A model for the gradual evolution of dioecy and heterogametic sex determination

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Abstract. In plants with separate sexes, the development of an individual as male or female is controlled by a dominant allele at a sex-determining locus - the fundamental basis of XY and ZW systems. The many independent transitions from hermaphroditism to dioecy that have taken place in flowering plants must therefore often have entailed the emergence of such a locus. One proposition is that this evolution occurs in two major steps, with the initial invasion of a male-sterility mutation at one gene followed by mutations causing female sterility at a second closely linked gene. Here, we show that dioecy with heterogametic sex determination can also emerge in a gradual adaptive process, involving the co-evolution of resource allocation to different sexual functions jointly with its genetic architecture. Our model further reveals that the evolution of an XY versus a ZW system depends on the mating system in ancestral hermaphrodites as well as the trade-off they face between allocating resources to male and female functions. In particular, selfing and inbreeding depression systematically favour the evolution of XY systems, which may help to explain why the vast majority of dioecious flowering plants have this sex determination system. Taken together, our results throw new light on the possible origins of dioecy from hermaphroditism by revealing a hitherto unrecognised link between the ecology and economics of sex allocation and the genetic basis of sex determination.

Keywords. Gradual evolution, quantitative traits, genetic architecture, separate sexes, sex determination.

Introduction

Many plants have evolved separate sexes (or dioecy) from hermaphroditism (Charlesworth, 1985; Renner, 2014; Henry et al., 2018). Explanations for these repeated transitions have come from two types of models. First, sex allocation theory uses optimality arguments to identify conditions in which natural selection favours individuals allocating all their resources to one sexual function over those allocating to both (Charnov et al., 1976; Charlesworth and Charlesworth, 1981; Charnov, 1982). Whether this happens depends on how resource allocation affects fitness, which may be influenced by a number of ecological and physiological factors (Givnish, 1982; Lloyd, 1982; Renner and Ricklefs, 1995; Freeman et al., 1997; Pannell and Jordan, 2022; Masaka and Takada, 2023). The joint effect of these factors is usefully summarised in male and female 'gain curves', which relate fitness gained through each sexual function to the amount of resources allocated to it (Charnov et al., 1976). Gain curves that increase in an accelerating manner indicate increasing returns on investment and therefore an advantage to sexual specialisation (Charnov et al., 1976; Charnov, 1982). The second strand of theory uses population genetic arguments, which have revealed that dioecy is further favoured by inbreeding depression (Charlesworth and Charlesworth, 1978a,b, 1981). When inbreeding depression is strong, a population of partially self-fertilising hermaphrodites can be invaded by a male-sterility mutation because male-sterile individuals (i.e. females) cannot self-fertilise and thus escape the deleterious effects of inbreeding (this also favours partial male sterility provided it reduces selfing, Charlesworth and Charlesworth, 1978b). In turn, the presence of females favours the invasion of female-sterility mutations turning hermaphrodites into males.

Selection may favour separate sexes, but whether dioecy evolves depends on the genetic architecture of sex allocation (Charlesworth, 1999; Beukeboom and Perrin, 2014). Because sex is often determined by a locus where one sex is heterozygous and the other is homozygous (XX/XY or ZW/ZZ females and males, Ming et al., 2011; Bachtrog et al., 2014; Beukeboom and Perrin, 2014), the transition from hermaphroditism to dioecy must in many cases have involved the emergence of such a locus. Optimality models rely on the 'phenotypic gambit' and are thus mute about genetics (Charnov et al., 1976; Charnov, 1982). Population genetic models, meanwhile, suggest that sex-determining loci evolve through the invasion of an initial male-sterility mutation at a first gene, followed by one or more mutations causing female sterility at a second, closely linked gene (the 'two-gene model', Charlesworth and Charlesworth, 1978a,b, 1981; Charlesworth, 1991; Charlesworth et al., 2005; Beukeboom and Perrin, 2014; Olito and Connallon, 2019). Depending on whether that initial male sterility allele is fully recessive or fully domi-

nant, this scenario leads to XY or ZW sex determination, respectively. Here, we propose an alternative model where instead of being fixed and pre-determined, both dominance and sex-specific fecundity arise gradually through the co-evolution of sex allocation and its underlying genetic architecture. We show that XY and ZW systems readily emerge from this co-evolution, and that whether selection promotes one or the other depends on the strength of inbreeding depression and the shape of gain curves.

Model

The ecological scenario we envisage follows closely from Charlesworth and Charlesworth (1978b, 1981). We consider a large population in which individuals allocate a proportion x of their reproductive resources to their female and $1-x$ to their male function, leading to a trade-off between both functions. Strategy x results in female and male fecundities $F(x) = F_0 x^{\gamma_♀}$ and $M(x) = M_0(1-x)^{\gamma_♂}$, respectively, where F_0 and M_0 correspond to the maximum achievable fecundity, and exponents $\gamma_♀$ and $\gamma_♂$ 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. $\alpha'(x) \leqslant 0$; where necessary, we specifically assume that $\alpha(x) = \alpha_0(1-\beta x)$ where $0 \leqslant \alpha_0 < 1$ denotes the maximum achievable selfing rate and $0 \leqslant \beta \leqslant 1$ 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. Finally, adults die and a new generation is formed from viable seeds (Figure 1B; Appendix A for more details).

