürger *et al.*, 2006; Pennings *et al.*, 2008; Ripa, 2008), the exact conditions that allow for speciation without geographic isolation remain a matter of debate. Some of these conditions have been addressed in several recent studies, including the number of loci determining the trait under disruptive selection (e.g. Bolnick, 2004; Gourbiere, 2004; Bürger and Schneider, 2006; Bürger *et al.*, 2006; Rettelbach *et al.*, 2011), the strength of assortative mating (e.g. Kirkpatrick and Nuismer, 2004; Doebeli *et al.*, 2007; Otto *et al.*, 2008), and the cost of choosiness (e.g. Matessi *et al.*, 2002; Bürger and Schneider, 2006; Schneider and Bürger, 2006; Kopp and Hermisson 2008; Otto *et al.*, 2008).

The number of loci determining phenotypic traits directly affects the phenotypic resolution at which these traits can be expressed: a larger number of loci result in a larger number of possible phenotypic classes. This interferes with the competition strength between individuals (Bürger *et al.*, 2006) and affects the number of mates that fall within a given individual's range of acceptable phenotypes (Bolnick, 2004). It has been shown that the likelihood of speciation decreases when a large number of loci determine the traits under disruptive selection, with speciation then being possible only when the level of assortative mating is high (Gourbiere, 2004; Bürger and Schneider, 2006). Similarly, a large number of loci have been shown to increase the waiting time until sympatric speciation (Dieckmann and Doebeli, 1999, 2004; Bolnick, 2004). However, the opposite effect on the likelihood of speciation has also been reported (Kondrashov and Kondrashov, 1999; Bürger *et al.*, 2006; Rettelbach *et al.*, 2011).

Reproductive isolation in sympatry usually results from a form of assortative mating, which may be pre-established or may evolve simultaneously with divergence in the trait under disruptive selection. In the case of pre-established assortative mating, reproductive isolation is more likely to emerge under a moderate level of assortativity, while very strong assortative mating can in fact act against speciation, by reducing polymorphism and by generating stabilizing sexual selection (Kirkpatrick and Nuismer, 2004; Bürger *et al.*, 2006; Otto *et al.*, 2008). On the other hand, assortative mating might evolve simultaneously with ecological divergence under a complex interplay of natural and sexual selection. It has been established that the evolution of mating preference (from random to assortative) is generally favoured when intermediate phenotypes are less fit (Dieckmann and Doebeli, 1999; Otto *et al.*, 2008; Pennings *et al.*, 2008; Ripa, 2008). It has been reported that if selection against intermediate phenotypes ceases once they are sufficiently rare, evolution of assortative mating might stop at an intermediate level, thus preventing speciation (Matessi *et al.*, 2002; Pennings *et al.*, 2008). In contrast, in a model of secondary contact, an intermediate level of assortative mating has been found to promote maximal trait differentiation (Servedio, 2011). And even though it is widely understood that recombination in sexual populations tends to obstruct adaptive speciation (Maynard Smith, 1966; Felsenstein, 1981), it has also been highlighted that under conditions of frequency-dependent selection recombination kernels of intermediate width can promote ecological diversification and the evolution of assortative mating (Noest, 1997; Doebeli *et al.*, 2007).

Costs of choosiness restrict the number of mating trials per female and/or otherwise decrease the reproductive success of individuals that prefer rare phenotypes. Recent findings confirm the intuitive expectation that when high costs are associated with assortative mating, this can prohibit the latter's evolution, thus reducing the range of conditions under which speciation is possible (Matessi *et al.*, 2002; Bürger and Schneider, 2006; Schneider and Bürger, 2006; Kopp and Hermisson, 2008; Otto *et al.*, 2008). It has also been reported that when the costs of choosiness are incorporated into models of adaptive speciation, waiting times until speciation are prolonged (Bolnick, 2004).

The aforementioned studies considering conditions for non-allopatric speciation do not take into account spatial interactions among individuals, but instead assume that organisms compete and form reproductive pairs irrespective of the relative spatial location of other individuals. However, local interactions are important and inherent to most biological systems, and the spatial distribution of individuals within populations is therefore bound to influence the level of gene flow and the degree of intraspecific competition among the resident phenotypes. Local interactions between individuals are defined by spatial population structure, which broadly speaking can arise in two forms. First, spatial structuring can be induced by environmental heterogeneity. The evolutionary dynamics of populations with environmentally induced spatial structure have been investigated both in metapopulations comprising discrete spatially segregated patches (Gavrilets *et al.*, 1998, 2000; Day, 2001; Gavrilets and Vose, 2005) and along continuous environmental gradients (Endler, 1977; Day, 2000; Doebeli and Dieckmann, 2003, 2004, 2005; Mizera and Meszéna, 2003; Heinz *et al.*, 2009; Payne *et al.*, 2011). Second, if a spatial environment is homogeneous and uniform, the creation and maintenance of spatial structure occurs only through self-structuring. Self-structuring emerges spontaneously as a result of intrinsic ecological dynamics (Lion and van Baalen, 2008), including those that give rise to reproductive pair correlations (Young *et al.*, 2001). For populations with asexual reproduction, it has recently been reported that the coexistence of species, as well as their emergence through evolutionary branching, occurs for more restrictive parameter combinations when modelled on a lattice than when modelled under well-mixed conditions (Mágori *et al.*, 2005).

