

An explanation for the prevalence of XY over ZW sex determination in species derived from hermaphroditism

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Abstract. The many independent transitions from hermaphroditism to separate sexes (dioecy) in flowering plants and some animal clades must often have involved the emergence of a heterogametic sex-determining locus, the basis of XY and ZW sex determination (i.e. male and female heterogamety). Current estimates indicate that XY sex determination is much more frequent than ZW, but the reasons for this asymmetry are unclear. One proposition is that separate sexes evolve through the invasion of sterility mutations at closely linked loci, in which case XY sex determination evolves if the initial male sterility mutation is fully recessive. Alternatively, dioecy may evolve via the gradual divergence of male and female phenotypes, but the genetic basis of such divergence and its connection to XY and ZW systems remain poorly understood. Using mathematical modelling, we show how dioecy with XY or ZW sex determination can emerge from the joint evolution of resource allocation to male and female function with its genetic architecture. Our model reveals that whether XY or ZW sex determination evolves depends on the trade-off between allocation to male and female function, and on the mating system of the ancestral hermaphrodites, with selection for female specialisation or inbreeding avoidance both favouring XY sex determination. Together, our results cast light on an important but poorly understood path from hermaphroditism to dioecy, and provide an adaptive hypothesis for the preponderance of XY systems. Beyond sex and sex determination, our model shows how ecology can influence the way selection shapes the genetic architecture of polymorphic traits.

Introduction

Many plants and some animals have evolved separate sexes (or dioecy) from hermaphroditism (Charlesworth, 1985; Renner, 2014; Henry et al., 2018; Leonard, 2018; Pannell and Jordan, 2022). In these species, sex is typically determined at a sex-determining locus with either male heterogamety, where males are XY heterozygotes and females are XX homozygotes, or female heterogamety, where females are ZW heterozygotes and males are ZZ homozygotes (Bachtrog et al., 2014; Beukeboom and Perrin, 2014). Although the basis of sex determination is unknown for the vast majority of the >15,000 dioecious plant species, current estimates indicate that male heterogamety (XY) is much more frequent than female heterogamety (ZW) in this clade (approximately 85%, Ming et al., 2011; Leite Montalvão et al., 2021), so that transitions from hermaphroditism to dioecy must more often have involved the evolution of an XY rather than a ZW sex-determining locus. The reasons behind this asymmetry remain poorly understood.

One possible explanation for the prevalence of XY systems comes from population genetics models, where dioecy evolves via the spread of sterility mutations in response to selection to avoid self-fertilisation and inbreeding depression (Charlesworth and Charlesworth, 1978a,b, 1981). Under strong inbreeding depression, a population of partially selfing hermaphrodites can be invaded by a male-sterility mutation (i.e., by females), which then favours the spread of female-sterility mutations turning hermaphrodites into males. During this step-wise evolution, which is commonly known as the “gynodioecy pathway” to dioecy, an XY system emerges when the initial male-sterility mutation is fully recessive, whereas a ZW system evolves when it is fully dominant (Charlesworth and Charlesworth, 1978a,b). It has thus been argued that the high frequency of XY systems in dioecious plants might be a by-product of the nature of the initial sterility mutation, which, according to this argument, would most often be a fully recessive ‘loss-of-function’ mutation (Charlesworth and Charlesworth, 1978a).

Although evidence suggests that gynodioecy may often have been an intermediate state in transitions to dioecy (Charlesworth, 1999; Spigler and Ashman, 2012; Dufaÿ et al., 2014; see also Weeks, 2012 and Chap. 1 in Leonard, 2018 for a discussion of androdioecy as a possible intermediate state in some invertebrate animals), dioecy may also have evolved through the divergence of increasingly male- and female-biased phenotypes leading to sexual specialisation (Charnov et al., 1976; Lloyd, 1980; Renner and Ricklefs, 1995; Freeman et al., 1997; Käfer et al., 2017; Pannell and Jordan, 2022). This gradual

process, which is often referred to as the “monoecy-parodioecy pathway” to dioecy (Lloyd, 1980), has been studied through the lens of sex allocation theory. This theory uses optimality arguments to identify conditions under which selection favours individuals allocating all their resources to one sexual function over those allocating to both (Charnov, 1982; West, 2009). Whether selection favours specialisation depends on the shape of the male and female ‘gain curves’, which are functions that relate resource allocation to fitness gained through each sex, and are influenced by a number of ecological and physiological factors that roughly relate to the advantages or disadvantages of sexual specialisation over hermaphroditism (Charnov et al., 1976; Charnov, 1982; Givnish, 1982; Lloyd, 1982; Renner and Ricklefs, 1995; Freeman et al., 1997; Pannell and Jordan, 2022; Masaka and Takada, 2023). However, the optimality approach used in sex allocation theory is mute about the genetic basis of sex determination. Accordingly, we lack theory on how the gradual divergence in hermaphroditic sex allocation between increasingly male- and female-biased phenotypes might be achieved at the genetic level, and especially how this might lead to either XY or ZW sex-determining systems.

Here, we show how the joint evolution of sex allocation with its underlying genetic architecture readily leads to the gradual emergence of a heterogametic sex-determining locus. Our model reveals that selection shapes dominance relationships between alleles at nascent sex-determining loci, and thus influences whether XY or ZW sex determination evolves. This evolution depends both on the shape of gain curves and on the mating system in the hermaphroditic ancestor, with partial selfing and inbreeding depression promoting XY. Overall, our model therefore provides a new and adaptive hypothesis for why most species transitioning to dioecy appear to acquire XY rather than ZW sex determination.

Model

Our model should apply generally to any animal or plant population that evolves gradually from hermaphroditism to dioecy, but we frame it explicitly in terms relevant to plants, both for conciseness and because of the very frequent transitions plants have made from hermaphroditism to dioecy (Charlesworth, 1985; Renner, 2014).

We consider a large population in which diploid individuals allocate a proportion x of their reproductive resources to their female function and $1 - x$ to their male function, leading to a trade-off between the two (Supplementary Table S1 for a list of key symbols). Sex allocation x results in female and male

fecundities $F(x) = F_0 x^{\gamma_{\text{♀}}}$ and $M(x) = M_0 (1 - x)^{\gamma_{\text{♂}}}$, respectively, where F_0 and M_0 correspond to the maximum achievable fecundity, and exponents $\gamma_{\text{♀}}$ and $\gamma_{\text{♂}}$ control the shape of each gain curve and thus the nature of the trade-off between male and female functions (Figure 1A; many of our results are derived for functions $F(x)$ and $M(x)$ that are more general than these power functions; see Appendix). Following pollen and ovule production, individuals first self-fertilise a fraction $\alpha(x)$ of their ovules ('prior selfing'; Lloyd, 1975), and then outcross the remaining $1 - \alpha(x)$ via random mating. We assume that self-fertilisation (selfing hereafter) does not affect siring success through male function, but may decrease with allocation x to female function (i.e. $\alpha'(x) \leq 0$; where necessary, we specifically assume that $\alpha(x) = \alpha_0(1 - \beta x)$, where $0 \leq \alpha_0 < 1$ denotes the maximum achievable selfing rate and $0 \leq \beta \leq 1$ controls the degree to which $\alpha(x)$ depends on female allocation, as in Charlesworth and Charlesworth, 1978b, 1981). Outcrossed offspring develop into viable seeds with probability 1, whereas selfed offspring develop into viable seeds with probability $1 - \delta$, where δ measures the magnitude of inbreeding depression (Charlesworth and Charlesworth, 1987). Finally, adults die and a new generation is formed from viable seeds (Figure 1B; see Appendix A for more details).