When gain curves are accelerating ($\gamma_♀ > 1$ and $\gamma_♂ > 1$, Charnov et al., 1976; Charnov, 1982) or when inbreeding depression is sufficiently strong (Charlesworth and Charlesworth, 1981), a hermaphrodite individual in a population of males and females has lower than average fitness; and conversely, a unisexual of either sex has greater than average fitness in a population of hermaphrodites. Dioecy should thus be evolutionarily stable under these conditions, and may 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, 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 ('continuum-of-alleles' model; Fig. 1C; Kimura, 1965, p. 883 in Walsh and Lynch, 2018). This locus could be a pleiotropic gene, such as a regulatory element that influences the development of female and male traits, or fully-linked genes that are independent targets of partial female and male sterility mutations (where in both cases there is a physiological trade-off among female and male functions, as in e.g., Charlesworth and Charlesworth, 1978a,b, 1981). Genetic effects on x are initially additive but translate to non-additive effects on fitness when $F(x)$ and $M(x)$ are non-linear. To investigate the emergence of sex-determining systems, we allow later for the evolution of the genetic architecture of sex allocation x (i.e. allow for non-additive genetic effects on x to evolve).

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 that evolution occurs in two phases (Appendix B.1). First, the population converges gradually via a sequence of substitutions of mutations of small effect to the intermediate strategy $x^* = \gamma_♀/(\gamma_♀ + \gamma_♂)$, with all individuals being hermaphrodites (Appendix B.1.2.1). Second, the population experiences either stabilising selection and therefore remains hermaphroditic, or negative frequency-dependent disruptive selection (Geritz et al., 1998; Metz and Leimar, 2011; Avila and Mullon, 2023), which results in the gradual differentiation of two types of alleles: one that causes its carrier to allocate more resources to female function, and the other to male function. The distribution of allelic effects thus goes from being unimodal to bimodal. Which of these two outcomes unfolds depends on the shape of gain curves, with disruptive selection requiring at least one of them to be sufficiently accelerating (specifically that $2\gamma_♀\gamma_♂ > \gamma_♀ + \gamma_♂$; Fig. 2A; Appendix B.1.2.2). When both gain curves are accelerating ($\gamma_♀ > 1$ and $\gamma_♂ > 1$), 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 (Fig. 2C). 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 (Fig. 2D,E; Appendix B.2.3 for details). These results align with classical optimality models in that they

delineate the same conditions for hermaphroditism, dioecy, andro- and gynodioecy to be evolutionarily stable (Charnov et al., 1976; Charnov, 1982, see Appendix B.4 for more details on this connection). However, gradual evolution to polymorphic sexual systems here leads to the coexistence of three types: two homozygotes that express female- and male-biased sex allocation strategies, respectively; and a heterozygote with an intermediate hermaphroditic strategy (Figure 2C-E).

Emergence of XY and ZW sex determination. To examine how dioecy might ultimately evolve, we allow for the co-evolution of sex allocation with its underlying genetic architecture. We first assume that the evolving locus is composed of two linked elements, a sex allocation gene, where alleles code for different sex allocation strategies, and its promoter, where alleles determine the level of expression of their linked 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; Rueffler et al., 2006). We let the sex allocation gene and its promoter each undergo recurrent mutations of small effect, so that dominance and sex allocation co-evolve (Appendix C.1 for details on the model). We investigate this model using stochastic simulations, first under conditions predicted to lead to pure male and female alleles (so when $\gamma_{♀} > 1$ and $\gamma_{♂} > 1$). In these simulations, complete dominance of one sex allocation allele always evolves, so that eventually dioecy is complete and the population comprises only males and females (Figure 3B-C). Remarkably, whether the male or the female allele becomes dominant depends strongly on male and female gain curves (i.e. on $\gamma_{♀}$ and $\gamma_{♂}$, Figure 3D). Provided 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 $\gamma_{♀} > \gamma_{♂}$), leading to the emergence of an XY system. Conversely, when fitness returns increase more steeply via male function (i.e., when $\gamma_{♂} > \gamma_{♀}$), the female allele most often becomes dominant, leading to a ZW system. When both gain curves are close to being linear (i.e. when $\gamma_{♂}$ and $\gamma_{♀}$ are close to one), this correspondence is reversed so that XY is favoured when $\gamma_{♂} > \gamma_{♀}$, and ZW when $\gamma_{♀} > \gamma_{♂}$. 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 $\gamma_{♀} > 1$ or $\gamma_{♂} > 1$), and obtained the same results qualitatively: the allele encoding 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 $\gamma_{♀} > 1$), or heterozygote (ZW) females and homozygote (ZZ) hermaphrodites (when $\gamma_{♂} > 1$).