Here we incorporate sexual reproduction into a model of adaptive speciation and investigate the effect of spatial self-structuring on the waiting time until speciation. In this context, we also investigate the interactions of spatial self-structuring, first, with the effect of the number of loci determining the trait under disruptive selection, and second, with the consequences of mating costs for individuals that prefer rare phenotypes.

METHODS

Model description

Overview

Our individual-based model describes the genotypic and phenotypic evolutionary dynamics of sexual populations. The phenotypic traits of individuals are determined by several loci, which allows for a gradual evolution of resource specialization and mating behaviour. The model is defined in continuous time and continuous space, with periodic boundary conditions in a uniform environment on the unit square. Algorithmically, the model is implemented according to the minimal-process method (Gillespie, 1976).

Individuals

Each individual possesses two phenotypic traits, each of these being determined by two sets of diallelic diploid loci with equal additive effect. The first trait is an ecological character, which controls resource use and thus affects competition. The second trait is a mating preference, which regulates the degree of assortativeness when mating. Each trait is defined by the difference between the number of '+' and '−' alleles, divided by the total number of alleles, so that both traits can vary from −1 to +1. The ecological trait u determines the type of resource or environment to which an individual is best adapted. Specifically, the function

$K(u) = K_0 N_{\sigma_\mathrm{K}}(u)$ describes how u determines an individual's carrying-capacity density, where $N_\sigma(z) = \exp(-\frac{1}{2}\, z^2/\sigma^2)$ and K_0 is the maximally attainable carrying-capacity density. The mating trait a determines the mating preference of individuals, based on similarity in the ecological trait. Mating preference can vary from disassortative ($a < 0$) to assortative ($a > 0$), with random mating occurring for $a = 0$. All individuals in the model are characterized by the rates at which births, deaths, and dispersals occur, as well as by their spatial location (x, y), with $0 \le x, y \le 1$.

Events

All individuals i are assigned birth rates b_i, death rates d_i, and dispersal rates m_i, for $i = 1, \ldots, N$, where N is the current population size. These rates are updated after each event. The time that elapses until the next event is based on the total rates $B = \sum_{i=1}^{N} b_i$, $D = \sum_{i=1}^{N} d_i$, $M = \sum_{i=1}^{N} m_i$, and $E = B + D + M$, being drawn from an exponential probability density with mean $1/E$. The affected individual i for the next event (birth, death, or dispersal) of the process is then chosen with probability $(b_i + d_i + m_i)/E = e_i/E$. The type of event is chosen according to probabilities b_i/e_i, d_i/e_i, and m_i/e_i, respectively. Accordingly, the affected individual will reproduce by giving birth to one offspring, will die, or will perform a dispersal step. Unless stated otherwise, the parameter values we use for model runs are shown in Table 1.

Reproduction

The mating probability between individuals i and j is given by the product of a phenotypic weight p_{ij} and a spatial weight q_{ij} (Doebeli and Dieckmann, 2003). For $a < 0$, the phenotypic weight is defined as $p_{ij} = 1 - N_{\sigma_-}(\Delta u_{ij})$, where $\sigma_- = a^2$, and Δu_{ij} is the phenotypic difference

Table 1. Overview of model parameters

Parameter	Description	Default value
b	Birth rate	1.0
m	Dispersal rate after birth	0.0
σ_c	Phenotypic competition width (= phenotypic standard deviation of competition function)	1.0
σ_s	Spatial competition radius (= spatial standard deviation of competition function)	0.2
σ_K	Phenotypic resource width (= phenotypic standard deviation of resource distribution)	2.0
σ_m	Dispersal radius (= spatial standard deviation of probability density for dispersal distance)	0.01
σ_p	Mating radius (= spatial standard deviation of probability density for mate choice)	0.1
K_0	Maximal carrying-capacity density	500
μ	Mutation probability	0.002
c	Mating cost	0
l_e	Number of loci determining ecological trait	15
l_m	Number of loci determining mating trait	5

between the potential mates i and j. For $a > 0$, $p_{ij} = N_{\sigma_+}(\Delta u_{ij})$, where $\sigma_+ = 1/(20a^2)$. For $a = 0$, $p_{ij} = 1$. The spatial weight q_{ij} decreases with the spatial distance $r_{ij} = \sqrt{\Delta x_{ij}^2 + \Delta y_{ij}^2}$ between potential mates i and j according to $q_{ij} = N_{\sigma_\mathrm{p}}(r_{ij})/(2\pi\sigma_\mathrm{p}^2)$. The offspring inherits alleles from both of its parents at each locus independently, implying free recombination. Random mutations that switch alleles from '+' to '−', and vice versa, occur with a small probability μ. A cost for individuals preferring to mate with locally rare phenotypes arises from a birth rate defined as $b_i = bN_{\mathrm{p},i}/(c + N_{\mathrm{p},i})$, where $N_{\mathrm{p},i} = \sum_{j=1,j\neq i}^{N} p_{ij}q_{ij}$ is the number of suitable mating partners in the neighbourhood of individual i, and c is the strength of the cost.

Death

An individual's death rate depends both on local logistic competition and its carrying-capacity density. Specifically, the death rate of individual i with ecological trait u_i at location (x_i, y_i) is defined as $d_i = [2\pi\sigma_\mathrm{s}^2 K(u_i)]^{-1}\sum_{j=1,j\neq i}^{N} N_{\sigma_\mathrm{c}}(\Delta u_{ij}) N_{\sigma_\mathrm{s}}(\Delta x_{ij}) N_{\sigma_\mathrm{s}}(\Delta y_{ij})$, where the competition function's standard deviations are denoted by σ_c for phenotypic differences and by σ_s for spatial distances.

