Divergence and Evolution of Assortative Mating in a Polygenic Trait Model of Speciation with Gene Flow

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Abstract

Assortative mating is an important driver of speciation in populations with gene flow and is predicted to evolve under certain conditions in few-locus models. However, the evolution of assortment is less understood for mating based on quantitative traits, which are often characterized by high genetic variability and extensive linkage disequilibrium between trait loci. We explore this scenario for a two-deme model with migration, by considering a single polygenic trait subject to divergent viability selection across demes, as well as assortative mating and sexual selection within demes, and investigate how trait divergence is shaped by various evolutionary forces. Our analysis reveals the existence of sharp thresholds of assortment strength, at which divergence increases dramatically. We also study the evolution of assortment via invasion of modifiers of mate discrimination and show that the evolutionarily stable assortment strength has an intermediate value under a range of migration-selection parameters, even in diverged populations, due to subtle effects which depend sensitively on the extent of phenotypic variation within these populations. The evolutionary dynamics of the polygenic trait is studied using the hypergeometric and infinitesimal models. We further investigate the sensitivity of
our results to the assumptions of the hypergeometric model, using individual-based simulations.

The extent of gene flow between diverging populations and its implications for speciation have been extensively investigated in both empirical and theoretical studies (Dobzhansky 1940; Felsenstein 1981; Neimiller et al. 1997; Servedio and Kirkpatrick 1997; Wang et al. 1997; Kirkpatrick 2000; Servedio 2000; van Doorn et al. 2000; Servedio and Noor 2003; Coyne and Orr 2004; Gavrilets 2004; Hey 2006; Bolnick and Fitzpatrick 2007; Servedio 2011). A typical scenario involves divergence of two populations in allopatry followed by secondary contact; selection against the resultant, possibly inviable, hybrids can spur the reinforcement of prezygotic mating preferences, leading to complete reproductive isolation and the emergence of ‘good species’ (Dobzhansky 1940; Servedio and Noor 2003; Coyne and Orr 2004). Alternatively, divergence may occur in the face of continuous gene flow even without an initial allopatric phase, if populations face divergent selection due to ecological heterogeneity, competition and/or selective mating (Bolnick and Fitzpatrick 2007). Prezygotic isolation is in this case both a driver of initial divergence, and may itself be selected for or against as divergence increases.

In this paper, we focus on the latter case of parapatric populations with ongoing migration and ask: How do the competing forces of divergent selection and homogenizing gene flow shape the evolution of prezygotic isolation and resultant divergence levels between populations, when the traits under natural and sexual selection are highly polygenic?

In considering this question, it is useful to distinguish between two scenarios. Reinforcement may occur via the divergence of an assortment trait between populations, on a timescale for which the strength of assortment is assumed fixed. Here, strength of assortment refers to female ‘choosiness’ or the the extent to which females discriminate between similar and dissimilar males. Alternatively, if there is heritable variation in the degree of mate discrimination, as observed in several natural populations (Butlin 1993;
Ortiz-Barrientos and Noor (2005), then the assortment strength may itself evolve due to direct or indirect selection. Reinforcement, in this case, involves co-evolution of the degree of discrimination with the assortment traits on which it acts. These two views of reinforcement are complementary—the ‘established assortment’ model is useful in surveying possible outcomes, while the ‘evolving assortment’ model elucidates whether outcomes are evolutionary attractors, i.e., if long-term evolution over a higher-dimensional trait space is likely to converge to them.

Both established and evolving assortment scenarios have been studied extensively using Adaptive Dynamics (AD) and in models with one or two (or very few) loci under disruptive selection (Felsenstein 1981; Kelly and Noor 1996; Servedio 2000; Matessi et al. 2001; Pennings et al. 2008; Ripa 2009; Servedio 2011; Rettelbach et al. 2013). These models are often chosen for their analytical tractability and can disentangle the roles of different evolutionary processes during divergence in a simple setting. However, many putative assortment traits, such as body size, beak length or display traits such as colorful plumage may be highly polygenic and differ from oligogenic traits in two key ways.

First, polygenic traits harbour substantial genetic variation in spite of being under stabilizing selection (Barton and Keightley 2002) and typically exhibit a continuous range of phenotypes. Frequency-dependent selection acts on this continuous variation very differently from how it acts on few-locus traits, with divergence in the latter case sometimes arising only as an artefact of the small number of accessible phenotypes (Polechová and Barton 2005). Moreover, as we argue in this paper, even within diverged populations, the extent of genetic variation and the frequency of atypical, ‘outlier’ phenotypes can qualitatively impact whether these populations evolve complete reproductive isolation.

A second distinctive feature of polygenic traits is that the response of their distribution to selection is driven primarily by changes in associations or linkage disequilibria
(LD) between loci (Bulmer 1980). Assortative mating, especially, generates strong LD
(Felsenstein 1981; Barton and de Cara 2009), which inflates trait variance. For highly
polygenic traits, this LD-driven increase in variance can be stronger and more rapid than
loss of variation due to sexual selection (Kirkpatrick and Nuismer 2004; Bürger and
Schneider 2006). In fact, we find that the buildup of LD across loci triggers synergistic
changes in allele frequencies, resulting in a steep increase in divergence between the two
populations beyond a threshold assortment strength, akin to a speciation event.

To clarify shared features as well as key differences between assortment based on highly
polygenic traits versus assortment based on similarity at a few loci, we consider a well-
studied ‘magic trait’ scenario of speciation (Gavrilets 2004; Servedio et al 2011), wherein
two initially identical populations with ongoing gene flow express a continuous trait that
is subject to divergent viability selection across demes and is also the basis of assorta-
tive mating by female choice, which generates sexual selection on males. We focus on
the following questions: First, are there general conditions on the strengths of selec-
tion, migration and assortment for which polygenic traits diverge? In particular, what
role does assortative mating play in generating divergence? Second, when assortment
strength can evolve through the invasion of modifiers of mate discrimination, is there
an evolutionarily stable (ES) level of assortment? Is it sufficient to produce divergence
and eventually complete reproductive isolation? Third, under what conditions is genetic
variation maintained within demes, and how does the extent of variation affect modifier
evolution?

In considering the last question, it is important to distinguish between genetic (and
phenotypic) variation that exists in populations before the onset of divergent selection
(for instance due to migration or frequency-dependent or fluctuating selection in the past)
and variation that is dynamically maintained during divergence by de novo mutation or
gene flow between demes. Here, we take the initial phenotypic variance as a parameter,
but assume that it is not so low as to inhibit a response to selection. In principle,
initial variation may be depleted by stabilizing selection within each deme, but for highly polygenic traits, this occurs more slowly than the changes in trait mean involved in divergence. Further, even for traits determined by a moderate number of loci, variation may be replenished by the influx of genetically dissimilar individuals. In order to clarify when stable variation is maintained simply by gene flow, we mostly study the model with no mutation. The effects of mutation are discussed in Appendix S6.

It is also useful to contextualize the model within the main themes emerging from other theoretical models of prezygotic isolation and divergence (Kirkpatrick and Ravigne 2002). A crucial determinant of prezygotic isolation is whether the isolating mechanism has a one-allele or two-allele basis (Felsenstein 1981). One-allele mechanisms, e.g., those involving the spread of modifiers that increase habitat preference or mate discrimination, are not hindered by migration or recombination, as they require substitution of the same allele in both populations. By contrast, two-allele mechanisms, e.g., those involving divergence of sexual display or assortment traits, require different alleles to be maintained in incipient species (possibly at multiple loci), and are unlikely to evolve with high gene flow. However, many plausible scenarios of reinforcement have both one and two-allele components (Kirkpatrick and Ravigne 2002; Servedio and Noor 2003). For instance, in our model, while isolation increases through substitution of modifiers that increase mate discrimination (one-allele mechanism), it also requires the emergence of distinct phenotypes in each deme (which has a two-allele basis, in that different alleles must be maintained in the two populations at several trait loci). Moreover, migration influences these two components in opposite directions, with high migration promoting hybridization and making it harder for distinct phenotypes to emerge, while also increasing the tendency of populations to evolve stronger discrimination that reduces hybridization. We explore the dual role of migration in assortment evolution subsequently.