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 the model in which dominance is a quantitative trait. In this version, two sex allocation alleles segregate, $x_♀$ and $x_♂$, where one encodes a more female strategy than the other ($x_♀ > x_♂$, hereafter referred to as 'female' and 'male' alleles for brevity). In $x_♂/x_♀$ heterozygotes, the female allele is expressed proportionally to a dominance coefficient h, so that the sex allocation strategy of a $x_♂/x_♀$ heterozygote is given by $h\ x_♀ + (1-h)\ x_♂$. We assume this h is controlled by a quantitative trait locus that is 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). 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. $h \to 0$ when $h < h^*$) and above which selection favours ever higher values of h (i.e. $h \to 1$ when $h > h^*$). Complete dominance of either the male or female allele therefore always evolves, 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 indicates that whether selection promotes XY or ZW sex determination is independent from the particular mechanisms responsible for variation in dominance (whether through *cis* or *trans* effects), but rather comes down to gain curves in the absence of selfing.

A decomposition of the selection gradient on dominance reveals that selection on sex-determining systems and its relationship with gain curves can be understood as follows (see Appendix C.2.4 for details). Selection on dominance h acts only in $x_♂/x_♀$ heterozygotes, that are hermaphrodites. Such a heterozygote can either become more female or become more male through an increase or a decrease in h, respectively. But whatever the change in dominance, this heterozygote will always be less fit than female homozygotes through female function and than male homozygotes through male function. In fact, homozygotes typically impose such strong competition owing to their fecundity advantage that it is best for a heterozygote to allocate more to the sex in which this advantage is the weakest. This entails becoming more female when $\gamma_♂ > \gamma_♀$ and more male when $\gamma_♂ < \gamma_♀$, leading to ZW and XY

systems, respectively. When both gain curves are close to linear ($\gamma_♀$ and $\gamma_♂$ close to one), the advantage of homozygotes is reduced and it is then best for a heterozygote to allocate to the function that leads to the greatest increase in fecundity, i.e. becoming more female when $\gamma_♀ > \gamma_♂$ and more male when $\gamma_♀ < \gamma_♂$.

Partial selfing and inbreeding depression favour XY sex determination. Our results so far assume complete outcrossing, but dioecy and other polymorphic sexual systems are also known to evolve in partially selfing populations subject to inbreeding depression (e.g. gyno- and androdioecy, Charlesworth and Charlesworth, 1978a,b, 1981). To examine how partial selfing and inbreeding depression influence the evolution of sexual systems and sex determination, we analyse our model with $\alpha_0 > 0$ and $\beta > 0$ in Appendix D. Where selection leads to polymorphic sexual systems, we find that partial selfing always favours the evolution of XY over ZW sex determination, especially when inbreeding depression is high (Fig. 4C). This is because selfing increases competition through female function, while inbreeding depression reduces the reproductive value of offspring produced via this function (Appendix D.3.2 for details). The combination of these effects favours dominance of the male allele and thus the emergence of XY sex determination.

Discussion

Dioecy is commonly thought to evolve from hermaphroditism 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 is fully recessive or fully dominant, respectively (the 'gynodioecy' pathway, Charlesworth and Charlesworth, 1978a,b, 1981). Our analyses indicate that dioecy underlain by an XY or a ZW system can also be the outcome of a gradual adaptive process consisting of the joint evolution of sex allocation with its genetic architecture. Our model thus gives formal support to the alternative idea that dioecy may result from the divergence of male and female morphs without going through an intermediate gynodioecious state (the 'monoecy-paradioecy' pathway; Lloyd, 1980; Pannell and Jordan, 2022). Additionally, we show that selection can influence whether XY or ZW sex determination evolves, and that which of these two systems is favoured depends on the mating system of ancestral hermaphrodites as well as the trade-off between male and female function (i.e. gain curves). Under complete outcrossing, the conditions favouring XY or ZW sex determination are symmetrical, with selection typically favouring

dominance of the allele for the sex where the benefits of sexual specialisation are the weakest (Fig. 4B). This symmetry is broken by selfing in favour of XY sex determination (Fig. 4C). Our model therefore provides a new explanation for the observation that most dioecious plant species have XY rather than ZW sex determination (about 85%, Ming et al., 2011). Specifically, given the high frequency of XY sex determination in dioecious plants, our results suggest that dioecy might often evolve from partially selfing hermaphroditic ancestors (as previously suggested, but for very different reasons; Charlesworth and Charlesworth, 1978a), or in situations where the benefits of sexual specialisation are particularly pronounced for female function (a completely new result), which could for instance be the case under conditions of predator satiation (Janzen, 1971; Lloyd, 1982) or when animal seed dispersers are particularly attracted to plants with larger crops of fleshy fruits (Givnish, 1982; Vamosi et al., 2007; Biernaskie, 2010; Appendix E for an example).