Dispersal

There are two types of dispersal events. First, each newborn individual undergoes natal dispersal from the location of its mother, i.e. of the parent that has chosen its mate. Second, the subsequent dispersal of all individuals occurs at a constant rate $m_i = m$. In either case, individuals are changing their locations by random displacements in the directions x and y, each drawn from a normal distribution with mean 0 and standard deviation σ_m.

Identification of speciation

To identify speciation, we apply the following criterion. We count the number of individuals for each of the phenotypic classes of the ecological trait (the number of these classes equals twice the number of loci determining the ecological trait plus 1). In the resulting histogram, we identify the two most prevalent phenotypic classes, denoting the corresponding number of individuals by h_1 and h_2, while denoting the total number of individuals in all intermediate phenotypic classes by h_min. We recognize speciation if three conditions are met simultaneously: (i) the two peaks are sufficiently separated, i.e. the phenotypes u_1 and u_2 that correspond to h_1 and h_2 differ by at least 0.5, $|\, u_1 - u_2 \,| \geq 0.5$; (ii) hybrids in between the two peaks are sufficiently rare, i.e. the total number h_min of intermediate individuals is less than 5% of the average of h_1 and h_2, $h_\mathrm{min} < 0.05(h_1 \text{ and } h_2)/2$; and (iii) the heights of the two peaks are sufficiently similar, i.e. h_1 and h_2 differ by a factor of less than 2, $0.5 < h_1/h_2 < 2$. Extensive numerical explorations confirm that this criterion ensures the stability of the phenotypic clusters resulting from speciation, across the full parameter range we investigate: if speciation is recognized, we never observe the subsequent collapse of those phenotypic clusters. We refer to the time at which this criterion is first met as the waiting time T until speciation. To explore stochastic variation in this waiting time, we employ replicate model runs (using different random seeds). We perform these model runs across the parameter range that has previously been identified as allowing for speciation (Dieckmann and Doebeli, 1999, 2004). To ensure that all model runs have enough time to result in speciation, we continued them until a sufficiently long maximal duration (5000 generations).

Identification of the average size of spatial clusters

In our model, spatial self-structuring implies the emergence of spatial clusters that are dynamic and have self-organized shapes and sizes. To measure the average size of these spatial clusters for different degrees of spatial self-structuring, we calculate the pairwise distances r between all individuals of the population. For well-mixed populations in two-dimensional environments, the expected number $C(r)$ of pairs of individuals with distances between r and $r + dr$ for small dr increases linearly with r, so we construct correlation histograms as $c(r) = C(r)/r$. In well-mixed populations, there are no spatial aggregations of individuals, so the corresponding function $c_{\mathrm{m}}(r)$ is flat. In contrast, self-structuring results in the emergence of spatial clusters, so the function $c_{\mathrm{s}}(r)$ shows a peak at small values of r. With increasing r, $c_{\mathrm{s}}(r)$ decreases at a speed proportional to the level of self-structuring, first dropping below and then eventually converging to $c_{\mathrm{m}}(r)$. The drop below $c_{\mathrm{m}}(r)$ corresponds to the empty areas around the spatial clusters. Thus, we identify the average cluster size as the distance at which the function $c_{\mathrm{s}}(r)$ describing a self-structured population intersects with the function $c_{\mathrm{m}}(r)$ for the corresponding well-mixed population (for the latter, we set $\sigma_{\mathrm{m}} = 0.2$). Since the mating radius σ_{p} also influences the size of spatial clusters, we consider different values of σ_{p} for each of the 15 analysed values of σ_{m} ($0.01 \leq \sigma_{\mathrm{m}} \leq 0.08$ and $0.01 \leq \sigma_{\mathrm{p}} \leq 0.1775$; Fig. 2). For each of these 225 combinations of σ_{m} and σ_{p}, we analyse 5000 snapshots of spatial structure. The average cluster size for each σ_{m} is averaged over the considered 15 values of σ_{p}.

RESULTS

Adaptive speciation is faster in self-structured than in well-mixed sexual populations

Figure 1 shows typical results for the joint evolution of resource utilization and mating preference in spatially well-mixed populations and spatially self-structured populations, accompanied by snapshots of the corresponding initial and resulting spatial patterns. Initially, individuals are either randomly distributed in space (Fig. 1a) or aggregated in spatial clusters (Fig. 1d). The evolution of resource utilization starts from monomorphic populations located at the resource optimum (Figs. 1b and 1e, top panels). The mating preference first gradually changes from random to slightly assortative (Figs. 1b and 1e, bottom panels); this reduces gene flow and allows for diversification of the ecological trait, with two phenotypic clusters emerging (Figs. 1b and 1e, top panels). The degree of assortative mating eventually becomes stronger, and this allows reproductive isolation to be established between those two phenotypic clusters.

In self-structured populations, assortatively mating individuals limit their partner search to spatial clusters, thus decreasing the probability of recombination between phenotypic morphs occupying different clusters. As some phenotypes that prevail transiently become extinct only after more extreme phenotypes become locally established, the reduced supply of recombinants means that the distribution of phenotypes across phenotypic clusters remains polymorphic for longer periods.