Previous theory demonstrates that dioecy is evolutionarily stable when gain curves are accelerating ($\gamma_{\text{♀}} > 1$ and $\gamma_{\text{♂}} > 1$, Charnov et al., 1976; Charnov, 1982) or when inbreeding depression is sufficiently strong (Charlesworth and Charlesworth, 1981). Under these conditions, a hermaphrodite in a population of males and females will have lower than average fitness, and a population of hermaphrodites will be invadable by unisexuals. Dioecy may then evolve from hermaphroditism through sequential invasions of fully dominant or fully recessive mutations causing complete (Charlesworth and Charlesworth, 1978a, 1981) or partial sterility (Charlesworth and Charlesworth, 1978b), most likely first of male and then female function.

Rather than fixing the nature and dominance of mutations *a priori*, we assume here that sex allocation x is influenced by a quantitative trait locus subject to recurrent mutations of small effects, leading to gradual evolution (i.e., mutations create new alleles whose value deviates from the original allele by a small amount, the 'continuum-of-alleles' model; Fig. 1C; Kimura, 1965, p. 883 in Walsh and Lynch, 2018). This locus could be a regulatory element that influences the development of female and male traits, or one or more fully linked genes that are independent targets of partial female and male sterility mutations (where in both cases there is a physiological trade-off between female and male function). Genetic effects on sex allocation x are initially assumed to be additive, meaning that the two alleles carried by an individual at the quantitative trait locus contribute equally to its phenotype (note that

although genetic effects on the phenotype are additive, they may translate to non-additive effects on fitness, as described by gain curves). To investigate the emergence of sex-determining systems, we later allow for the evolution of the genetic architecture of sex allocation x (i.e., we allow non-additive genetic effects on the phenotype x to evolve), first by considering the evolution of dominance at the quantitative trait locus, and then by extending our model to a case where sex allocation is influenced by multiple loci.

Results

Gradual evolution of sexual systems under complete outcrossing. We first assume that the population is fully outcrossing ($\alpha_0 = 0$) and focus on the effects of selection for sexual specialisation, as in classical sex allocation theory (Charnov et al., 1976; Charnov, 1982). We show in Appendix B.1 that the population either converges and remains monomorphic for an optimal intermediate sex allocation $x^* = \gamma_{\text{♀}} / (\gamma_{\text{♀}} + \gamma_{\text{♂}})$, with all individuals being hermaphrodites; or experiences negative frequency-dependent disruptive selection ('disruptive selection' hereafter for short), resulting in the gradual differentiation of two types of alleles: one that causes its carrier to allocate more resources to female function, and the other more resources to male function. Which of these two outcomes occurs depends on the shape of gain curves, with disruptive selection requiring at least one of them to be sufficiently accelerating (specifically that $2\gamma_{\text{♀}}\gamma_{\text{♂}} > \gamma_{\text{♀}} + \gamma_{\text{♂}}$; Fig. 2A). When both gain curves are accelerating ($\gamma_{\text{♀}} > 1$ and $\gamma_{\text{♂}} > 1$), disruptive selection leads to the co-existence of two alleles: one for a pure male ($x = 0$) and another for a pure female ($x = 1$) strategy. When only one curve is accelerating, one allele encodes a unisexual strategy (female or male), while the other encodes a hermaphroditic strategy, albeit biased towards the opposite sex (Appendix B.2 for analysis). Figs. 2B-E show how these different possible evolutionary dynamics unfold in individual-based simulations (detailed in Appendix B.3). These results align with classical optimality models in that they delineate the same conditions for the evolutionary stability or instability of hermaphroditism (Charnov et al., 1976; Charnov, 1982, see Appendix B.4 for more details in this connection; see also Appendix B.5 for the connection between our results and population genetics models, Charlesworth and Charlesworth, 1978a,b).

Emergence of XY and ZW sex determination through dominance evolution. Because we have assumed so far that alleles have additive effects on sex allocation, disruptive selection leads to the

coexistence of not two but three types of individuals: two homozygotes that express female- and male-biased sex allocation strategies, respectively, and a heterozygote with an intermediate hermaphroditic strategy (Figure 2C-E), so that dioecy is incomplete. To examine how complete dioecy might ultimately evolve, we next model the joint evolution of sex allocation with dominance at the underlying locus. We first investigate this joint evolution using computer simulations, and then analyse a mathematical model to better understand the mechanisms governing it. In the simulations, we assume that the evolving locus is composed of two elements: a sex allocation gene, where alleles code for different sex allocation strategies; and a linked promoter that determines the level of expression of the sex allocation allele (Figure 3A). Variation at the promoter leads to variation in allelic expression through *cis* effects, which in turn determine the dominance relationships among sex allocation alleles (Van Dooren, 1999). We let the sex allocation gene and its promoter each undergo recurrent mutations of small effect (i.e. each follow the continuum-of-alleles model), so that dominance and sex allocation evolve jointly (see Appendix C.1 for details on these simulations).

We first run simulations under conditions predicted to lead to pure male and female alleles (so when $\gamma_{\text{♀}} > 1$ and $\gamma_{\text{♂}} > 1$). In these simulations, complete dominance of one sex allocation allele always evolves, so that the population ultimately comprises only males and females, and dioecy is complete (Figure 3B-C). Remarkably, whether the male or the female allele becomes dominant depends strongly on male and female gain curves (i.e., on $\gamma_{\text{♀}}$ and $\gamma_{\text{♂}}$, Figure 3D). Provided that neither curve is close to being linear, the male allele is more likely to become dominant when fitness increases more steeply via female function (i.e., when $\gamma_{\text{♀}} > \gamma_{\text{♂}}$), leading to the emergence of an XY system. Conversely, when fitness returns increase more steeply via male function (i.e., when $\gamma_{\text{♂}} > \gamma_{\text{♀}}$), the female allele most often becomes dominant, leading to a ZW system. We also simulated scenarios predicted to lead to gyno- and androdioecy, where pure females and pure males coexist with hermaphrodites, respectively (i.e., with either $\gamma_{\text{♀}} > 1$ or $\gamma_{\text{♂}} > 1$), and obtained qualitatively similar results: the allele for the unisexual strategy most often becomes dominant (Figure 3D), so that the population typically ends up being composed of either heterozygote (XY) males and homozygote (XX) hermaphrodites (when $\gamma_{\text{♀}} > 1$), or heterozygote (ZW) females and homozygote (ZZ) hermaphrodites (when $\gamma_{\text{♂}} > 1$). Finally, we ran simulations allowing for mutations causing unisexuality to occur at the sex allocation locus, i.e. mutations encoding $x = 0$ and $x = 1$, which in the context of our model correspond to sterility mutations. Our results show that this has very little effect on whether XY or ZW evolves (Supp. Fig. S1). If anything, the association between gain curves and the evolution of XY vs. ZW sex determination is strengthened by

the occurrence of sterility mutations (compare dashed and full lines in Supp. Fig. S1).