The evolutionary dynamics envisioned by our model rely on the availability of heritable and continuous variation for being more female or male. While there is ample evidence for such variation in hermaphrodites across multiple taxa (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), the specific loci responsible for this variation are not yet known for any species. In dioecious plants, the genetic basis of sex determination has been described in only 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 (e.g. in asparagus and kiwifruit, Akagi et al., 2019; Harkess et al., 2020). Either is compatible with the outcome of our model, which sees dioecy ultimately achieved through a single dominant Mendelian element. In fact, we assumed that the development of sexual characters is controlled by a major-effect locus, but evolutionary dynamics would unfold similarly if many loci were initially involved, because disruptive selection always favours a concentration of genetic variation (Rueffler et al., 2006; Kopp and Hermisson, 2006; Yeaman and Whitlock, 2011).

Our model is particularly relevant to cases where dioecy evolved from monoecy in flowering plants, with individuals gradually diverging in the number of their male and female flowers (Renner and Ricklefs, 1995; Cronk, 2022). Nonetheless, our predictions should also apply to plants with bisexual flowers, and to animal taxa in which dioecy evolved from hermaphroditism, such as the *Ophryotrocha* genus in polychaete annelids or flatworms of the *Schistosoma* genus (Ramm, 2016; Picchi and Lorenzi, 2018; Leonard, 2018; Wang et al., 2022). Our model may also be useful to understand '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; Kuemmerli and Keller, 2009; Lagunas-Robles et al., 2021).

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References

T. Akagi, I.M. Henry, R. Tao, and L. Comai. A Y-chromosome–encoded small RNA acts as a sex determinant in persimmons. *Science*, 346(6209):646–650, 2014.

T. Akagi, S.M. Pilkington, E. Varkonyi-Gasic, I.M. Henry, S.S. Sugano, M. Sonoda, A. Firl, M.A. McNeilage, M.J. Douglas, T. Wang, R. Rebstock, C. Voogd, A.C. Allan, K. Beppu, I. Kataoka, and R. Ryutaro. Two Y-chromosome-encoded genes determine sex in kiwifruit. *Nature plants*, 5(8): 801–809, 2019.

T-L. Ashman. Constraints on the evolution of males and sexual dimorphism: field estimates of genetic architecture of reproductive traits in three populations of gynodioecious fragaria virginiana. *Evolution*, 57(9):2012–2025, 2003.

Piret Avila and Charles Mullon. Evolutionary game theory and the adaptive dynamics approach: adaptation where individuals interact. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 378(1876):20210502, 2023. doi: 10.1098/rstb.2021.0502.

D. Bachtrog, J.E. Mank, C.L. Peichel, M. Kirkpatrick, S.P. Otto, T.-L. Ashman, M.W. Hahn, J. Kitano, I. Mayrose, R. Ming, N. Perrin, L. Ross, N. Valenzuela, J.C. Vamosi, and The Tree of Sex Consortium. Sex determination: why so many ways of doing it? *PLoS Biology*, 12(7):e1001899, 2014.

L.W. Beukeboom and N. Perrin. *The evolution of sex determination*. Oxford University Press, USA, 2014.

J.M. Biernaskie. The origin of gender dimorphism in animal-dispersed plants: disruptive selection in a model of social evolution. *The American Naturalist*, 175(6):E134–E148, 2010.

S. Billiard, V. Castric, and V. Llaurens. The integrative biology of genetic dominance. *Biological Reviews*, 96(6):2925–2942, 2021.

D.R. Campbell, A.K. Sakai, S.G. Weller, T.M. Culley, A.K. Dunbar-Wallis, A.M. Andres, T.G. Wong, T. Dang, B. Au, M. Ku, A.R. Marcantonio, P.J. Ngo, A.A. Nguyen, M.H. Tran, and Q-P. Tran. Genetic potential for changes in breeding systems: Predicted and observed trait changes during artificial selection for male and female allocation in a gynodioecious species. *American Journal of Botany*, 109(11):1918–1938, 2022.

B. Charlesworth. The evolution of sex chromosomes. *Science*, 251(4997):1030–1033, 1991.

B. Charlesworth and D. Charlesworth. A model for the evolution of dioecy and gynodioecy. *The American Naturalist*, 112(988):975–997, 1978a.

D. Charlesworth. Distribution of dioecy and selfincompatibility in angiosperms. In *Evolution - essays in honour of John Maynard Smith*, pages 237–268. Cambridge University Press, 1985.

D. Charlesworth. Theories of the evolution of dioecy. In *Gender and sexual dimorphism in flowering plants*, pages 33–60. Springer, 1999.

D. Charlesworth and B. Charlesworth. Population genetics of partial male-sterility and the evolution of monoecy and dioecy. *Heredity*, 41(2):137–153, 1978b.

D. Charlesworth and B. Charlesworth. Allocation of resources to male and female functions in hermaphrodites. *Biological Journal of the Linnean Society*, 15(1):57–74, 1981.

D. Charlesworth, B. Charlesworth, and G. Marais. Steps in the evolution of heteromorphic sex chromosomes. *Heredity*, 95(2):118–128, 2005.