After adaptive speciation, more individuals mate assortatively in self-structured populations (Fig. 1e, bottom panel) than in well-mixed populations (Fig. 1b, bottom panel). Individuals of the two newly formed species are distributed across the whole habitat either randomly (Fig. 1c) or in spatial clusters (Fig. 1f). The resulting mosaic of spatial clusters

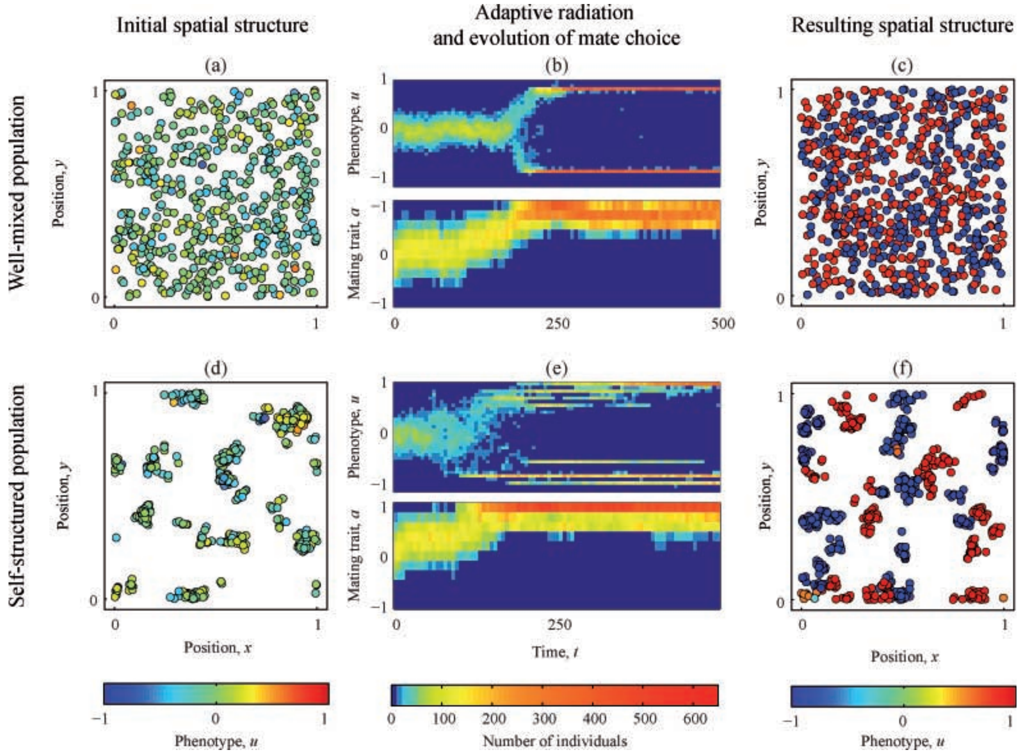

Fig. 1. Comparison of initial spatial structure, evolutionary dynamics of ecological trait and mating trait, and resulting spatial structure in spatially well-mixed ($\sigma_m = 0.08$; a, b, c) and spatially self-structured ($\sigma_m = 0.01$; d, e, f) populations. In the snapshots of spatial structures, taken at times $t = 50$ and $t = 500$, the horizontal and vertical axes measure the spatial position of individuals, while the colour scale indicates the ecological trait u. In the panels showing evolutionary dynamics, the colour scale indicates the number of individuals within the shown phenotypic classes.

is endogenously generated by intrinsic ecological dynamics, even though the considered habitat is continuous and completely homogeneous. Spatial clusters dynamically arise as self-organized entities with characteristic average diameters (see below). The number of individuals inside a cluster depends on the balance between the local birth and death processes (source–sink dynamics). The distance between clusters is defined by the spatial competition radius, and also arises endogenously.

It is noteworthy that inside the spatial clusters of self-structured populations, assortatively mating individuals are likely to encounter appropriate mating partners; this provides conditions for assortative mating ‘for free’, which may in turn be responsible for the higher proportion of individuals mating assortatively, and thus for the earlier speciation in these populations. The next subsection confirms this interpretation.

Optimal ratio of mating radius and dispersal radius promotes early speciation

To understand in greater detail how spatial self-structuring provides conditions for assortative mating ‘for free’, and thus accelerates speciation, we compare waiting times until