Competition through male and female functions determines whether XY or ZW evolves. To better understand the nature of selection on dominance, we analyse mathematically a version of our model in which dominance is treated as a quantitative trait. In this version, two sex allocation alleles are maintained as a polymorphism by disruptive selection, $x_{\text{♀}}$ and $x_{\text{♂}}$, where one allele encodes a more female strategy than the other ($x_{\text{♀}} > x_{\text{♂}}$, hereafter referred to as ‘female’ and ‘male’ alleles). In $x_{\text{♂}}/x_{\text{♀}}$ heterozygotes, the female allele is expressed proportionally to a dominance coefficient h , so that the sex allocation strategy of a $x_{\text{♂}}/x_{\text{♀}}$ heterozygote is given by $h x_{\text{♀}} + (1 - h) x_{\text{♂}}$. We assume that the value of h is determined by a quantitative trait locus subject to recurrent mutations of small effect and unlinked to the sex allocation locus. This allows us to investigate the nature of selection on other mechanisms that may modify dominance (e.g. *trans* effects, Billiard et al., 2021; see Appendix C.2 for details on this model and its analysis).

The selection gradient on h , which gives the direction and strength of selection acting on mutations modifying dominance in a population expressing h , reveals that there exists a threshold h^* below which selection favours ever lower values of h (i.e. $h \rightarrow 0$ when $h < h^*$) and above which selection favours ever higher values of h (i.e., $h \rightarrow 1$ when $h > h^*$). Complete dominance of either the male or female allele therefore also always evolves here, resulting in the emergence of XY or ZW sex determination, respectively (Fig. 4A). Computing h^* explicitly is difficult, but its position relative to $1/2$ can be inferred from the sign of the selection gradient at $h = 1/2$, with a positive gradient indicating that $h^* > 1/2$ (such that XY is favoured), and a negative gradient indicating that $h^* < 1/2$ (such that ZW is favoured). In fact, we observe an almost perfect correspondence between this analysis and the outcome of our earlier individual-based simulations (compare Fig. 3D with Fig. 4B). This shows that whether selection promotes XY or ZW sex determination is independent of the particular mechanisms responsible for variation in dominance (whether through *cis* or *trans* effects), but rather comes down to the shape of the gain curves here.

Decomposing the selection gradient on dominance reveals that selection on sex-determining systems and its relationship with gain curves can be understood as follows (Appendix C.2.4 for details). Selection on dominance h acts only in $x_{\text{♂}}/x_{\text{♀}}$ heterozygotes, which are hermaphrodites. Such a heterozygote can become more female (or more male) through an increase (or a decrease) in h . But whatever the change in dominance, this heterozygote will always be less fit than female homozygotes through female

function and less fit than male homozygotes through male function. In fact, homozygotes are typically so competitive because of their fecundity advantage, that it is best for a heterozygote to allocate more to the sex in which this advantage is weakest. This scenario favours heterozygote individuals that are more female when $\gamma_{\sigma} > \gamma_{\varphi}$ and more male when $\gamma_{\sigma} < \gamma_{\varphi}$, leading to the evolution of ZW and XY systems, respectively. When both gain curves are close to linear (γ_{φ} and γ_{σ} close to one), the advantage of homozygotes over heterozygotes is reduced, and it is then best for a heterozygote to allocate to the sexual function that leads to the greater increase in fecundity, i.e., to become more female when $\gamma_{\varphi} > \gamma_{\sigma}$ and more male when $\gamma_{\varphi} < \gamma_{\sigma}$.

Partial selfing and inbreeding depression favour XY sex determination. Our analysis so far has assumed that hermaphrodites are completely outcrossing. However, partial selfing and inbreeding depression can play an important role in the evolution of dioecy and other polymorphic sexual systems such as gyno- and androdioecy (Charlesworth and Charlesworth, 1978a,b, 1981). To examine how these factors influence the gradual evolution of sexual systems and sex determination, we now analyse our model for $\alpha_0 > 0$ and $\beta > 0$ (see Appendix D for details).

To investigate the influence of selfing on the gradual emergence of polymorphism, we first fix dominance at the sex allocation locus (see Appendices D.1-D.2). Previous analyses have found that the invasion of a partial male-sterility mutation in a population of hermaphrodites is either facilitated or hindered by partial selfing, depending on whether inbreeding depression is high or low, respectively (Charlesworth and Charlesworth, 1978b). Consistent with these observations, we find that selfing favours disruptive selection, and thus the emergence of polymorphism in sex allocation, when inbreeding depression is high ($\delta > 1/2$), whereas it inhibits polymorphism when inbreeding depression is low ($\delta < 1/2$, see Fig. D2 in Appendix D). By decomposing the disruptive selection coefficient (eq. D17 in Appendix D), we further reveal that this effect of selfing stems from the interplay between its twofold transmission advantage and the deleterious effects of inbreeding depression (Fisher, 1941), which influences fitness gained through female function. In particular, when $\delta > 1/2$ (i.e., when a selfed individual is less than half as fit as an outcrossed individual), an individual transmits on average more copies of its genes to the next generation by outcrossing than by self-fertilising its seeds. In this case, increased allocation into female function leads to multiplicative fitness benefits, as it allows individuals to produce not only more seeds but also seeds that transmit on average more copies of their genes due to increased outcrossing (since $\beta > 0$). Such multiplicative benefits favour sexual specialisation, and allow the emergence of dioecy even when

both gain curves are saturating (i.e. where $\gamma_{\text{♀}} < 1$ and $\gamma_{\text{♂}} < 1$; Fig. 4C).

To study the effect of partial selfing on the evolution of sex determination, we next investigate selection on dominance when disruptive selection favours polymorphic sexual systems (as in section “Competition through male and female functions determines whether XY or ZW evolves”; Appendix D.3 for details on these analyses). We show that partial selfing favours the evolution of XY over ZW sex determination, especially when inbreeding depression is high (Fig. 4C). This is because selfing increases competition for reproduction through female relative to male function, and inbreeding depression reduces the reproductive value of offspring produced via the female function (i.e., it reduces the relative influence of self-fertilised offspring on the long-term demography of the population; Charlesworth, 1980; Caswell, 2001; Rousset, 2004). The combination of these two effects means that, in a population where male and female alleles segregate, an intermediate, hermaphroditic heterozygote is better off allocating more resources to its male function, as this reduces the competition from homozygotes and boosts the reproductive value of its offspring. Together, these conditions favour the evolution of dominance of the male over the female allele, and therefore the emergence of XY sex determination.