While populations can split purely due to strong assortment under certain special conditions (Kondrashov and Shpak 1998), divergence is greatly facilitated if the as-
sortment trait is a ‘magic trait’ under direct disruptive selection (Servedio et al. 2011), which leads to a strong coupling between postzygotic and prezygotic isolation. Here, we consider a magic assortment trait subject to both viability and sexual selection, and demonstrate how these two components of direct selection can drive mate discrimination antagonistically—an effect also observed in few-locus models (Kelly and Noor 1996; Matessi et al. 2001; Kirkpatrick and Nuismer 2004).

Even with direct selection on the assortment trait, selection on modifiers of assortment may be indirect, e.g., when it is due to linkage disequilibrium between the modifier locus and assortment trait loci. Direct selection on modifiers arises if choice is ‘costly’, for instance, if more discriminating females suffer reduced mating opportunities. Such costs, unless very minor, inhibit the evolution of mate discrimination (Kopp and Hermisson 2008; Otto et al. 2008) and are excluded from the model.

The model

Our model assumes two demes, in which haploid organisms undergo viability selection towards distinct optima in each deme, followed by migration between demes, and finally assortative mating within each deme, driven by female preference for phenotypically similar males. We consider a scenario especially favourable to speciation, namely, where the phenotype \( X \), expressed in both sexes, simultaneously affects viability and assortment. The phenotypic distributions in the two demes are assumed to be initially identical and Gaussian (with mean \( X_0 \) and variance \( V_0 \)), but evolve differently over time due to divergent selection.

Generations are assumed to be discrete and non-overlapping. In each generation, populations first undergo stabilizing selection with fitness \( W_i(X) = \exp \left( -\frac{(X - \mu_i)^2}{2V_s} \right) \) for deme \( i \). Density is regulated independently in each deme (‘soft selection’). Selection is strongly divergent across the two demes when the difference between the optima \( \mu_1 \) and
\[ \mu_2 \text{ is large, and the strength of stabilizing selection (} \sim 1/V_{s1}, 1/V_{s2} \text{) high. Selection is followed by migration, where a fraction } m_{ij} \text{ of the population of deme } i \text{ is replaced by migrants from deme } j. \]

After migration, each population mates assortatively, followed by free recombination. Assortment is based on female choice, with females preferentially mating with males within a phenotypic range \( \alpha \). We consider a Gaussian preference function: the probability of mating, given an encounter between a female with phenotype \( Y \) and a male with phenotype \( Z \) is proportional to \( \exp[-(Y - Z)^2/2\alpha^2] \), where \( \alpha \) is the preference range of the female, and \( 1/\alpha^2 \) represents the degree of mate discrimination. If all females have the same preference range, then \( 1/\alpha^2 \) also represents the strength of assortative mating in the population. Each female, irrespective of phenotype, has the same probability of mating, but males with common phenotypes have a mating advantage, resulting in sexual selection on males. Population census is carried out after mating and recombination to obtain the distribution \( P(X) \) of phenotypes.

The preference range \( \alpha \) is determined by a single unlinked locus which is present in both sexes, and can be inherited from either parent. However, strength of preference is expressed only by females. In the established assortment case, a single allele with preference range \( \alpha \) is fixed at this locus, while in the evolving assortment scenario, alleles with preference ranges \( \alpha_1, \alpha_2, \ldots \) segregate.

The magic trait \( X \) is determined additively by \( L \) autosomal, haploid, unlinked, diallelic loci. Allelic effects at each locus are assumed to be identical, and chosen to ensure that the typical segregation variance, i.e., the phenotypic variance of offspring of parents near the center of the phenotypic range is 1 in the large \( L \) limit (Appendix S1); then, the phenotypic range extends from \( -\sqrt{2L} \) to \( \sqrt{2L} \). Further, all phenotypic ‘distances’ such as \( \mu, \sqrt{V_s}, \sqrt{V_0} \) and \( \alpha \) are specified in units of this segregation variance, which can be easily measured in populations.
We study the evolutionary dynamics of the trait $X$ using the hypergeometric model (HM) which assumes that all genotypes corresponding to any phenotype are represented equally in the population (‘symmetry assumption’, details in Appendix S1), resulting in all trait loci being polymorphic with allele frequencies equal to $1/2$ for $X=0$ (Kondrashov 1984; Barton 1992; Doebeli 1996). In the large $L$ limit, our results are also recovered from the infinitesimal model (Bulmer 1980), which makes the less restrictive assumption of a constant, non-zero segregation variance (which nevertheless requires high genetic polymorphism). The infinitesimal model encompasses a wider class of genetic architectures and also describes traits determined by many loci of unequal effects with weak, random epistasis (Barton et al. 2016).

A limitation of this approach is that small deviations from the symmetry assumption can be amplified by stabilizing selection, resulting in much less genetic variation than predicted by the HM (Barton and Shpak 2000). To test the stability of HM predictions, we perform individual-based simulations of finite populations, for which deviations from symmetry assumptions arise simply due to drift. To suppress other confounding effects of genetic drift (for instance, in small populations, where it may swamp weak, indirect selection on modifiers), we simulate very large populations ($N\sim10^6$), for which changes due to the intrinsic instability of the HM are expected to dominate over stochastic fluctuations due to drift.

Individual-based simulations are initialized by assigning to each individual in the two demes a phenotype $X$ drawn from a Gaussian distribution with mean $X_0$ and variance $V_0$, and a uniformly distributed genotype corresponding to this phenotype. Selection is implemented by drawing $N$ individuals in each deme (with replacement) from the previous generation with probability proportional to their fitness. Subsequently, a fraction $m_{12}$ of individuals in deme 1 is replaced by randomly chosen individuals from deme 2 and vice versa. Assortative mating is implemented by choosing a female at random, and then iteratively drawing males (allowing for mating with probability equal to the Gaussian
preference function) until mating is successful. The offspring genotype has loci drawn with equal probability from either parent. This procedure is repeated until $N$ offspring are created. Simulations are run for $2-5 \times 10^4$ generations to test for deviations from the HM, which emerge slowly.

Most of our analysis deals with a highly symmetric scenario with reciprocal migration between demes ($m_{12}=m_{21}=m$), and equally strong selection ($V_{s1}=V_{s2}=V_s$) on the two populations towards optima with $\mu_1=-\mu_2=\mu$, which are symmetric about $X=0$. We explore both the established and evolving assortment scenarios for the symmetric model in detail, and then briefly comment on versions with asymmetric gene flow (see Appendix S7).

Established assortment

With established assortment, every female has the same preference range $\alpha$. Starting with identical Gaussian phenotypic distributions with mean $X_0=0$ and low initial variance ($\sqrt{V_0} \ll \mu$), the two populations evolve under divergent selection, migration and assortative mating (see Appendix S1), until a long-term steady state is reached (see Appendix S2 for a discussion of alternative initial conditions). We first characterize how divergence between populations in this long-term state depends on various evolutionary parameters under HM assumptions.