E.L. Charnov. *The Theory of Sex Allocation (MPB-18)*. Princeton University Press, 1982.

E.L. Charnov, J.J. Bull, and J. Maynard Smith. Why be an hermaphrodite? *Nature*, 263(5573):125–126, 1976.

G. Cossard, J.F. Gerchen, X. Li, Y. Cuenot, and J.R. Pannell. The rapid dissolution of dioecy by experimental evolution. *Current Biology*, 31(6):1277–1283, 2021.

Q. Cronk. The distribution of sexual function in the flowering plant: from monoecy to dioecy. *Philosophical Transactions of the Royal Society B*, 377(1850):20210486, 2022.

D.C. Freeman, J.L. Doust, A. El-Keblawy, K.J. Miglia, and E.D. McArthur. Sexual specialization and inbreeding avoidance in the evolution of dioecy. *The Botanical Review*, 63(1):65–92, 1997.

S.A.H. Geritz, E. Kisdi, and J.A.J. Metz. Evolutionarily singular strategies and the adaptive growth and branching of the evolutionary tree. *Evolutionary Ecology*, 12(1):35–57, 1998.

T.J. Givnish. Outcrossing versus ecological constraints in the evolution of dioecy. *The American Naturalist*, 119(6):849–865, 1982.

A. Harkess, K. Huang, R. van der Hulst, B. Tissen, J.L. Caplan, A. Koppula, M. Batish, B.C. Meyers, and J. Leebens-Mack. Sex determination by two Y-linked genes in garden asparagus. *The Plant Cell*, 32(6):1790–1796, 2020.

I.M. Henry, T. Akagi, R. Tao, and L. Comai. One hundred ways to invent the sexes: theoretical and observed paths to dioecy in plants. *Annual review of plant biology*, 69:553–575, 2018.

D.H. Janzen. Seed predation by animals. *Annual review of ecology and systematics*, 2(1):465–492, 1971.

M. Kimura. A stochastic model concerning the maintenance of genetic variability in quantitative characters. *Proceedings of the National Academy of Sciences*, 54(3):731–736, 1965.

M. Kopp and J. Hermisson. The evolution of genetic architecture under frequency-dependent disruptive selection. *Evolution*, 60(8):1537–1550, 2006.

R. Kuemmerli and L. Keller. Patterns of split sex ratio in ants have multiple evolutionary causes based on different within-colony conflicts. *Biology Letters*, 5(5):713–716, 2009.

G. Lagunas-Robles, J. Purcell, and A. Brelsford. Linked supergenes underlie split sex ratio and social organization in an ant. *Proceedings of the National Academy of Sciences*, 118(46):e2101427118, 2021.

J.L. Leonard. *Transitions between sexual systems: understanding the mechanisms of, and pathways between, dioecy, hermaphroditism and other sexual systems*. Springer, 2018.

D.G. Lloyd. The maintenance of gynodioecy and androdioecy in angiosperms. *Genetica*, 45(3):325–339, 1975.

D.G. Lloyd. The distributions of gender in four angiosperm species illustrating two evolutionary pathways to dioecy. *Evolution*, 34(1):123–134, 1980.

D.G. Lloyd. Selection of combined versus separate sexes in seed plants. *The American Naturalist*, 120 (5):571–585, 1982.

K. Masaka and T. Takada. Transition model for the hermaphroditism-dioecy continuum in higher plants. *Ecological Modelling*, 475:110135, 2023.

S.J. Mazer, V.A. Delesalle, and H. Paz. Evolution of mating system and the genetic covariance between male and female investment in clarkia (onagraceae): selfing opposes the evolution of trade-offs. *Evolution*, 61(1):83–98, 2007.

T.R. Meagher. The quantitative genetics of sexual dimorphism. In *Gender and sexual dimorphism in flowering plants*, pages 275–294. Springer, 1999.

J.A.J. Metz and O. Leimar. A simple fitness proxy for structured populations with continuous traits, with case studies on the evolution of haplo-diploids and genetic dimorphisms. *Journal of Biological Dynamics*, 5:163–190, 2011.

J. Meunier, S.A. West, and M. Chapuisat. Split sex ratios in the social hymenoptera: a meta-analysis. *Behavioral Ecology*, 19(2):382–390, 2008.

R. Ming, A. Bendahmane, and S.S. Renner. Sex chromosomes in land plants. *Annual review of plant biology*, 62(1):485–514, 2011.

N.A. Müller, B. Kersten, A.P. Leite Montalvão, N. Mähler, C. Bernhardsson, K. Bräutigam, Z. Carracedo Lorenzo, H. Hoenicka, V. Kumar, M. Mader, B. Pakull, K.M. Robinson, M. Sabatti, C. Vettori, P.K. Ingvarsson, Q. Cronk, N.R. Street, and M. Fladung. A single gene underlies the dynamic evolution of poplar sex determination. *Nature plants*, 6(6):630–637, 2020.

C. Olito and T. Connallon. Sexually antagonistic variation and the evolution of dimorphic sexual systems. *The American Naturalist*, 193(5):688–701, 2019.