Disruptive selection promotes the concentration of the genetic basis of sex. For practical reasons, we have assumed that sex allocation is the outcome of allelic expression at a single locus. However, sex allocation in hermaphroditic populations may often be a quantitative trait influenced by many loci (Meagher, 1999; Ashman, 2003; Mazer et al., 2007). This possibility raises the question of how dioecy might evolve in a hermaphroditic population in which variation in sex allocation has a polygenic basis. Previous modelling has shown that disruptive selection promotes the concentration of the genetic basis of traits from many to few or only one locus, as this results in greater heritability of the differentiated phenotypes (van Doorn and Dieckmann, 2006; Kopp and Hermisson, 2006). To study how this might occur in the evolution of dioecy, we extend our simulations to a scenario where sex allocation is initially determined by L freely-recombining sex allocation loci. In addition, we introduce a modifier locus at which alleles that determine the contribution of each locus to the phenotype can segregate (for instance, one allele may code for an equal contribution of each of the L sex allocation loci, while another may cause one of the L loci to determine most of the variation in sex allocation, Kopp and Hermisson, 2006; Appendix E for details). Alleles at the modifier locus are subject to small-effect mutations, so that the relative contribution of loci to sex allocation evolves jointly with allelic effects and dominance at each locus, all in a gradual manner.

To see the effects of disruptive selection on the genetic basis of sex, we assume that each of the L sex allocation loci initially contributes equally to the trait and that conditions are such that selection initially favours hermaphroditism (e.g., because gain curves saturate). Simulations show that, in this case, the contributions of the different loci to the phenotype, though variable, remain similar (Fig. 5A, shaded area). The population, meanwhile, shows a unimodal trait distribution centred around the optimal value x^* (Fig. 5B, shaded area). Suppose then that, at some given generation, conditions change such that selection on sex allocation now favours dioecy (e.g., gain curves now accelerate). When this occurs, we observe the progressive silencing of all but one locus, whose relative contribution to the trait keeps increasing until it explains all variation in sex allocation (Fig. 5A, non-shaded area). This concentration of sex allocation to a single locus allows for the concomitant evolution of separate sexes in the population via the gradual divergence of males and females (Fig. 5B, non-shaded area).

Discussion

The frequent evolution of dioecy from hermaphroditism in flowering plants is thought to have often occurred in a step-wise process that involves gynodioecy as an intermediate step, with XY or ZW sex determination emerging if the initial mutation causing male sterility was fully recessive or fully dominant, respectively (the ‘gynodioecy’ pathway, Charlesworth and Charlesworth, 1978a, 1981). An alternative scenario for transitions to dioecy, relevant to many plants but also animals in clades in which dioecy has evolved from hermaphroditism, invokes the gradual divergence in sex allocation of hermaphrodites in response to selection for sexual specialisation (the ‘monoecy-paradioecy’ pathway, Lloyd, 1980). This scenario has been much discussed (Lloyd, 1980; Renner and Ricklefs, 1995; Cronk, 2022; Pannell and Jordan, 2022), but there has so far been little theoretical investigation of how it might unfold and lead to XY or ZW sex determination (Charlesworth and Charlesworth, 1978b). Here, we conducted a formal analysis of the gradual evolution of dioecy from hermaphroditism, and showed that heterogametic sex determination can be the outcome of a gradual adaptive process involving the joint evolution of sex allocation with its genetic architecture.

Our results demonstrate that selection can act on dominance at a sex-determining locus, thereby providing an adaptive hypothesis for why some species transitioning to dioecy acquire XY while others acquire ZW sex determination. Namely, we found that selection can influence whether XY or ZW sex determination evolves, and that which of these two systems is more likely to emerge depends on the mating

system of ancestral hermaphrodites as well as on the trade-off between male and female allocation (as described by fitness gain curves). Under complete outcrossing, the conditions favouring XY or ZW sex determination are symmetrical, with selection favouring dominance of the allele for the sex where the benefits of sexual specialisation are the weakest (Fig. 4B). However, this symmetry is broken when dioecy evolves in populations of partially self-fertilising hermaphrodites, in which case the emergence of XY sex determination is more likely, especially when inbreeding depression is high and selfing is frequent (Fig. 4C). Given that most dioecious plants documented so far have XY systems, albeit based on a small fraction of the thousands of species with separate sexes (about 85%, Ming et al., 2011; Leite Montalvão et al., 2021), our results yield a new argument in support of the suggestion that dioecy might often evolve from hermaphroditism as a device to avoid inbreeding (Charlesworth and Charlesworth, 1978a,b).

In addition to evolving in response to selection for inbreeding avoidance, dioecy may also evolve when the ecological context favours sexual specialisation (Charnov et al., 1976; Freeman et al., 1997). In this case, our model predicts that whether an XY or a ZW system evolves should depend on how ecology influences the relative shapes of the male and female fitness gain curves, with XY favoured over ZW when the female gain curve is more accelerating than the male one, i.e., when benefits of specialisation are enjoyed more by females than males. There are still very few empirical estimates of the shape of these curves, but it is generally thought that they are more likely to be saturating than accelerating, e.g., due to local mate and resource competition under limited pollen or seed dispersal, respectively (Hamilton, 1967; Taylor and Bulmer, 1980; Charnov, 1982; Brunet, 1992; Charlesworth, 1999; Pannell and Jordan, 2022), potentially explaining the high prevalence of hermaphroditism in flowering plants (Käfer et al., 2017). Nevertheless, several ecological mechanisms that may cause gain curves to accelerate have been proposed in the literature (Bawa, 1980; Givnish, 1982; Freeman et al., 1997; Charlesworth, 1999; Pannell and Jordan, 2022). In plants with fleshy fruits, for instance, individuals producing larger crops of fruits (i.e., allocating more heavily to female function) may achieve more efficient seed dispersal due to increased attractiveness to animal dispersers. This coupling of sex allocation with seed dispersal can generate multiplicative benefits to specialising into female function through reduced kin competition among seeds of more female individuals, thereby causing the female gain curve to accelerate (Givnish, 1982; Vamosi et al., 2007; Biernaskie, 2010, see also Appendix F for a mathematical formalisation of this argument). Similarly, seeds of plants producing larger seed crops may benefit from a lower predation risk due to 'predator satiation' (Janzen, 1971; Lloyd, 1982), which could also lead the female gain curve to accelerate through a coupling between seed survival and seed production. To the extent that dioecy

might have evolved in response to selection for sexual specialisation, our results thus suggest that the observed excess of XY systems in dioecious plants may in part be the outcome of selection in populations in which the female gain curve was more accelerating than the male one. All else being equal, we should thus expect to find a greater prevalence of XY sex determination in dioecious species in which females benefit from sexual specialisation more than males, and so to find a statistical association between the prevalence of XY and the presence of ecological features most conducive to female specialisation such as, e.g., seed dispersal by animals (Givnish, 1982), in recently evolved dioecious species.