In general, strongly divergent selection (low $V_s$, high $\mu$) facilitates local adaptation while strong migration (high $m$) tends to create homogenized, generalist populations. In an intermediate selection regime, where these two opposing forces are comparable in magnitude, assortment plays a crucial role. An increase in assortment strength, i.e., a decrease in $\alpha$, has two somewhat contrary effects—first, it reduces the mating success of rare, outlier males by creating positive frequency-dependent sexual selection (especially at intermediate $\alpha$); second, it leads to a stronger correlation between male and female
Figure 1: (a) Long-term phenotypic distributions $P(X)$ vs. $X$ for a single deme with optimum at $+\mu$, for various values of $\alpha$ (HM predictions). The unimodal distribution becomes broader as $\alpha$ decreases and switches to a bimodal distribution at a threshold preference range $\alpha_c/2\mu$, here approximately 0.254. The bimodal distribution has clearly differentiated peaks at $+\mu$ and $-\mu$ corresponding respectively to diverged resident and migrant phenotypes, and may also have a small number of hybrids at $X=0$ (not visible on this plot), depending on the value of $\alpha_c$. (b) Various statistics of the population (as predicted by the HM) vs. relative width ($\alpha/2\mu$) of preference function. Statistics include (i) trait divergence measured as the relative difference between the trait means ($X_1$ and $X_2$) of the two demes (ii) variance of the phenotypic distribution in a deme (iii) variance due to LD (iv) hybridization rate. All statistics exhibit a sharp change at $\alpha=\alpha_c$. (c) Allele frequency vs. time for randomly chosen loci in individual-based simulations for a population near the divergence threshold ($\alpha\sim\alpha_c$). Allele frequencies increase synergistically over a short period of time, resulting in a sharp increase in divergence and the emergence of bimodal $P(X)$.
phenotypes within each mating pair—thus when outlier males do mate, they mate primarily with outlier females and produce outlier offspring. This increased correlation builds up LD between loci, increasing the variance of the unimodal trait distribution as well as its skew towards the optimum (fig. 1a), in spite of sexual selection against outlier phenotypes. This, in turn, leads to a stronger response to natural selection; in fact at a critical preference range $\alpha_c$, the LD becomes high enough for selection to drive synergistic changes in allele frequencies across all loci (fig. 1c), causing the mean phenotype to shift towards the selection optimum of the deme. Thus populations with $\alpha<\alpha_c$ have clearly distinguishable resident and migrant phenotypes in each deme (represented by the two peaks of the bimodal distribution in fig. 1a), along with a small fraction of hybrids.

The qualitative change in the phenotypic distribution at $\alpha=\alpha_c$ manifests itself as a sharp increase in the divergence, defined as the difference between mean trait values in the two demes, as well as in the trait variance within each deme (fig. 1b, also fig. 2a). The divergence in figs. 1b and 2a is scaled by $2\mu$, which is the maximum divergence possible (with zero migration), while the variance is scaled by $\mu^2$. The increase in variance at $\alpha_c$ is due to an increase in the disequilibrium component of the variance (see fig. 1b), which is just the pairwise LD summed over all pairs of loci. Elevated genome-wide LD and variance simply reflect the coexistence of diverged residents and migrants within each deme. Note also the corresponding drop in the rate of hybridization $H$ at $\alpha_c$, where $H$ is defined as the fraction of individuals in a deme produced by resident-migrant pairings in each generation ($H=2m(1-m)$ in a randomly mating population).

In the following, we refer to populations with bimodal phenotypic distributions within demes (having $\alpha<\alpha_c$) as diverged, and populations with unimodal distributions ($\alpha>\alpha_c$) as hybridized (even though trait means may differ slightly in the latter state). Some degree of gene flow can persist between diverged populations, as evinced by the small number of hybrids in populations with $\alpha<\alpha_c$. Thus divergence, as defined here, represents an important step in the speciation process, but does not necessarily complete reproductive
isolation. We refer to $\alpha_c$, the preference range at which phenotypic distributions become bimodal, as the preference threshold for divergence, and typically specify it as the ratio $\alpha_c/2\mu$, thus indicating how narrow preferences must be relative to the phenotypic distance between selection optima, for divergence to occur. Alternatively, we can specify the threshold assortment strength $(\alpha_c/2\mu)^{-2}$.

Note that $\alpha_c$ decreases as selection becomes weaker or migration stronger (fig. 2c), pointing towards the high levels of assortment required for divergence under these conditions. We also develop a Gaussian approximation for the infinitesimal model (Appendix S4) and find that this predicts the divergence threshold very well, especially for moderate selection (fig. 2c).

In addition to selection and migration parameters, $\alpha_c$ also depends on the initial phenotypic variance $V_0$ of the populations (fig. 2d). With no selection or assortment, $V_0$ rapidly equilibrates to twice the segregation variance, but diversifying selection, assortative mating and/or a history of secondary contact can cause it to differ significantly from this value; we thus treat $V_0$ as a parameter which encapsulates population history.

First consider populations with mean phenotype $X \sim 0$ and $\sqrt{V_0}/\mu \ll 1$. Such populations are unlikely to include the optimal phenotype at $t=0$, and divergence, if it occurs, is preceded by a gradual buildup of variance via strong assortative mating. On the other hand, for $\sqrt{V_0}/\mu \gg 1$, optimal phenotypes are present in the populations at the outset, irrespective of assortment level (as would be natural for populations that have just come into secondary contact after an allopatric phase). This results in an initial divergence, which is eroded subsequently due to continued migration and hybridization if assortative mating is weak. Crucially, stronger assortment is required to create divergence in unimodal populations than to prevent hybridization among diverged populations, as also noted in Kondrashov and Shpak (1998). Thus for assortment strengths which lie within the rising part of the $\alpha_c$ vs. $\sqrt{V_0}/\mu$ curve (fig. 2d), divergence is possible if $V_0$ is high and optimal phenotypes already present (i.e., for $V_0$ to the right of the $\alpha_c$ vs. $\sqrt{V_0}/\mu$ curve).
Divergence level \(\frac{X_2 - X_1}{\mu}\) for divergence

Preference threshold (\(\alpha_{c}/2\mu\)) for divergence

Migration fraction \(m\)

Selection thresholds \(\sqrt{V_s}/\mu\) and \(\sqrt{V_s}/\mu\) for migration

Strong selection regime: divergence for all \(\alpha\)

Intermediate selection regime: divergence for \(\alpha<\alpha_{c}\)

Weak selection regime: No divergence for any \(\alpha\)

Selection-migration parameters corresponding to the three selection regimes (HM predictions): Populations are always bimodal (or trimodal) for strong selection (for \(V_s\) below the \(V_s^{SS}\) threshold) and always unimodal for weak selection (for \(V_s>V_s^{WS}\), irrespective of \(\alpha\). For \(V_s^{SS}<V_s<V_s^{WS}\), phenotypic distributions shift from unimodal to bimodal at \(\alpha=\alpha_{c}\).

(c) Preference threshold \(\alpha_{c}/2\mu\) vs. migration rate \(m\): Predictions for \(\alpha_{c}\) from a Gaussian approximation of the infinitesimal model (lines) are in good agreement with HM predictions (points).

(d) Preference threshold \(\alpha_{c}/2\mu\) vs. the initial phenotypic variance \(V_0\) of populations (HM predictions): Stronger assortment is required for divergence (lower \(\alpha_{c}\)) when initial variance is low.

Figure 2: (a) Divergence measured as the difference between the trait means of the two demes vs. relative width (\(\alpha/2\mu\)) of preference function, for various \(V_s\). Lines represent HM predictions and points are from individual-based simulations with \(N=10^5\). For intermediate selection (\(\sqrt{V_s}/\mu=0.8, 1.2\)), trait divergence undergoes a sharp drop at a threshold \(\alpha_{c}\), signifying a switch from a bimodal to a unimodal \(P(X)\). For strong selection (\(\sqrt{V_s}/\mu=0.4\)) and weak selection (\(\sqrt{V_s}/\mu=2.5\)), no sharp transitions occur and populations remain diverged and hybridized respectively at all values of \(\alpha\). HM correctly predicts the qualitative state (diverged vs. hybridized) and \(\alpha_{c}\) in individual-based simulations, but not the exact divergence levels.