J.R. Pannell and C.Y. Jordan. Evolutionary transitions between hermaphroditism and dioecy in animals and plants. *Annual Review of Ecology, Evolution, and Systematics*, 53, 2022.

L. Picchi and M.C. Lorenzi. Polychaete worms on the brink between hermaphroditism and separate sexes. In *Transitions Between Sexual Systems: Understanding the Mechanisms of, and Pathways Between, Dioecy, Hermaphroditism and Other Sexual Systems*, pages 123–163. Springer, 2018.

S.A. Ramm. Exploring the sexual diversity of flatworms: Ecology, evolution, and the molecular biology of reproduction. *Molecular reproduction and development*, 84(2):120–131, 2016.

S.S. Renner. The relative and absolute frequencies of angiosperm sexual systems: dioecy, monoecy, gynodioecy, and an updated online database. *American Journal of botany*, 101:1588–1596, 2014.

S.S. Renner and R.E. Ricklefs. Dioecy and its correlates in the flowering plants. *American journal of botany*, 82(5):596–606, 1995.

C. Rueffler, T.J.M. Van Dooren, O. Leimar, and P.A. Abrams. Disruptive selection and then what? *Trends in Ecology & Evolution*, 21(5):238–245, 2006.

J.C. Vamosi, Y. Zhang, and W.G. Wilson. Animal dispersal dynamics promoting dioecy over hermaphroditism. *The American Naturalist*, 170(3):485–491, 2007.

T.J.M. Van Dooren. The evolutionary ecology of dominance-recessivity. *Journal of Theoretical Biology*, 198(4):519–532, 1999.

B. Walsh and M. Lynch. *Evolution and selection of quantitative traits*. Oxford University Press, 2018.

W. Wang, R.B. Gasser, D. Charlesworth, and Q. Zhou. Evolution of sexual systems, sex chromosomes and sex-linked gene transcription in flatworms and roundworms. *Nature Communications*, 13(1):3239, 2022.

S. Yeaman and M.C. Whitlock. The genetic architecture of adaptation under migration–selection balance. *Evolution*, 65(7):1897–1911, 2011.

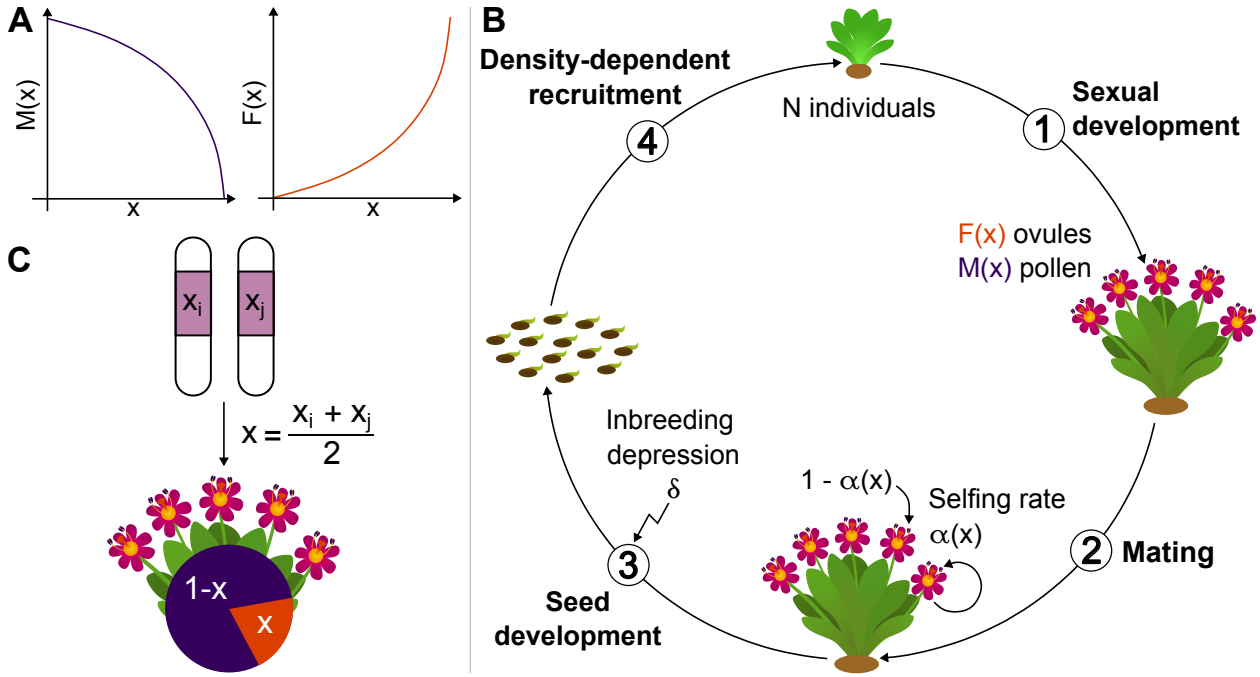

Figure 1: Life cycle and genetic architecture of sex allocation. A Male ($M(x)$, dark purple) and female ($F(x)$, orange) gain curves as functions of the fraction x of resources allocated to female function. In this example, the male gain curve is saturating, reflecting diminishing fitness returns through 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.