Irrespective of why selection promotes dioecy, our model also throws light on the emergence of single-locus sex determination from an initially polygenic basis of sex allocation in hermaphrodites. Specifically, our multilocus results reveal that selection for dioecy favours the concentration of genetic variation in sex allocation at a single (sex-determining) locus. Empirically, the way and the speed at which this concentration materialises will depend on the amount of available standing variation and on the genomic processes involved, which may include, for example, rearrangements of the regulatory network, recombination suppression, or gene duplication (Bachtrog et al., 2014; Henry et al., 2018). There is ample evidence for polygenic variation for sex allocation in many hermaphroditic taxa (as recently shown in e.g. *Mercurialis annua*, Cossard et al., 2021, or *Schiedea salicaria*, Campbell et al., 2022; for reviews see Meagher, 1999, Table 1 in Ashman, 2003 and in Mazer et al., 2007), but the specific loci involved are not yet known for any species. In dioecious plants, meanwhile, the specific genes involved in sex determination have only been described in a handful of species, with sex-determining loci consisting of either one master switch (e.g., in persimmon, poplar and willow, Akagi et al., 2014; Müller et al., 2020) or two fully linked genes at which sterility mutations segregate as expected if dioecy evolved via the gynodioecy pathway (e.g., in asparagus and kiwifruit, Akagi et al., 2019; Harkess et al., 2020; see also Westergaard, 1958 for phenotypic evidence consistent with this type of architecture). Either of these genetic architectures is compatible with the outcome of our model, which sees dioecy ultimately achieved through a single dominant Mendelian element. Whether this element involves one or more genes will depend on the genetic basis of sex allocation in the ancestral hermaphrodite, indicating that single-gene sex determination could sometimes evolve from hermaphroditism directly rather than derive from a previously established two-gene system (Charlesworth, 2019; Renner and Müller, 2021). Together, our results suggest that valuable insights could be gained from studying the role played in the genetic control of sex allocation in hermaphrodites by genes involved in sex determination in closely related dioecious taxa.

The gradual scenario we describe might be especially relevant to transitions to dioecy from monoecy in flowering plants, with individuals gradually diverging in the number of their male and female flowers; phylogenetic evidence suggests that such transitions may have been frequent (Renner and Ricklefs, 1995; Cronk, 2022). Taxa comprising closely related dioecious and monoecious species might in fact be particularly well-suited to investigate the evolutionary dynamics outlined in our model, as sex allocation is more easily quantified in monoecious plants (where male and female flowers can be counted) than in species with bisexual flowers. In animals, our model might be useful to understand the evolution of separate sexes from hermaphroditism in taxa such as polychaete annelids (e.g., in the genus *Ophryotrocha*; Picchi and Lorenzi, 2018) and flatworms (e.g., in the genus *Schistosoma*; Ramm, 2016). However, the few independent transitions to dioecy that have occurred in these clades limit the power of comparative studies to test our results on the evolution of XY vs. ZW sex determination. Experimental evolution may provide a more productive alternative. When subjected to sex-limited selection, lines of the hermaphroditic flatworm *Macrostomum lignano* evolve female- and male-biased phenotypes in remarkably few generations (Nordén et al., 2023; Cirulis et al., 2024). Selection in these experiments relied on a GFP marker that effectively fixes the nature of the sex-determining locus, so that unfortunately their results cannot be used to assess whether XY or ZW evolution is more likely. Apart from plants and hermaphroditic animals, our model may also be useful to understand the emergence of ‘split sex-ratios’ in ants and other social Hymenoptera, where colonies produce either male or female sexuals leading to a form of colony-level dioecy (Meunier et al., 2008; Kueimmerli and Keller, 2009). Interestingly, split sex-ratio is determined by a single non-recombining region acting like a W chromosome in *Formica glacialis* (Lagunas-Robles et al., 2021). According to our model, this may be the result of strong benefits to specialisation into the production of males, but here at the colony rather than individual level.

In conclusion, our analyses indicate an evolutionary pathway from hermaphroditism to dioecy through the joint evolution of sex allocation and its genetic architecture. This gradual process readily leads to a heterogametic sex-determining locus, paving the way for further genetic changes underlying the evolution of sex chromosomes such as recombination suppression, genetic degeneration and dosage compensation (Ellegren, 2011; Bachtrog et al., 2014; Charlesworth, 2019; Lenormand and Roze, 2022). Our model also provides an adaptive hypothesis for the apparently high frequency of XY sex determination in dioecious plants, which we have shown is especially favoured under inbreeding avoidance. Beyond sex determination, our model showcases how ecology can influence the way selection shapes the genetic basis of polymorphic traits.

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Data and code availability: Simulation programs and scripts are available at <https://zenodo.org/doi/10.5281/zenodo.13378508> (Lesaffre et al., 2024)

Authors contributions: TL, JRP and CM conceptualised the study. TL performed the analysis under the supervision of CM. TL wrote the initial draft, and all three authors contributed to the final version. JRP and CM acquired the funding for the project.

Declaration of interests: The authors declare no conflict of interest.

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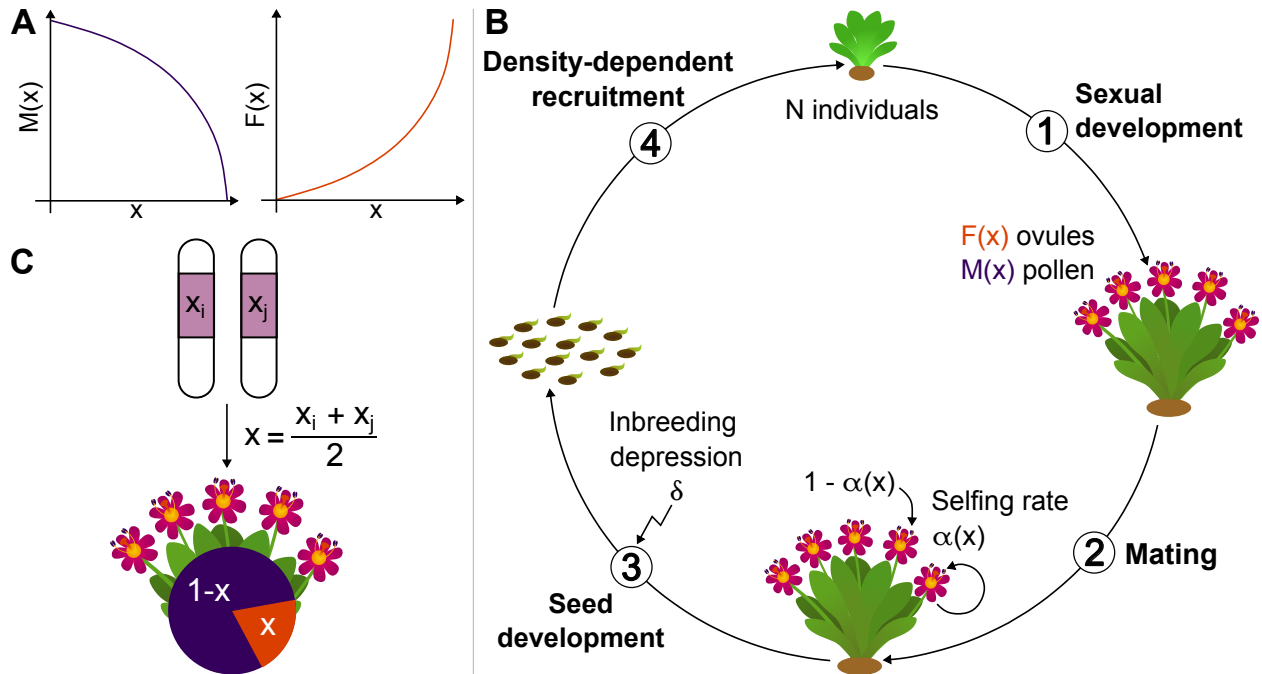


Figure 1: Life cycle and genetic architecture of sex allocation. **A** Male ($M(x)$, dark purple) and female ($F(x)$, orange) gain curves as functions of the fraction x of resources allocated to female function. In this example, the male gain curve is saturating, reflecting diminishing fitness returns through male function, whereas the female gain curve is accelerating, reflecting increasing fitness returns through female function. **B** Life cycle assumed in the model. See main text for details. **C** Genetic architecture of sex allocation in our baseline model. The sex allocation strategy x expressed by an individual is determined by its genotype at a quantitative trait locus where alleles are additive.