(b) Selection-migration parameters corresponding to the three selection regimes (HM predictions): Populations are always bimodal (or trimodal) for strong selection (for \(V_s\) below the \(V_s^{SS}\) threshold) and always unimodal for weak selection (for \(V_s>V_s^{WS}\), irrespective of \(\alpha\). For \(V_s^{SS}<V_s<V_s^{WS}\), phenotypic distributions shift from unimodal to bimodal at \(\alpha=\alpha_{c}\).
curve), but cannot be induced in low-$V_0$ populations ($V_0$ to the left of the curve), leading to a bistability, wherein the initial variance determines whether divergence is possible in the long run (see also Appendix S4). This bistability has important consequences for modifier evolution, as discussed later.

In contrast to the intermediate selection regime, divergence levels change very little with assortment strength when selection is much stronger or weaker than migration (fig. 2a). In the strong selection regime, i.e., for $V_s$ smaller than the threshold $V_s^{SS}$ in fig. 2b, the distribution in each deme is bimodal (or trimodal if $m$ is large and hybrids numerous enough), and divergence correspondingly high even with random mating ($\alpha \to \infty$). At the other extreme, in the weak selection regime, i.e., for $V_s$ larger than the weak selection threshold $V_s^{WS}$ in fig. 2b, populations remain hybridized and exhibit a unimodal distribution even for maximum assortment ($\alpha \to 0$).

The existence of a weak selection threshold $V_s^{WS}$ is explained by considering the lifetime fitness of different phenotypes in the $\alpha \to 0$ limit. Neglecting the effect of segregation (due to mating between genotypically distinct but phenotypically identical individuals), the relative change in frequency of phenotype $X$ in deme 1 in one generation is $\sim (1 - m)W_1(X)/\bar{W}_1 + mW_2(X)/\bar{W}_2$, where $\bar{W}_1$ and $\bar{W}_2$ denote the mean fitness in the two demes. For $m=0.5$ and $\bar{W}_1 \sim \bar{W}_2$ (as expected for a hybridized population), this relative change is maximum for the generalist phenotype $X=0$ when selection is weak ($\sqrt{V_s} > \mu$), but is (locally) minimum at $X=0$ and maximum near the optima $\pm \mu$ for stronger selection ($\sqrt{V_s} < \mu$). Thus, weak stabilizing selection within demes effectively generates stabilizing selection on the whole population around the generalist phenotype. The threshold $V_s^{WS}$ for $m<0.5$ can be derived similarly; see also van Doorn et al. (2000). Even in the weak selection regime, the HM does predict a modest assortment-driven increase in divergence ($\sqrt{V_s}/\mu = 2.5$ curve in fig. 2a) due to a shift of the distributions towards extreme or edge phenotypes. However, finite populations cannot sustain these shifts and congeal into a few genotypes near $X=0$, ultimately resulting in zero divergence (illustrated in detail in
Figure 3: Long-term phenotypic distribution $P(X)$ of the whole population comprising both demes from individual-based simulations (for $N=10^5$) vs. HM predictions, $t=50000$ generations after onset of divergent selection. (a) HM accurately predicts $P(X)$ for diverged populations in individual-based simulations if there is significant hybridization between them (close match between squares and the solid line for trimodal distribution with numerous hybrids), but not if hybridization is low (triangles vs. dashed line). (b) HM predictions are accurate for hybridized populations when they are subject to strong divergent selection (squares), but not if selection on populations is weak (triangles vs. dashed line). The HM predicts the bimodal/trimodal (fig. 2(a)) or unimodal (fig. 2(b)) character of the phenotypic distributions accurately.

Appendix S5 for very weak selection).

Thus, a scan across parameter space reveals three qualitatively different scenarios: the strong selection scenario with purely ecological divergence, the intermediate selection scenario with assortment-dependent divergence and the weak selection scenario with no divergence. Figure 2b depicts typical ($V_s, m$) combinations corresponding to the three scenarios, by plotting the strong selection $V_s^{SS}$ and weak selection $V_s^{WS}$ thresholds against migration rate $m$.

**Stability of hypergeometric model (HM) predictions.** While the HM correctly predicts the qualitative state (diverged vs. hybridized) of finite populations, it may not always predict the exact divergence level (fig. 2a). This discrepancy, when it appears, is due to the fact that the high genetic polymorphism, implicit in the HM, is disfavored by stabilizing selection (Barton and Shpak 2000). With migration, however, each deme
can also replenish genetic variation by mating between phenotypically distinct residents and migrants, raising the possibility that the HM is more robust in a two-deme than in a one-deme scenario.

To test this, we compare the long-term phenotypic distributions \( P(X) \) of large populations \((N=10^5 - 10^6)\) from individual-based simulations with the corresponding HM predictions (fig. 3). This reveals certain general trends. First, the HM correctly predicts \( P(X) \) for finite, initially polymorphic populations, whether diverged (bimodal) or hybridized (unimodal) over short timescales (results not shown). Second, for diverged populations, long-term stability of the HM prediction for \( P(X) \) depends on the extent of gene flow: populations with minimal gene flow between migrant and resident phenotypes (as indicated by rare hybrids) eventually lose phenotypic variation around the two optima due to stabilizing selection, while diverged populations with significant hybridization maintain variation and have distributions that are accurately predicted by the HM (fig. 3a). Thus in the diverged state, strong assortment (low \( \alpha \)), reduced migration (low \( m \)) or strong selection (low \( V_s \)) tend to destabilize the HM prediction.

Finally, for hybridized populations, the unimodal distribution \( P(X) \) agrees with the HM for intermediate selection, but collapses into a single-phenotype distribution if \( V_s \) is large (fig. 3b). As discussed above, this is due to the fact that weak stabilizing selection within demes generates net stabilizing selection about \( X \sim 0 \). In fact, an increase in assortment in the weak-selection regime can actually destabilize \( P(X) \) by depleting polymorphic loci, an effect which precludes the buildup of LD with assortment. Loss of variation in the weak selection limit is also observed in single diploid-locus and oligogenic models (van Doorn et al. 2000; Kirkpatrick and Nuismer 2004; Bürger and Schneider 2006; Pennings et al. 2008; Rettelbach et al. 2013).

The instabilities discussed above merely cause loss of variation around the peak(s) of the phenotypic distributions, while typically maintaining their bimodal or unimodal...
character (fig. 3, see Appendix S5 for some exceptions). Thus, the HM accurately predicts the qualitative state of populations, as well as the threshold $\alpha_c$ for divergence (fig. 2a), as long as populations have a sufficient number of polymorphic loci in the initial state.

Evolving assortment

We now consider the evolving assortment scenario, where a modifier (associated with preference range $\alpha_{mod}$) is segregating at a small frequency $p_0$ in an ancestral population (preference range $\alpha_{anc}$). Our goal is to understand how modifier frequency changes in response to selective forces, identify conditions for invasion of assortment modifiers, and use this to determine the evolutionarily stable (ES) assortment strength for various migration-selection scenarios.

To study modifier evolution, we make two simplifying assumptions: that there is no initial asymmetry between demes (modifier frequency in each deme is $p_0$ at $t=0$), and that there is no initial disequilibrium between the modifier locus and the trait loci ($P(X, \alpha_{mod})=p_0P(X)$ at $t=0$). We first examine HM predictions in detail, and then compare these with individual-based simulations.