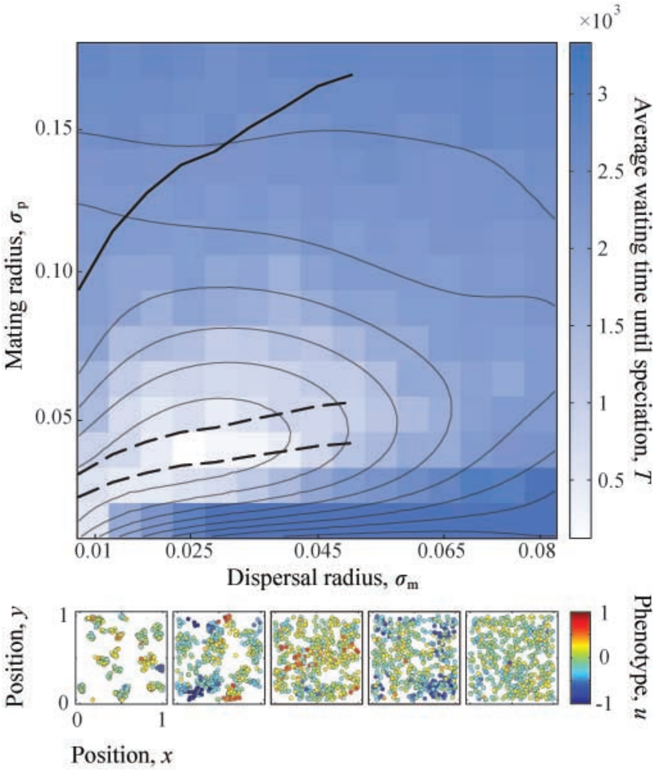

Fig. 2. Dependence of the average waiting time until speciation on the dispersal radius σ_m and on the mating radius σ_p. Each cell shows an average over 100 replicate model runs. The thin grey contour lines are inferred from a polynomial approximation of the data. The thick black curve describes how the average size of spatial clusters varies with the dispersal radius σ_m. Dashed black curves correspond to one-third and one-quarter of this average cluster size. The bottom row shows snapshots of spatial structures, for $\sigma_p = 0.1$ and values of σ_m shown along the main panel's horizontal axis.

speciation for many different combinations of dispersal radius and mating radius. The degree of spatial self-structuring in sexually reproducing populations is determined by both of these parameters. While the dispersal radius directly affects the spatial population structure, the influence of the mating radius is indirect, by defining the spatial area across which mate search occurs: if this area is large, spatial population structure, even if present, has no impact on the availability of phenotypes that can be chosen as mates.

Figure 2 shows the dependence of the average waiting time until speciation on the dispersal radius and the mating radius. Light and dark areas correspond to short and long waiting times until speciation, respectively. In populations with the highest considered level of self-structuring ($\sigma_m = 0.01$), an increase in mating radius delays speciation. For intermediate levels of self-structuring ($0.02 \leq \sigma_m \leq 0.05$), a very small or very large mating radius delays speciation. A further increase in dispersal radius (beyond $\sigma_m = 0.05$) makes the spatial clusters indistinguishable, so the waiting time until speciation is no longer affected.

The thick curve in Fig. 2 shows the average size of spatial clusters for different dispersal radii. Comparing the mating radii enabling the earliest speciation with these sizes of

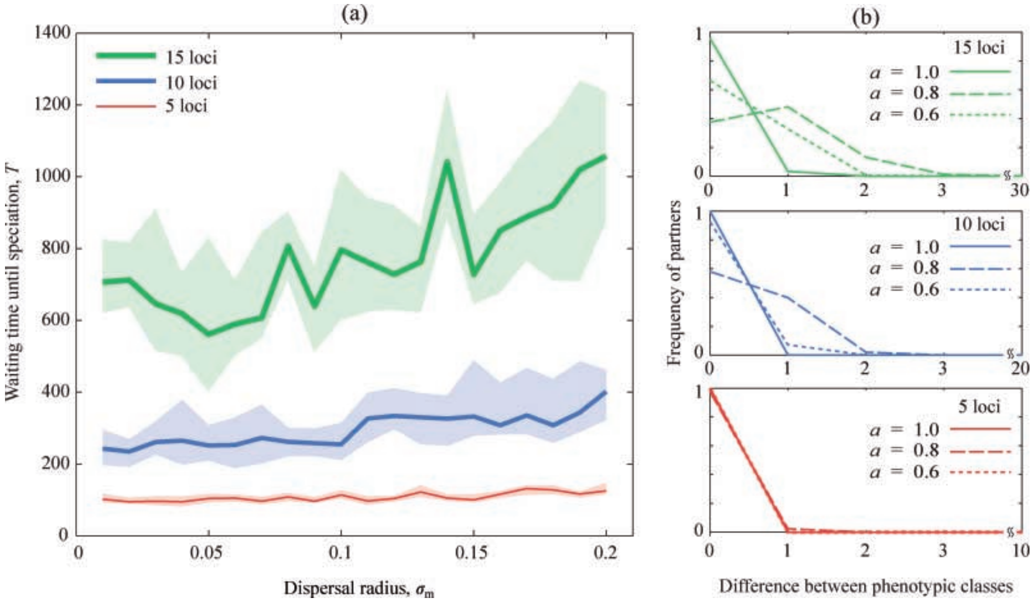

Fig. 3. (a) Dependence of the waiting time until speciation on the level of spatial self-structuring for different numbers of loci determining the ecological trait. The shaded areas extend between the 40% and 60% percentiles of the distribution of waiting times until speciation for 100 replicate model runs, while the curves show the corresponding medians. (b) Corresponding frequencies of mates, according to the difference between the phenotypic classes of mating partners. Other parameters: $\sigma_p = 0.2$ and $K_0 = 800$.

spatial clusters reveals that speciation times are shortest when the mating radius corresponds to one-quarter to one-third of the cluster size, as indicated by the two dashed curves in Fig. 2.

Spatial self-structuring weakens the effect of a large number of loci

Figure 3 shows that increasing the number of loci determining the ecological trait delays speciation. As we explain below, this delay is caused by the diminished level of strict assortative mating when a large number of loci result in a higher resolution of the phenotypes that can be expressed for the ecological trait.

For a small number of loci, assortative mate choice becomes virtually restricted to partners with identical phenotypes (Fig. 3b, panel for 5 loci), whereas for a large number of loci, the same degree of assortativity (as measured by the mating trait a) leads to mating individuals accepting mates from a larger number of phenotypic classes (Fig. 3b, panels for 10 and 15 loci). This occurs because mating probabilities are a function of the absolute phenotypic difference between potential partners. Therefore, if a large number of loci determine the ecological trait, the relative proportion of strictly assortative mating is smaller. This decreases the probability of alleles increasing assortativity spreading in the populations, and thereby delays speciation.