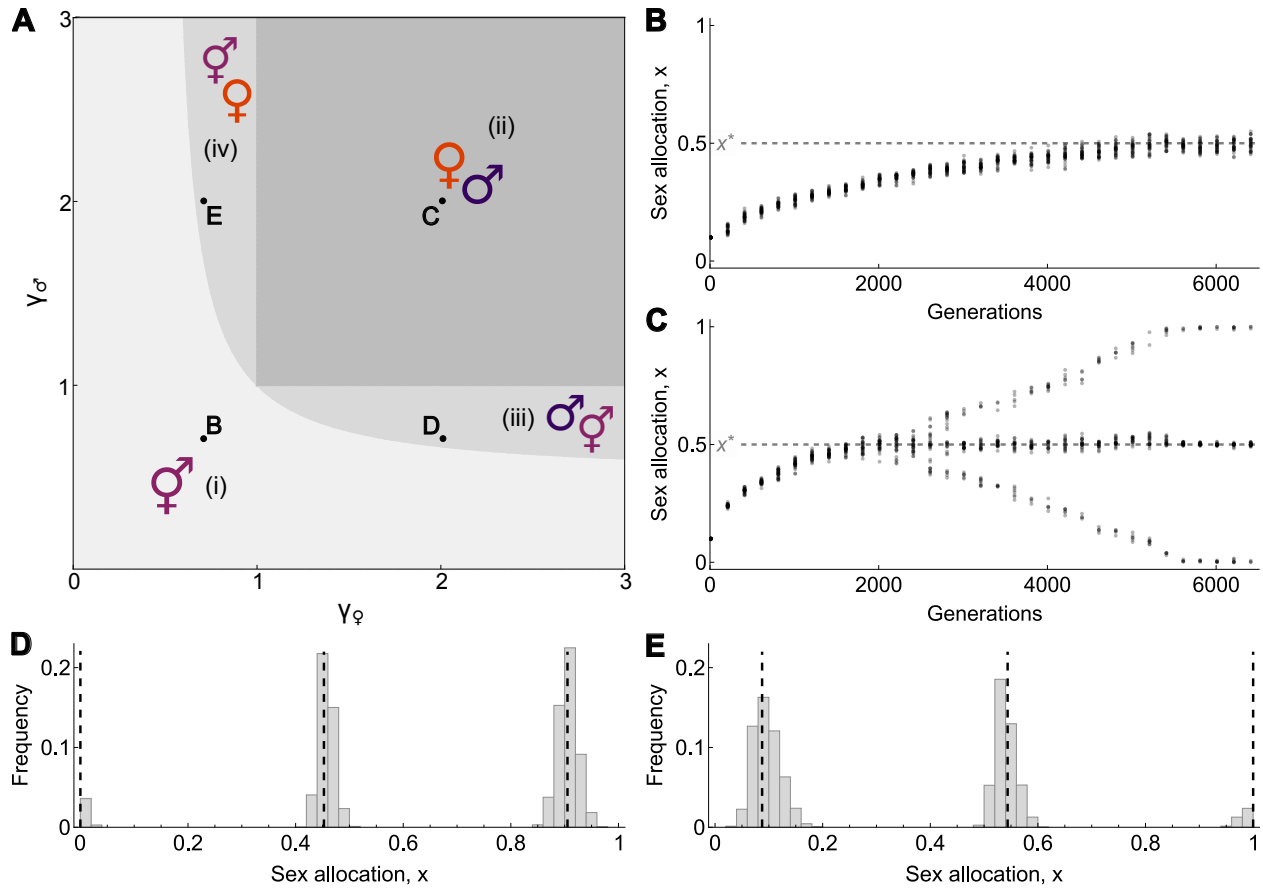


Figure 2: The gradual evolution of sex allocation and sexual systems under complete outcrossing. **A** The four outcomes of evolution according to γ_ϕ and γ_σ (Appendix B.1 for analysis): (i) hermaphroditism (light grey); (ii) dioecy (dark grey); (iii) androdioecy (medium light grey) and (iv) gynodioecy (medium light grey), where pure males and females coexist with hermaphrodites, respectively. **B-E** Results from individual based simulations showing the four possible outcomes outlined in Panel A. Simulations follow the evolution of a population of $N = 10^4$ individuals, with a per-locus mutation rate of $\mu = 5 \times 10^{-3}$, and where a mutation creates a new allele whose genetic effect consists of its original value to which is added a small value randomly sampled from a Normal distribution with mean 0 and standard deviation $\sigma = 10^{-2}$ (Appendix B.3 for details on simulations). **B** The phenotypes expressed by 30 randomly sampled individuals every 200 generations under conditions predicted to lead to hermaphroditism (with $\gamma_\phi = \gamma_\sigma = 1/\sqrt{2}$). The population converges to express the equilibrium strategy $x^* = \gamma_\phi / (\gamma_\phi + \gamma_\sigma) = 1/2$, indicated by the light grey dashed line. **C** Same as B under conditions predicted to favour dioecy (with $\gamma_\phi = \gamma_\sigma = 2$). Disruptive selection leads to the coexistence of pure male ($x = 0$) and female ($x = 1$) alleles. At equilibrium, the population is composed of homozygous males (with genotype 0/0), homozygous females (with genotype 1/1), and heterozygous hermaphrodites (with genotype 1/0). **D** Distribution of phenotypes at equilibrium in a simulation where androdioecy evolves (with $\gamma_\phi = 2$ and $\gamma_\sigma = 1/\sqrt{2}$). Dashed vertical lines indicate the equilibrium strategies the analytical model predicts, which are calculated according to the method described in Appendix B.2. **E** Same as D where gynodioecy evolves (with $\gamma_\phi = 1/\sqrt{2}$ and $\gamma_\sigma = 2$).