Assortment ESS and its dependence on the evolutionary history of the ancestral population. Consider an ancestral population with selection-migration parameters ($\mu=7.5$, $\sqrt{V_s}=0.8\mu$, $m=0.2$) for which divergence occurs at a threshold $\alpha_c$ that depends on $V_0$, the initial phenotypic variance of the population (before it equilibrated at $\alpha_{anc}$). For various values of $\alpha_{anc}$, this population may equilibrate to qualitatively different (unimodal vs. bimodal) states depending on $V_0$ (see fig. 2d). Thus the fate of an assortment modifier introduced in this population depends not only on the preference ranges ($\alpha_{anc}$ and $\alpha_{mod}$) of the ancestral and modifier alleles, but also on the evolutionary history of the ancestral population. To explore this dependence, we contrast how modifiers evolve in ancestral populations with a history of low variance ($\sqrt{V_0}/\mu \ll 1$) with
Figure 4: (a)-(b) Pairwise invasibility plots (as predicted by HM) for modifier with preference range $\alpha_{\text{mod}}$ introduced in an ancestral population in a long-term stationary state at some preference range $\alpha_{\text{anc}}$, where the long-term state depends on the initial (pre-equilibration) variance $V_0$ of the ancestral population. PIPs are shown for the case where $V_0$ is (a) low ($\sqrt{V_0} \ll \mu$) and (b) high ($\sqrt{V_0} > \mu$). A modifier may invade and go to fixation (filled region of both PIPs) or invade but remain in a polymorphic equilibrium with the ancestral allele (diagonally shaded regions), or transiently invade an ancestral population with (historically) low $V_0$, induce divergence, and then decline in frequency due to negative selection on the modifier in the diverged state (chequer shaded region in fig. 4a). The unusual topology of the PIP in fig. 4a is due to the fact that diverged populations ($\alpha_{\text{anc}} < \alpha_c$) can be invaded by any modifier with $\alpha_{\text{mod}}$ sufficient to maintain divergence. (c) Modifier frequency as a function of time $t$ for four different parameter combinations ($\alpha_{\text{anc}}, \alpha_{\text{mod}}$) corresponding to the four scenarios: invasion and fixation, invasion and stable polymorphism at the preference locus, transient invasion and subsequent decline of modifier, and no invasion of modifier (HM predictions).
modifier evolution in ancestral populations which had high initial variance ($\sqrt{V_0/\mu}>1$), by plotting pairwise invasibility plots (PIPs) for ($\alpha_{anc}$, $\alpha_{mod}$) combinations in both cases (figs. 4a and 4b). Since the PIPs assume a specific evolutionary history of the ancestral population, they only illustrate the outcome of a single mutation event and cannot be used to infer the outcome of a sequence of mutations at the modifier locus.

Consider first the PIP for the ancestral population with high $V_0$ before equilibration (fig. 4b). This plot reveals the existence of an intermediate evolutionarily stable (ES) preference range $\alpha_*$, somewhat lower than $\alpha_c$. Ancestral populations with $\alpha_{anc} > \alpha_c$ are invaded by modifiers that reduce the preference range (filled region to the right of $\alpha_*$ in fig. 4b), thus driving populations towards the divergence threshold. However, diverged ancestral populations with $\alpha_{anc} \ll \alpha_c$, are invaded by modifiers that increase $\alpha$ (filled region to the left of $\alpha_*$) and introduce some hybridization between resident and migrant phenotypes in each deme. Positive selection on such modifiers is due to their preferential association with relatively fit hybrids at the expense of highly unfit migrant phenotypes (details below).

The PIP also reveals various combinations of very high assortment and very low assortment alleles which form protected polymorphisms (diagonally shaded region in fig. 4b; the phase boundary of this region can be also derived from a simple geometric construction, see Geritz et al. (1998)). High-assortment alleles ($\alpha_{mod} \ll \alpha_*$) have a fitness advantage in weakly assortative, unimodal populations ($\alpha_{anc} \gg \alpha_*$), as they tend to associate with phenotypic outliers close to the selection optimum. This causes the high-assortment allele to invade and the populations to diverge. In the bimodal state, low-assortment alleles associate with more hybrids and fewer phenotypes near the migrant optimum, giving them a selective advantage, which persists as long as they are too rare to collapse divergence. Thus both high and low assortment alleles have a fitness advantage at low frequencies, resulting in a polymorphic equilibrium between them, which allows populations to remain diverged while maintaining significant hybridization. Such polymorphisms are, however,
ultimately unstable—alleles with α value intermediate to these may either supplant both of the original alleles or form a new dimorphism with the low-assortment or the high-assortment allele, eventually bringing the population close to $\alpha^* \text{(Geritz et al. 1998)}$.

We next examine the PIP (fig. 4a) for an ancestral population with a history of low variance $V_0$ (before equilibration) and a correspondingly stringent divergence threshold (low $\alpha_c$). Consider a situation with $\alpha_{anc}$ slightly higher than $\alpha_c$, for which the ancestral populations are hybridized, but could have diverged had the initial variance been sufficiently high. As before, small-effect modifiers that reduce preference range ($\alpha_c<\alpha_{mod}<\alpha_{anc}$), successfully invade and fix. However, when modifiers that reduce $\alpha$ below the divergence threshold ($\alpha_{mod}<\alpha_c<\alpha_{anc}$) are introduced, very different dynamics ensue—the modifier initially shows a sharp increase in frequency, causing the populations to diverge, but once divergence sets in, there is a resurgence of the ancestral allele which pushes modifier frequency back to zero (solid curve in fig. 4c), with diverged sub-populations now being maintained at $\alpha_{anc}$ itself.

This sort of ‘resident strikes back’ dynamics also emerges in other evolutionary models with multiple attractor states [Mylius and Diekmann 2001], and in the present model, occurs when the ancestral population has intermediate $\alpha_{anc}$ (chequer-shaded region of PIP in fig. 4a) for which divergence levels show a bistable dependence on $V_0$ (the initial variance of the population before equilibration). The invading high-assortment modifier merely increases population variance, causing the bistable system to switch to the alternative (bimodal) state in which the ancestral allele has an advantage due to its tendency to associate with relatively fit hybrids (fig. 5c). The range of $\alpha_{anc}$ allowing for the transient invasion of high-assortment modifiers shrinks with increasing $V_0$, and vanishes (fig. 4b) when $V_0$ is so high that there is no distinction between the assortment level required to induce or maintain divergence in the ancestral population.
Figure 4c illustrates the variety of dynamical behaviours that can occur when assortment modifiers invade an ancestral population with weak assortment \((\alpha_{anc} > \alpha_c)\) and low \(V_0\) (before equilibration). Modifiers that further widen preference range are eliminated, while modifiers that reduce \(\alpha\) typically invade the population in the short run, but suffer a long-term fate that depends sensitively on the values of \(\alpha_{anc}\) and \(\alpha_{mod}\). Thus, \(\alpha_{mod} < \alpha_{anc}\) modifiers either fix (corresponding to the filled region in fig. 4a), or decline towards zero frequency (typically after invading transiently and inducing divergence, chequer-shaded region in fig. 4a) or form a dimorphism with the ancestral allele (diagonally shaded region).

**Assortment ESS under different migration-selection scenarios.** Having analyzed modifier evolution in detail for one set of parameters, we now ask: how does the ES assortment level vary with migration and selection strengths, and is it always high enough to induce divergence, while simultaneously being too low to complete reproductive isolation between diverged sub-populations (as in fig. 4b and accompanying text)?