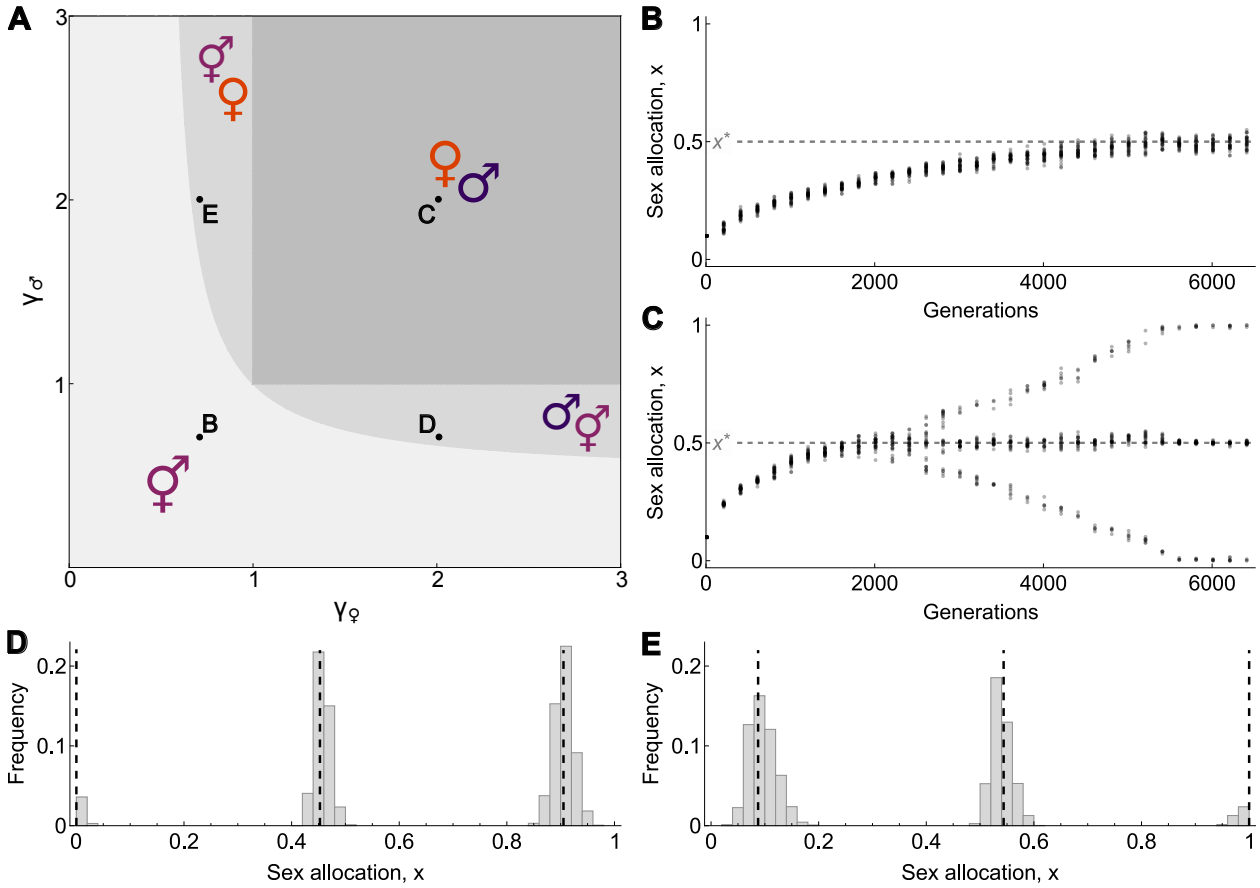

Figure 2: The gradual evolution of sex allocation and sexual systems under complete outcrossing. A The four outcomes of evolution according to $\gamma_♀$ and $\gamma_♂$ (Appendix B.1 for analysis): (i) hermaphroditism (light grey); (ii) dioecy (dark grey); (iii) androdioecy (medium light gray) and (iv) gynodioecy (medium light gray), where pure males and females coexist with hermaphrodites, respectively. **B** Phenotypes expressed by 30 randomly sampled individuals every 200 generations in a simulation under conditions predicted to lead to hermaphroditism (with $\gamma_♀ = \gamma_♂ = 1/\sqrt{2}$). The population converges to express the equilibrium strategy $x^* = \gamma_♀/(\gamma_♀ + \gamma_♂)$, indicated by the light grey dashed line (Appendix B.3 for simulation details). **C** Same as B under conditions predicted to favour dioecy (with $\gamma_♀ = \gamma_♂ = 2$). The population first converges to x^* and then experiences disruptive selection, leading to pure male ($x = 0$) and female ($x = 1$) alleles. At equilibrium, the population is composed of males, females and hermaphrodites. **D** Distribution of phenotypes at equilibrium in a simulation where androdioecy evolves (with $\gamma_♀ = 2$ and $\gamma_♂ = 1/\sqrt{2}$). Dashed vertical lines indicate the equilibrium strategies computed numerically in Appendix B.2.3. **E** Same as D where gynodioecy evolves (with $\gamma_♀ = 1/\sqrt{2}$ and $\gamma_♂ = 2$). Other parameters used in all simulations: $N = 10^4$, $\mu = 5 \times 10^{-3}$ and $\sigma = 10^{-2}$ (Appendix B.3 for description of parameters).