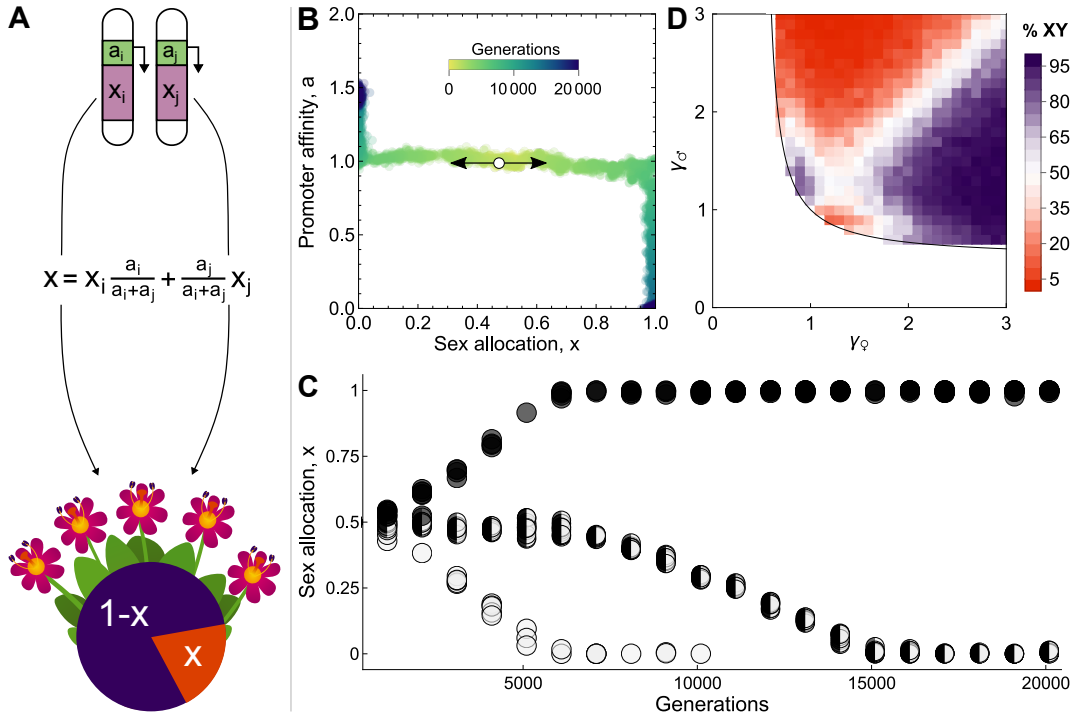


Figure 3: The joint evolution of sex allocation and dominance. **A** Genetic architecture of sex allocation. The sex allocation locus is composed of a sex allocation gene and its promoter. Transcription factors must bind to the promoter for the sex allocation gene to be expressed, which they do at a rate that depends on the promoter's affinity, a . Consequently, sex allocation alleles are expressed in proportion to their promoter's affinity, and promoter affinities encode the dominance relationship between sex allocation alleles. In this example, alleles x_i and x_j are associated with promoters with affinities a_i and a_j , so that they contribute in proportions $a_i/(a_i + a_j)$ and $a_j/(a_i + a_j)$ to the expressed sex allocation strategy x . **B** Phase diagram of sex allocation and promoter affinity when the two evolve jointly in a simulation under conditions predicted to lead to dioecy ($\gamma_\phi = \gamma_\sigma = 2$). Each dot depicts an allele, characterised by the sex allocation strategy it encodes and its promoter's affinity. Colour indicates time since the start of the simulation (in generations), with darker colours indicating later times. The population is initially monomorphic with $x_0 = 0.5$ and $a_0 = 1$ (white circle). Here, the male allele becomes associated with an increasingly high affinity promoter while the female allele becomes associated with an increasingly low affinity one, leading to complete dominance of the male allele and the emergence of XY sex determination. (Parameters: $N = 10^4$, Appendix C.1 for simulation details). **C** Phenotypes expressed by individuals as a function of time for the same simulation as figure B. Each circle depicts an individual. Fully black and white circles depict homozygotes for female- and male-biased alleles, respectively, whereas half black and white circles depict heterozygotes (defined as individuals bearing two alleles that are more different than the average difference between two alleles within the same individual). As sex allocation alleles diverge and dominance evolves, heterozygotes gradually become more male-biased, and eventually replace male homozygotes, thereby achieving dioecy with XY sex determination. **D** Proportion of XY systems evolving out of 200 simulations with $N = 10^3$, for values of γ_ϕ and γ_σ spanning the parameter range in which selection on sex allocation is disruptive. XY and ZW systems are equally likely to emerge when $\gamma_\phi = \gamma_\sigma$, whereas XY systems are more prevalent where $\gamma_\phi > \gamma_\sigma$ and ZW systems where $\gamma_\phi < \gamma_\sigma$ when gain curves are sufficiently accelerating. When gain curves are close to being linear, the correspondence between gain curve shape and the proportion of XY evolving is reversed. Parameters used in all simulations: mutation probability $\mu = 5 \times 10^{-3}$, standard deviation in mutational effect $\sigma = 10^{-2}$.