Figure 5a shows how the scaled ES assortment strength, given by \((\alpha^*_s/2\mu)^{-2}\), and the divergence threshold, \((\alpha_c/2\mu)^{-2}\), vary with \(2\mu\), the phenotypic distance between the selection optima, for two different migration rates. As selection across demes becomes more divergent \((2\mu \text{ increases})\), the ES assortment level changes in a rather complex way, revealing four qualitatively different regimes of assortment evolution. For small \(\mu\), random mating is the ESS, with \((\alpha^*_s/2\mu)^{-2} \sim 0\). For intermediate \(\mu\), the population evolves non-zero assortment, which is still lower than the threshold for divergence (dashed line), so that the populations are hybridized at the ESS. For larger \(\mu\), i.e., in the falling part of the \((\alpha^*_s/2\mu)^{-2}\) vs. \(2\mu\) plot in fig. 5a, assortment evolves exactly to the level required to induce divergence but no further, while for very large \(\mu\), the ES assortment strength is much higher than the divergence threshold \((\alpha_c/2\mu)^{-2}\), which is not even well-defined when \(\mu\) is very large and divergence is driven primarily by ecological selection.
Figure 5: (a) The scaled ES assortment strength \( (\alpha_s/2\mu)^{-2} \) and scaled threshold assortment strength for divergence, \( (\alpha_c/2\mu)^{-2} \), vs. \( 2\mu \), the difference between the selection optima, for two values of \( m \). (b) Coefficients of viability, sexual and net selection on a modifier that reduces preference range \( (\alpha_{mod}=0.98\alpha_{anc}) \) vs. assortment level \( (\alpha_{anc}/2\mu)^{-2} \) within the ancestral population, for \( \mu=8 \) (main plot) and \( \mu=6 \) (inset). Selection coefficients are measured 2000 generations after introduction of modifier at initial frequency \( p_0=0.1 \). Net selection on modifier changes sign at \( \alpha=\alpha_s \). For \( \mu=6 \) (inset), negative sexual selection on modifiers prevents assortment strength from evolving beyond the ES level, while for \( \mu=8 \), negative viability selection prevents a further increase. (c)-(d) Marginal phenotypic distributions \( P_a(X) = P(X, \alpha)/\sum_X P(X, \alpha) \) associated with an intermediate-assortment \( (\alpha=\alpha_s) \) and a high-assortment \( (\alpha=0.5\alpha_s) \) allele segregating at the modifier locus in one of the demes (with optimum at \( +x \)), 100 generations after the high-assortment modifier is introduced at frequency 0.1 in the ancestral population close to its ESS. Lower marginal fitness of the high-assortment modifier in a bimodal population may be due to the lower frequency of relatively fit hybrids and higher frequency of unfit migrant phenotypes in the associated phenotypic distribution (fig. 5(c)), or due to the higher frequency of outliers in the resident and migrant sub-distributions associated with the modifier (fig. 5(d)). All plots show HM predictions.
To understand why assortment strength cannot evolve to a level sufficient for divergence when $\mu$ is small, while evolving up to or beyond the divergence threshold for larger $\mu$, consider how assortment modifiers fare in hybridized (unimodal) populations. In such populations, modifiers that reduce $\alpha$ tend to associate with outlier or ‘extreme’ phenotypes—this generates indirect selection on the modifier, if outliers either have high viability (are close to the selection optimum) or low mating success (have phenotypes far from those of most individuals). We distinguish between these two possibilities by separately tracking the viability and sexual selection/mating success components of the net (indirect) selection acting on the modifier (see Appendix S1). Note that for the symmetric model, indirect selection is the sole driver of modifier evolution (neglecting drift).

For small $\mu$ (corresponding to the weak selection regime in fig. 2b), outliers are not favoured by viability selection since they are less fit than the generalist ($X \sim 0$) phenotype. Moreover, outliers are also chosen for mating with a probability less than their frequency, as they are farther from the majority. Thus, in this regime both viability and sexual selection disfavour modifiers that increase assortment, resulting in $(\alpha_\ast/2\mu)^{-2} \sim 0$ at the ESS.

For intermediate or large $\mu$ (corresponding to the assortment-dependent divergence regime in fig. 2b), outlier phenotypes associated with the modifier are fitter than phenotypes near $X \sim 0$, resulting in positive viability selection on the modifier. However, as long as the population is unimodal, the modifier still undergoes negative sexual selection due to the reduced mating success of outliers. Thus, natural and sexual selection drive modifier evolution in opposite directions, and the ensuing ES assortment level depends on the relative strength of the two, which depends on selection and migration parameters. To clarify this, we explicitly track, for two different selection parameters, how the coefficients of viability and sexual selection on a modifier of small effect ($\alpha_{mod}=(1-\delta)\alpha_{anc}$, $\delta=0.02$) vary with the assortment level, $(\alpha_{anc}/2\mu)^{-2}$, in the ancestral populations (fig.
For intermediate $\mu$, outliers enjoy a rather modest fitness advantage over hybrids. Thus, a modifier that increases discrimination in a randomly mating population experiences weak viability selection, which is just slightly higher than the sexual selection acting against it (inset, fig. 5b). In fact, as assortment builds up, i.e., with increasing $1/\alpha^2_{anc}$, sexual selection against modifiers (that reduce $\alpha$) becomes stronger than positive viability selection, inhibiting a further increase in assortment towards the divergence threshold (inset, fig. 5b). For larger $\mu$, phenotypes close to the deme optimum are much fitter than hybrids clustered around $X=0$ (strong selection for specialists over generalists). Thus, viability selection on modifiers that lower $\alpha$ is much stronger, and prevails over negative sexual selection (main plot, fig. 5b), driving assortment to a level sufficient for divergence.

Within diverged populations, assortment evolution is governed by somewhat different effects. Close to $\alpha_c$, when populations have just become bimodal, it is possible for highly unfit phenotypes that migrate into the deme to produce relatively fit hybrid offspring by mating disassortatively, i.e., with well-adapted residents. By contrast, modifiers with stronger assortment ($\alpha_{mod} < \alpha_c$) allow for almost no hybridization between phenotypes at the two optima and are hence associated with fewer hybrids and a higher fraction of phenotypes near the immigrant optimum (fig. 5c). While this may give rise to a weak sexual selection advantage for such modifiers (since migrant phenotypes have a mating advantage with respect to hybrids in bimodal populations, being more numerous), it also results in lower marginal fitness of the $\alpha<\alpha_c$ modifier. Thus high-assortment modifiers undergo negative viability selection within bimodal populations (main plot, fig. 5b), which prevents any further increase in assortment beyond the divergence threshold, at least when $\mu$ is not extremely large (falling part of the curve in fig. 5a).

As $\mu$ increases further, the divergence threshold $(\alpha_c/2\mu)^{-2}$ decreases, resulting in a fall in the ES assortment strength, $(\alpha_*/2\mu)^{-2}$, with $\mu$ (fig. 5a). For very large $\mu$, populations
approach the strong selection regime in fig. 2b, where divergence is driven more by ecological selection than assortment, and is thus accompanied by extensive hybridization between resident and migrant phenotypes (note, for instance, the trimodal distribution in fig. 3a). The high rate of hybridization pulls the means of the distributions around the two optima closer to $X=0$, resulting in somewhat reduced local adaptation. Modifiers that further increase assortment in such a population do associate more strongly with unfit migrant phenotypes than with fitter hybrids, but they also tend to form associations with better adapted (closer to optimal) phenotypes within the resident pool. Due to these two opposing effects, such modifiers may actually undergo positive or very weakly negative viability selection, causing assortment strength to evolve beyond the very low level required to split the unimodal population (very large $\mu$ regime in fig. 5a).