Importantly, we not only find that in self-structured populations the waiting time until speciation is shorter (Figs. 1 and 2), but also that this effect of spatial self-structuring

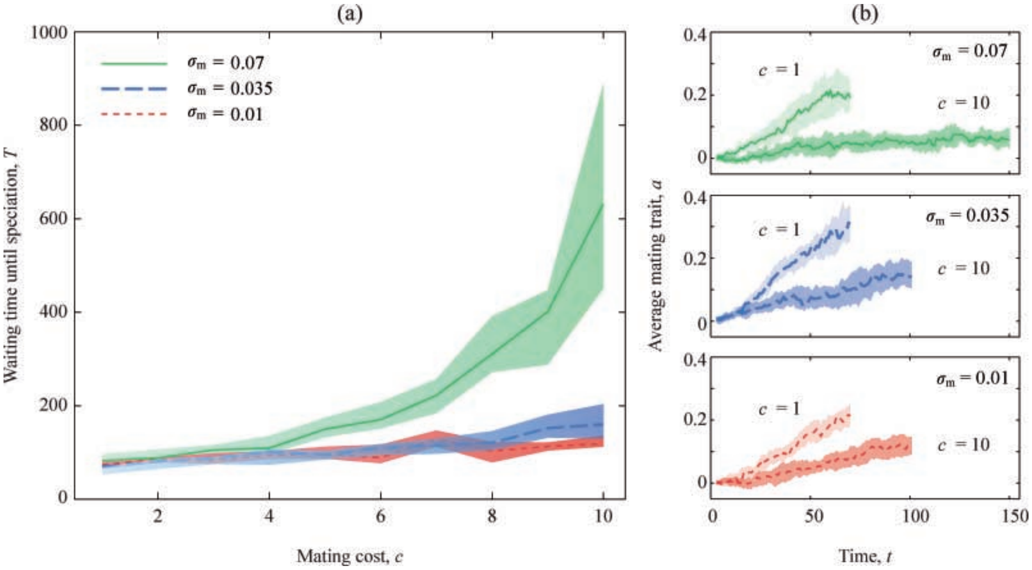

Fig. 4. (a) Dependence of the waiting time until speciation on the mating cost *c* for well-mixed ($\sigma_m = 0.07$), intermediately self-structured ($\sigma_m = 0.035$), and highly self-structured ($\sigma_m = 0.01$) populations. The shaded areas extend between the 40% and 60% percentiles of the distribution of waiting times until speciation for 100 replicate model runs, while the curves show the corresponding medians. (b) Corresponding evolution of the average mating trait *a*; time series end when reaching the average waiting time until speciation. Other parameters: $l_e = 5$.

becomes more noticeable with an increase in the number of loci determining the ecological trait. This suggests that in such populations the aforementioned effect of assortative mating 'for free' is increasingly important for promoting the establishment of assortative mate choice and for accelerating speciation, by providing an alternative mechanism for enhancing the relative proportion of strictly assortative mating. This explains why for a small number of loci the effect of spatial self-structuring is negligible, because strictly assortative mating is facilitated by the resultant low phenotypic resolution, so that speciation in this case occurs very quickly.

Spatial self-structuring renders mating costs less severe for rare phenotypes

Figure 4a shows the influence of the mating cost on the average waiting time until speciation. We find that in well-mixed populations ($\sigma_m = 0.07$), an increase in the mating cost for individuals that prefer rare phenotypes delays speciation. In contrast, in highly self-structured populations ($\sigma_m = 0.01$), as well as in populations with an intermediate level of spatial self-structuring ($\sigma_m = 0.035$), even a strong mating cost does not cause a significant delay in the average waiting time until speciation.

To find a mechanistic explanation for this observation, we track the evolution of a population's average level of assortative mating. The mean values of mating traits among individuals of populations for different degrees of spatial self-structuring and for different strengths of mating costs are shown in the small panels of Fig. 4b. Both for highly structured populations ($\sigma_m = 0.01$) and for intermediately structured populations

($\sigma_m = 0.035$), the evolution of mate choice proceeds in a similar way, with the average mating trait gradually evolving towards assortative mating. In contrast, in well-mixed populations ($\sigma_m = 0.07$), the average level of assortative mating fluctuates around random mating when the mating cost is strong ($c = 10$). From these observations, we can thus conclude that the mating cost affects the waiting time until speciation by inhibiting the evolution of assortative mating and that this effect can be overcome by the spatial self-structuring of populations.

DISCUSSION

In this study, we have investigated how the waiting time until adaptive speciation in a population with sexual reproduction is influenced by spatial self-structuring. We find that self-structuring generally facilitates the evolution of assortative mating and thus promotes earlier speciation. The main feature of a self-structured population is that individuals inside a spatial cluster tend to possess very similar phenotypes. This feature influences the evolutionary dynamics in several ways. First, it allows for assortative mating 'for free', since individuals typically find phenotypically similar mates inside their spatial clusters (Fig. 2), jump-starting the evolution of assortative mating required for speciation. Second, it allows individuals that prefer rare phenotypes to find mating partners from the same phenotypic class, implying strict assortative mating, even when a large number of loci determine the ecological trait (Fig. 3). Third, spatial self-structuring enables fast speciation even when individuals that prefer rare phenotypes experience additional fitness costs (Fig. 4).