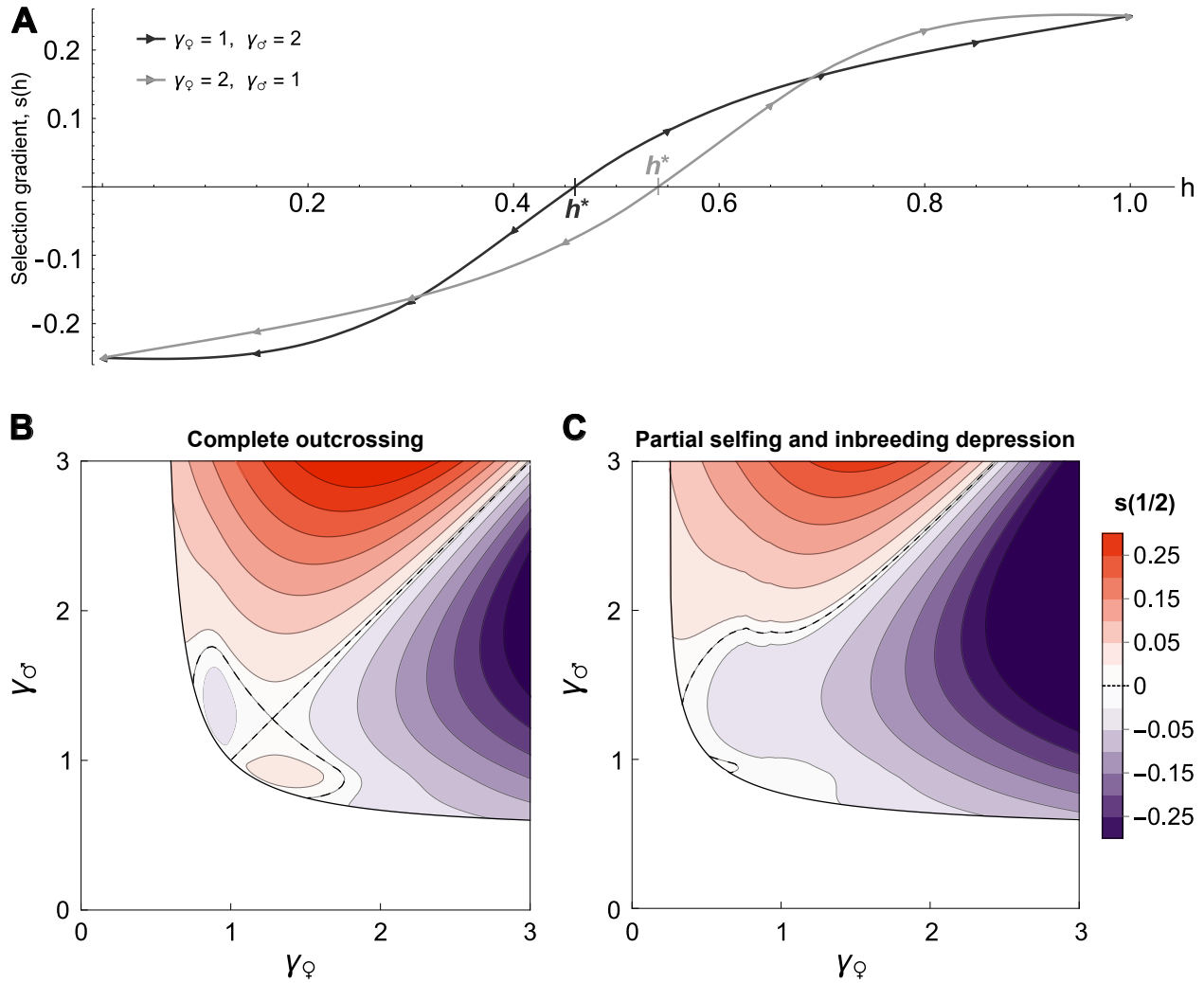


Figure 4: The nature of selection on dominance at a sex-determining locus. **A** Selection gradient $s(h)$ acting on the dominance h of the female allele $x_{\text{♀}} = 1$ over the male allele $x_{\text{♂}} = 0$ for two cases leading to dioecy (Appendix C.2.4 for how to compute this gradient). The selection gradient $s(h)$ is negative when h is smaller than the threshold h^* such that $s(h^*) = 0$, and positive when h is greater than h^* . Therefore, selection always eventually leads to either $h = 0$ (leading to an XY system) or $h = 1$ (leading to a ZW system). Additionally, the larger h^* is, the more readily an XY system should evolve and conversely, the smaller h^* , the more likely a ZW system evolves. For the examples shown here, we expect to see an XY in the case depicted in grey and a ZW in black. **B** Selection gradient on dominance at additivity, $s(1/2)$, in the complete outcrossing case ($\alpha_0 = 0$). Dashed lines indicate points where the gradient is zero so that XY and ZW sex determination are equally likely to evolve. Orange shades are for $s(1/2) > 0$, which indicates that $h^* < 1/2$ and thus that ZW sex determination is favoured, whereas purple shades are for $s(1/2) < 0$, which entails that $h^* > 1/2$ and XY sex determination is favoured. Variations in the sign and intensity of the selection gradient match almost perfectly with the proportion of XY systems evolving in simulations (Fig. 3D). **C** Same as B but with partial selfing and strong inbreeding depression ($\alpha_0 = 0.75$, $\delta = 0.75$, $\beta = 1$). The parameter space in which an XY system is favoured becomes much larger than the one in which a ZW system is favoured, indicating that selfing promotes XY over ZW sex determination.

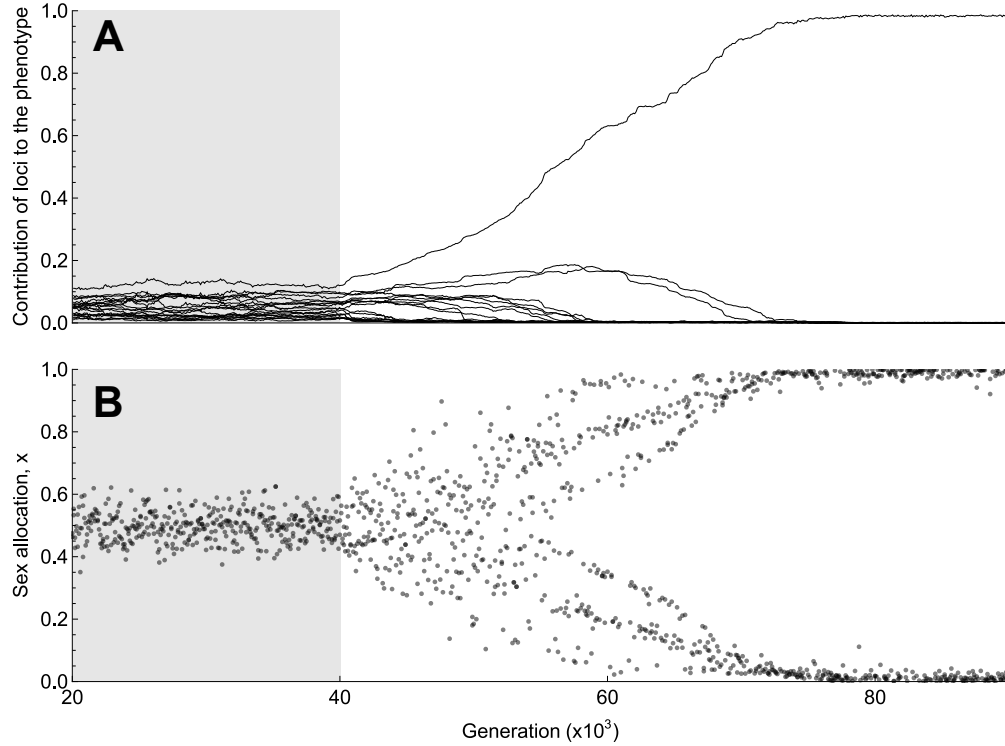


Figure 5: Concentration of the genetic architecture of sex allocation in response to selection for dioecy. Results of a simulation with $L = 20$ loci initially contributing equally to the sex allocation strategy expressed by individuals (Appendix E for details on these simulations). Selection favours hermaphroditism for the first 40,000 generations (i.e. gain curves are saturating, with $\gamma_{\text{♀}} = \gamma_{\text{♂}} = 1/2$; grey background in the plots). An ecological change then occurs, causing selection to favour dioecy for the rest of the simulations (i.e. gain curves become accelerating, with $\gamma_{\text{♀}} = \gamma_{\text{♂}} = 2$; white background in the plot). **A** Relative contributions of the 20 quantitative trait loci to the phenotype as a function of time (after a burn-in period of 20,000 generations). When hermaphroditism is favoured (before the ecological change), loci contributions vary due to drift but remain roughly equal (on average 0.05). In contrast, when dioecy is favoured, selection drives the evolutionary dynamics of loci contributions, leading all but one locus to become silenced (i.e. to not contribute to the sex allocation phenotype), with the remaining locus acting as the sex-determining locus. **B** Sex allocation strategies expressed in the population as a function of time. While selection favours hermaphroditism, the population remains unimodally distributed around $x^* = \gamma_{\text{♀}} / (\gamma_{\text{♀}} + \gamma_{\text{♂}})$ with little phenotypic variance. When dioecy becomes favoured, the phenotypic variance increases and the distribution gradually shifts from unimodal to bimodal, ultimately achieving dioecy. Parameters used in simulations: population size $N = 5 \times 10^3$; mutation probability $\mu = 10^{-2}$; standard deviation in mutational effect $\sigma = 5 \times 10^{-2}$.