Figure 5a also illustrates how migration influences the ES assortment strength. An increase in $m$ shifts the $(\alpha_s/2\mu)^{-2}$ vs. $2\mu$ curve towards larger $\mu$, while also increasing the ES assortment level attained at large $\mu$. This is explained by noting that the range of $\mu$ for which populations exist in the weak selection regime and consequently have random mating ESS, is larger for $m=0.4$ than for $m=0.2$ (fig. 2b). Even when assortment-dependent divergence becomes possible, high-assortment modifiers are less effective in generating increased phenotypic variance and skew towards the selection optimum in populations with high $m$, because of the homogenizing effects of gene flow. Thus, weak viability selection on modifiers is easily canceled out by negative sexual selection even for fairly large $\mu$, resulting in ES assortment levels that are insufficient for divergence. Only when $\mu$ is quite large does the indirect fitness advantage of such modifiers become strong enough to drive assortment to the threshold for divergence. Interestingly, for high $m$, this assortment threshold can be so high as to produce complete reproductive isolation (zero hybridization) between populations at the onset of divergence itself, in contrast to the moderate hybridization observed at the ESS for lower migration rates. A modifier that further increases assortment does not significantly reduce the (already
negligible) hybrid frequency. Instead, it tends to associate with outliers within resident and migrant sub-populations in each deme (see fig. 5d). These outliers, especially within the resident sub-population, are both less fit and less likely to be selected for mating than phenotypes at the selection optimum, resulting in negative viability and sexual selection against modifiers that increase assortment strength beyond the divergence threshold.

**Assortment evolution in individual-based simulations.** The preceding discussion highlights the sensitivity of modifier evolution to genetic variation within demes. Finite populations subject to stochastic fluctuations may, however, exhibit much less variation than predicted by the HM (see fig. 3). How does loss of variation affect modifier dynamics, and does the resultant ESS differ from the HM prediction?

Consider a situation with $\alpha_* \sim \alpha_c$ (as predicted by the HM). Figure 6 shows that the HM accurately predicts modifier dynamics in individual-based simulations when the ancestral population in which the modifier appears is weakly assortative and hybridized, i.e., $\alpha_{anc} > \alpha_{mod} > \alpha_* \approx \alpha_c$ (fig. 6a), but not within diverged ancestral populations with strong assortment, i.e., for $\alpha_{anc} < \alpha_{mod} < \alpha_*$ (fig. 6b). Diverged populations tend to lose phenotypic variation and congeal around the selection optima (fig 3a); thus the effects that drove modifier evolution under the HM (involving selection for a specific level of hybridization or against outliers), no longer operate in the absence of variation. Consequently, while weakly assortative populations in individual-based simulations can evolve towards the divergence threshold $\alpha_c \sim \alpha_*$ by fixing small-effect modifiers that reduce $\alpha$ (in agreement with the HM), once in the diverged state, modifiers that reduce $\alpha$ even further, evolve neutrally and are not selected against (fig. 6b).

The analysis so far assumes no mutation. However, mutation contributes substantially to polygenic variability (Barton and Keightley 2002). To test whether assortment evolution in populations with stable genetic variation agrees qualitatively with HM predictions, we perform individual-based simulations allowing for recurrent mutation at the
Figure 6: Modifier dynamics from individual-based simulations of populations with \( N = 10^6 \) (points) vs. HM predictions (lines). Modifier frequency vs. time \( t \) is accurately predicted by HM for \( \alpha_{\text{anc}} > \alpha_\ast \), i.e., when the ancestral population is hybridized (fig. 6a) but not for \( \alpha_{\text{anc}} < \alpha_\ast \), i.e., when the ancestral population is diverged (fig. 6b). Modifiers that change \( \alpha \) in finite populations with \( \alpha_{\text{anc}} < \alpha_\ast \) undergo nearly neutral evolution (see data points in fig. 6b, obtained by averaging over 5 replicates), and not the positive selection predicted by the HM.

trait loci (Appendix S6). These show that large, finite populations with mutation have a well-defined ES level of assortment, as long as the mutation rate is not too low, with modifiers that take the population towards this ESS undergoing positive selection in both strongly assortative and weakly assortative populations (fig. S5, Appendix S6).

**Asymmetric models**

Several theoretical studies have argued that reinforcement is strongly affected by the directionality of gene flow, and occurs under more stringent conditions for continent-island migration than with reciprocal introgression \( \text{[Servedio and Kirkpatrick 1997]} \) \( \text{[Servedio 2000]} \). To test this, we study our model with \( m_{12} \neq m_{21} \), and find that while asymmetric gene flow does make it more difficult for assortment-increasing modifiers to invade, it also facilitates higher divergence at any given assortment strength (see Appendix S7 and Discussion).
Our results highlight a number of subtle effects that arise in simple magic-trait scenarios of speciation when the trait is polygenic and can sustain high genetic variation. The core question addressed in the paper is: How does the interplay of gene flow, natural and sexual selection shape the evolution of such a trait along with the degree of mate discrimination for the trait? Studying the co-evolution of mate discrimination with the assortment trait on which it acts, sheds light on the evolutionary accessibility and stability of diverged states, thus providing a window into long-term divergence and speciation.

Established assortment

A striking feature of the onset of divergence in the model is its highly non-linear character, with small changes in the female preference range at $\alpha_c$ triggering a steep increase in trait differences between the two demes (figs. 1b, 2a). The existence of sharp divergence thresholds has important implications for reverse speciation (Seehausen 2006), suggesting that the collapse of diverged species into a hybrid swarm due to reduced mate discrimination may be an abrupt and unpredictable event, especially if the assortment trait is polygenic.

Threshold effects involving a precipitous rise in divergence over time are common in speciation models (Gavrilets 2004). The abrupt transition in this model at $\alpha_c$ has the same underlying cause, namely, the synergistic changes in allele frequency that occur when genome-wide LD builds up to a critical value. In fact, stronger assortment generates higher LD (fig. 1b), thus inflating the variance of polygenic traits despite sexual selection against phenotypic outliers. This effect contributes significantly to the divergence of polygenic traits determined by unlinked or weakly linked loci. However, when trait loci are tightly linked, assortative mating has a qualitatively different effect, with stronger assortment reducing rather than increasing (the already high) LD and trait variance (Kirkpatrick and Nuismer 2004; Bürger and Schneider 2006). Thus, extending the
model to include arbitrary linkage, as in de Cara et al. (2008), could provide a useful perspective on the conclusions of this study.

Sharp transitions to a diverged state only occur when selection and migration are competing evolutionary forces and divergence is assortment-dependent. As in the model of van Doorn et al. (2000), which considers preference-trait mating in a similar two-deme setting, this model also exhibits an ecological speciation (low $V_s, m$) and a weak selection (high $V_s, m$) regime, where assortment has little effect and populations exhibit high or low divergence, independently of $\alpha$ (fig. 2b). Weak selection thresholds emerge quite generally in two-deme models, even with single-locus and AD assumptions (Brown and Pavlovic 1992; Meszéna et al 1997), and reflect a switch in the topology of the fitness landscape (from disruptive to stabilizing selection) near the generalist phenotype.

Unlike the AD framework, which is mutation-limited, both the HM and the infinitesimal model assume high standing genetic variation—this allows for generation of new phenotypes via recombination, and long-term phenotypic change under selection, far beyond the initial phenotypic range of the population. Thus, as long as assortment is strong, divergence occurs even if populations have limited initial phenotypic variation ($\sqrt{V_0} \ll \mu$) and do not include optimal phenotypes at the outset. Further, the long-term state of populations is largely insensitive to where they start out in phenotypic space. For instance, under strongly divergent selection (large $\mu$) and low migration, sub-populations (with a modest segregation variance) can always evolve towards their respective optima via shifts in their phenotypic distributions, irrespective of whether they start out as generalist populations or being locally adapted to one of the optima or clustered around any intermediate phenotype (Appendix S2). This contrasts with asexual populations in AD models (Meszéna et al 1997), which undergo evolutionary branching under similar ecological conditions only if they start out exactly at the generalist strategy (or are invaded by mutants with very large phenotypic effects).
Both the HM and the more widely applicable infinitesimal model make qualitatively similar predictions (see Appendix S3), in particular, that phenotypic variance always increases with increasing assortment. However, in individual-based simulations with finite $L$, increasing assortment may collapse variance by destabilizing polymorphisms. This ‘loss of polymorphism’ regime has been highlighted in several oligogenic models (Kirkpatrick and Nuismer 2004; Pennings et al. 2008; Rettelbach et al. 2013), and becomes important in the present model under certain conditions (see fig. 3), e.g., for unimodal populations subject to stabilizing or weakly divergent selection across demes (resulting in reduced variation around the generalist phenotype), or for diverged populations which hybridize weakly (and undergo loss of variation about the selection optima). However, even under these conditions, as $L$ increases, selection coefficients responsible for loss of polymorphism at individual loci become very small, thus recovering the infinitesimal limit, in which polymorphic variation is more or less stable over other relevant timescales, e.g., the time required for assortment modifiers to fix within a population. Moreover, even for moderate values of $L$, mutation (with rate $U$~0.1) can maintain enough polymorphic variation for HM predictions to be valid over long timescales, at least in large populations (Appendix S6).