Why an optimal ratio of mating radius and dispersal radius accelerates speciation

We find that waiting times until speciation are shortest when there is a match between the mating radius and the (natal) dispersal radius of individuals (Fig. 2). Our comparison of the mating radius with the average size of spatial clusters suggests that speciation is fastest when the spatial mating radius is 3–4 times smaller than the average size of spatial clusters. This ratio guarantees that even individuals that prefer rare phenotypes find appropriate mates, and thus promotes the evolution of assortative mating. When the mating radius is very small ($\sigma_p = 0.01$), early speciation is only possible in highly self-structured populations.

Our results extend previous findings by Kawata (2002), who studied a spatially explicit model of sympatric speciation and found that the probability of speciation decreases with an increase in both mating area and dispersal radius. Kawata conjectured that an increase in both of these factors increases the dispersal of genes, which promotes recombination and thus homogenizes a population's genetic structure. As a result, it can destroy any association between alleles for ecological adaptation and alleles for assortative mating that might be created by natural selection (Felsenstein, 1981). Our results suggest a different interpretation. While Kawata (2002) investigated the influence of dispersal radius and of the size of the mating area independently from each other, here we have explored the joint effect of these factors on the evolutionary dynamics underlying speciation. We find that the interaction between these two factors is more complex, with our results suggesting that speciation is fastest for a certain ratio between the mating radius and dispersal radius.

Why spatial self-structuring weakens the effect of a large number of loci

Our results show that when the ecological trait is controlled by a large number of loci, the waiting time until speciation is longer (Fig. 3). The mechanism underlying this effect can be described as follows: a large number of loci results in more phenotypic classes, and as mating individuals accept a higher proportion of partners from different phenotypic classes, this hinders the establishment of assortative mating and delays speciation. Our results confirm and extend findings from previous studies in which a delay in speciation was observed resulting from a large number of loci determining the ecological trait (Dieckmann and Doebeli, 1999, 2004; Bolnick, 2004). Earlier, it was shown that (not surprisingly) increasing the phenotypic width of the mating function prolongs the waiting time until speciation (Bolnick, 2004). We find that this effect is weaker in self-structured populations, because appropriate mates are likely to be available in a mating individual's local neighbourhood, which allows those mating individuals to find a large proportion of mates with identical phenotypes.

It has been reported that the likelihood of speciation depends in a 'non-straightforward way' on the number of loci that determine the ecological trait (Bürger *et al.*, 2006). Specifically, Bürger and colleagues found that if disruptive selection is weak, the likelihood of speciation decreases with an increased number of loci. They suggest that, under these conditions, splitting the phenotypic distribution of ecological traits requires the emerging phenotypic clusters in that trait to be located near the boundary of the corresponding phenotypic range, which could be easier to achieve for a smaller number of loci. This is because, under these conditions, the average phenotypic distance between all resident phenotypes is larger, so the average mating probabilities across phenotypic classes are lower. For stronger disruptive selection, speciation is possible only with strong assortative mating, and speciation occurs more readily with more loci, since the self-organized fine-tuning of the evolutionary dynamics helps to keep phenotypic clusters at the optimal distance for coexistence. In our model, increasing the number of loci invariably results in delayed speciation. This is because we mostly consider relatively weak disruptive selection, which results in phenotypic clusters always being located at the boundary of the phenotypic range. When disruptive selection is strong, we also observe the emergence of more than two phenotypic clusters when ecological traits are determined by more than 15 loci. In such cases, evolutionary dynamics are more complex than those underlying the emergence of two species, and will benefit from additional investigation.

Why spatial self-structuring reduces mating costs for rare phenotypes

Our results confirm that high mating costs increase the waiting time until speciation in well-mixed populations (Fig. 4a), as mating individuals that prefer rare phenotypes are less likely to find appropriate mates. In well-mixed populations, potential mates for individuals with rare phenotypes will usually be located at a significant spatial distance from those individuals seeking a partner, so the mating cost reduces their chance to reproduce. This delays the evolution of assortative mating, which causes a longer waiting time until speciation (Fig. 3b). Conversely, in self-structured populations, individuals possessing similar phenotypes form spatial clusters: as mating individuals are then more likely to find appropriate mates in their local neighbourhood, the effect of mating cost is largely cancelled out.

Here we have modelled mating costs phenomenologically for individuals that prefer (locally) rare phenotypes, similar to Doebeli and Dieckmann (2003) and Gourbiere (2004). Other studies have examined models of sympatric speciation in which costs for choosy individuals are modelled more mechanistically, resulting from a restriction of their number of mating trials (Drossel and McKane, 2000; Doebeli and Dieckmann, 2005; Bürger and Schneider, 2006; Bürger *et al.*, 2006; Schneider and Bürger, 2006; Kopp and Hermisson, 2008). We expect the effect of spatial self-structuring on speciation readily to extend to those later models.

Comparison with other speciation modes

Throughout this article, we have referred to the examined diversification dynamics as adaptive speciation. This is because, in our model, the speciation process can be understood as an adaptive response that allows a population trapped at a fitness minimum through the action of frequency-dependent disruptive selection to escape from this trap (Dieckmann *et al.*, 2004).

To further contextualize our findings, it might be worthwhile highlighting that the speciation processes analysed here also meet the specifications of competitive speciation [which occurs when 'intermediate forms [are] fit if and only if some extreme forms are rare or absent' (Rosenzweig, 1978)] and of ecological speciation [defined as the 'evolution of reproductive isolation between populations as a result of ecologically-based divergent natural selection' (Schluter, 2000; Schluter and Conte, 2009)].