Evolving assortment

In the evolving assortment scenario, we explore how the evolutionarily stable (ES) assortment strength varies with selection and migration parameters, in order to determine when divergence and complete reproductive isolation occur at the ESS.

We identify several qualitatively different regimes of assortment evolution. With weak selection, divergence is not possible at any assortment strength, and randomly mating populations are immune to invasion by modifiers that increase assortment. Such random mating ESS also arise in oligogenic models (Pennings et al. 2008; Rettelbach et al. 2013) and simply reflect the absence of disruptive selection on the whole population.
Even when divergence is possible above a certain assortment threshold, the diverged state need not be an evolutionary attractor, in that the ES assortment may be lower than this threshold. This is typically the case when migration rates are high and/or selection across demes only moderately divergent, so that the gain in fitness due to local adaptation is offset by the loss in mating success that outliers suffer. Under these conditions, even though assortative mating increases trait variance, the accompanying sexual selection acts against assortment modifiers associated with the higher variance, thus constraining evolution of strong assortment and preventing divergence.

This sort of antagonism between natural and sexual selection also plays a role in diploid, single-locus models of competitive speciation, where assortment evolution stops at low values despite disruptive selection, precisely because of positive sexual selection on heterozygotes when they are widespread (Matessi et al. 2001; Otto et al. 2008; Pennings et al. 2008)—an effect similar to the one described above. Interestingly, this weak-assortment state is a global attractor in the polygenic model (with even highly diverged populations evolving towards it through the substitution of low-assortment modifiers, at least for the HM) but not in one-locus models.

As selection across demes becomes more divergent, positive viability selection on modifiers becomes strong enough to drive assortment levels up to the divergence threshold, so that populations are bimodal at the ESS. Significantly, there is effective stabilizing selection on the strength of assortment even within bimodal populations, with high-discrimination modifiers ($\alpha < \alpha_c \sim \alpha^*$) undergoing negative selection due to their association with certain phenotypes, at least in the HM and infinitesimal model. We identify two distinct explanations for this, which apply in different parameter ranges.

First, very high assortment depletes hybrids while simultaneously increasing the frequency of ill-adapted migrants within each deme (fig. 5c). The resultant selection against high assortment is essentially positive selection for moderate hybridization between di-
verged populations, which however must not be so high as to significantly reduce local adaptation. We verify that this kind of selection for hybridization is not sensitive to the ratio of hybrid to migrant fitness in each deme by also considering alternative (quadratic/stretched exponential) selection functions (results not shown).

Second, strong assortment increases the frequency of outliers within resident and migrant sub-populations (fig. 5d); the lower fitness and reduced mating success of such outliers selects against the associated high-assortment modifier.

The first explanation for selection against $\alpha<\alpha^*$ modifiers applies when there is significant hybridization between diverged populations, while the second is more relevant if there is complete reproductive isolation at the divergence threshold itself, i.e., if $\alpha_c$ is so low that the switch to bimodality is enough to ensure a close to zero probability of heterospecific matings. This is typically the case when both $2\mu$ and $m$ are high (fig. 5a); high migration, then, actually aids stronger reproductive isolation, by inducing females to evolve very restrictive preference ranges at the ESS (see Rettelbach et al. (2013) for a somewhat similar effect in a one-locus model). Thus selection for intermediate assortment in this situation does not reflect incomplete reproductive isolation between diverged populations, as found by Servedio (2011), but arises instead due to selection against assortment-driven increase in sub-population variance, as also observed in polygenic models of competitive speciation (Doebeli 1996).

In finite populations with zero or low mutational variance, complete reproductive isolation can also evolve via the action of stabilizing selection on diverged resident and migrant sub-populations in each deme. Stabilizing selection depletes standing variation within the sub-populations; as the phenotypic range of both migrants and residents shrinks, hybridization between the two becomes weaker, which further accelerates loss of variation, finally leading to the emergence of two distinct phenotypes, narrowly clustered around the optima, which are too ‘far apart’ to hybridize (fig. 3a). This finding has two general
implications. First, hybridization between incipient species may not be as much due to mating between the prototypical (fittest or most abundant) phenotypes, but is likely to involve outliers within each population. Thus the extent of hybridization between populations is intimately connected to the degree of phenotypic variation they harbour, or have harboured in the past. Second, contrary to the reinforcement view, in this situation, it is selection for increased discrimination that drives initial divergence, and stabilizing selection that causes populations to evolve complete reproductive isolation over longer timescales.

To assess the robustness of our results, we also analyze the model with asymmetric migration and unequal selection strengths in the two demes. Most qualitative conclusions remain unaltered in the presence of these asymmetries. However, asymmetric gene flow inhibits the evolution of assortment over a wider parameter range than symmetric migration (fig. S6b, Appendix S7), as is consistent with earlier studies which suggest that indirect, LD-mediated selection on modifiers can be washed out by net influx of a foreign allele at the modifier locus (Servedio and Kirkpatrick 1997; Servedio 2000). This is, however, partially offset by the fact that for a fixed strength of assortment, divergence is higher with more asymmetric migration (fig. S6a, Appendix S7). Thus, island populations subject to one-way introgression may evolve weaker assortment, but similar levels of divergence as populations with reciprocal introgression.

Many of our results depend on the fact that populations experience stabilizing selection around well-defined optima. Thus it would be useful to consider how these conclusions change when selection in each deme is directional (Cotto et al. in preparation). A limitation of the model is that the preference range is assumed to be determined by a single locus. Modeling the preference range as a polygenic trait with similar amounts of standing variation as the assortment trait could be another interesting direction for future work.
In conclusion, divergence and assortment evolution based on highly polygenic traits is well-described by phenotypic approaches such as the infinitesimal and the hypergeometric model, at least over short timescales. Polygenic traits can maintain substantial genetic and phenotypic variation in spite of stabilizing selection when there is gene flow between demes and if density regulation occurs independently in each deme. Assortative mating further amplifies phenotypic variation by building up associations between loci, thus facilitating a strong response to divergent selection. The extent of genetic variation also affects the degree of hybridization between diverged populations and the evolution of discrimination within these, and is thus a crucial determinant of the fate of incipient species.

**Author Contributions**

H.S. and N.H.B. designed the study, H.S. did the calculations, H.S. wrote the manuscript with input from N.H.B.

**Acknowledgements**

The research leading to these results has received funding from the People Programme (Marie Curie Actions) of the European Union’s Seventh Framework Programme (FP7/2007-2013) under REA grant agreement Nr. 291734 (H.S.) and ERC grant SelectionInformation 250152 (N.B.). We thank Maria Servedio, Olivier Cotto and Christelle Fraisse for useful comments on the manuscript, and two anonymous reviewers for detailed and insightful reviews.

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