In contrast to the aforementioned three process-based speciation modes of adaptive, competitive, and ecological speciation, traditional discussions of alternative speciation routes have instead focused on geographical patterns at the onset of species formation (e.g. Mayr, 1942, 1963; Dobzhansky, 1951). While the well-mixed populations we have analysed here, by considering large radii for dispersal and mating, are essentially sympatric, smaller such radii result in ecological settings traditionally explored in the context of parapatric speciation scenarios, with the role of isolation by distance (Wright, 1943) increasing as those radii become smaller relative to the average distance between neighbouring individuals and to the spatial scale of the considered habitat.

Last but not least, the speciation dynamics we have examined here are related to the notions of micro-allopatric speciation (Smith, 1955, 1965) and mosaic sympatry (Mallet, 2008; Mallet *et al.*, 2009). Both terms are used to refer to spatial patterns in which species can be viewed as coexisting sympatrically when assessed at larger spatial scales, yet are recognized as being spatially segregated when assessed at smaller spatial scales. This description fully matches the spatial patterns resulting from self-structuring in our model, which could be taken to suggest that both terms apply to our study. It must be borne in mind, however, that micro-allopatry and mosaic sympatry are meant to arise from a heterogeneous external environment to which the coexisting species differentially latch on through habitat choice or habitat-dependent reproductive success, whereas the small-scale spatial segregation between the co-existing species observed in our model arises in a homogeneous external environment through limited dispersal and phenotype-dependent local competition. Consequently, the spatial patterns emerging in our model should not be misunderstood as examples of either micro-allopatry or mosaic sympatry.

Comparison with related studies and extensions

While our results show that spatial self-structuring accelerates speciation in sexual populations, in populations with asexual reproduction the opposite effect has been found. Specifically, Day (2001) reported that limited dispersal in deme-structured metapopulations inhibits disruptive selection, because mutants rarely gain a fitness benefit when surrounded by very similar phenotypes. Mágori *et al.* (2005) investigated the coexistence of species, and their emergence through evolutionary branching, on a lattice and found that both of these occur only for more restrictive parameter combinations than found in well-mixed populations. Also, this latter result was explained by the reduced fitness advantage of rare mutant phenotypes.

To analyse the effects of spatial self-structuring on evolutionary branching in asexual populations, we can readily eliminate sexual reproduction and assortative mate choice from our model. Our corresponding investigations confirm the aforementioned findings of Day (2001) and Mágori *et al.* (2005), as well as the mechanism conjectured by those authors to underlie the observed delay of adaptive speciation. Going beyond those previous studies, we find that an additional mechanism contributes to the observed delay: in self-structured asexual populations, common phenotypes, being situated at the fitness minimum causing disruptive selection, escape extinction for longer durations than in well-mixed populations, due to their local coexistence with different phenotypes in spatial clusters (V. Fazalova and U. Dieckmann, submitted).

In sexual populations, by contrast, the two aforementioned delaying effects of spatial self-structuring arising from natural selection are overshadowed by the consequences of sexual selection: assortatively mating rare phenotypes gain an extra fitness benefit from co-occurring with similar phenotypes, while assortatively mating common phenotypes incur an extra fitness cost from co-occurring with other phenotypes.

In the present study, spatial self-structuring arises from limited offspring dispersal. The resultant spatio-phenotypic correlations facilitate the evolution of assortative mating, in turn promoting faster adaptive speciation. Analogous conditions favouring assortative mating may instead be generated through, or further enhanced by, other mechanisms, such as dispersal with philopatry, dispersal with natal homing, conditional dispersal triggered by phenotype-based quorum sensing, and/or dispersal concluding with habitat choice. All of these alternative or additional mechanisms – being widespread among animal species and occurring even for microorganisms – result in the kind of spatio-phenotypic correlations emerging in our model analysed here, and can thus be expected likewise to facilitate and accelerate adaptive speciation.

It also needs to be highlighted that spatial self-structuring, by increasing the mating frequency among relatives, can sometimes result in inbreeding depression. Hence, an interesting extension of our model would be to examine possible costs and benefits of inbreeding, and to ascertain their impacts on the waiting times until adaptive speciation.

While we have focused our analyses here on competition for a unimodal resource, we expect spatial self-structuring to promote adaptive speciation also in scenarios with bimodal or multi-modal resource distributions (e.g. Doebeli, 1996; Thibert-Plante and Hendry, 2011). For non-unimodal resource distributions, the inhibiting effect of stabilizing selection on adaptive diversification might be even weaker, and the resource distributions' intrinsic minima may further facilitate the evolution of assortative mating. In future studies, it would therefore be interesting to analyse interactions between the effects of non-unimodal resource distributions and spatial self-structuring in models of adaptive speciation.

CONCLUSIONS

The role of spatial self-structuring for adaptive speciation is complex. On the one hand, it delays adaptive speciation in populations with asexual reproduction (V. Fazalova and U. Dieckmann, submitted). On the other hand, as demonstrated in this study, self-structuring facilitates and accelerates speciation in sexually reproducing populations: this occurs by allowing for assortative mating 'for free', by reducing the effect of a large number of loci on the probability of strict assortative mating, and by cancelling out costs for assortative mating. Our results suggest that a very high level of spatial self-structuring is not necessary for fast speciation; intermediate levels can suffice, and are sometimes even optimal for accelerating speciation in sexual populations.

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