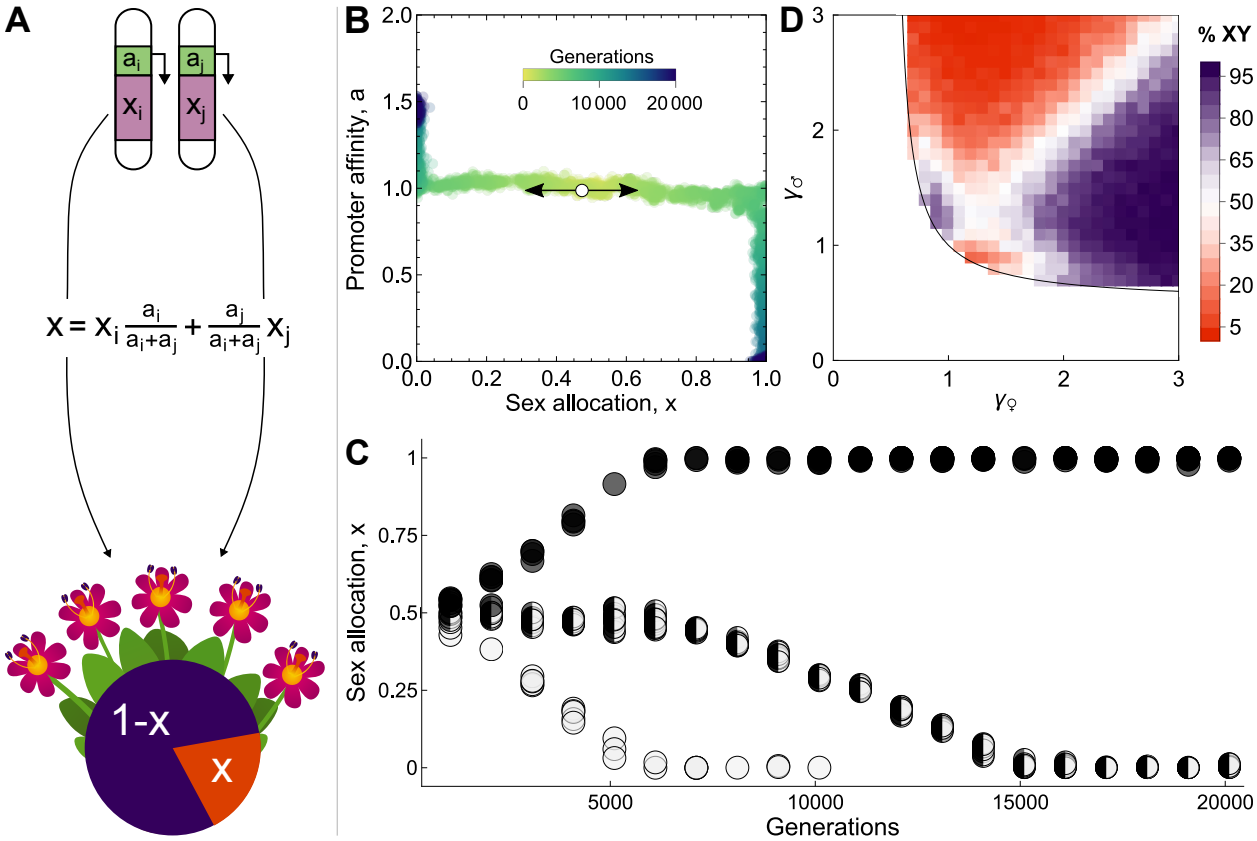

Figure 3: The co-evolution of sex allocation and gene-regulation. A Genetic architecture of sex allocation. The sex allocation locus is composed of a sex allocation gene and its promoter. Transcription factors must bind to the promoter for the sex allocation gene to be expressed, which they do at a rate 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 co-evolve in a simulation under conditions predicted to lead to dioecy ($\gamma_♀ = \gamma_♂ = 2$). 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 $\gamma_♀$ and $\gamma_♂$ spanning the parameter range in which selection on sex allocation is disruptive. XY and ZW systems are equally likely to emerge when $\gamma_♀ = \gamma_♂$, whereas XY systems are more prevalent where $\gamma_♀ > \gamma_♂$ and ZW systems where $\gamma_♀ < \gamma_♂$ 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: $\mu = 5 \times 10^{-3}$, $\sigma = 10^{-2}$.

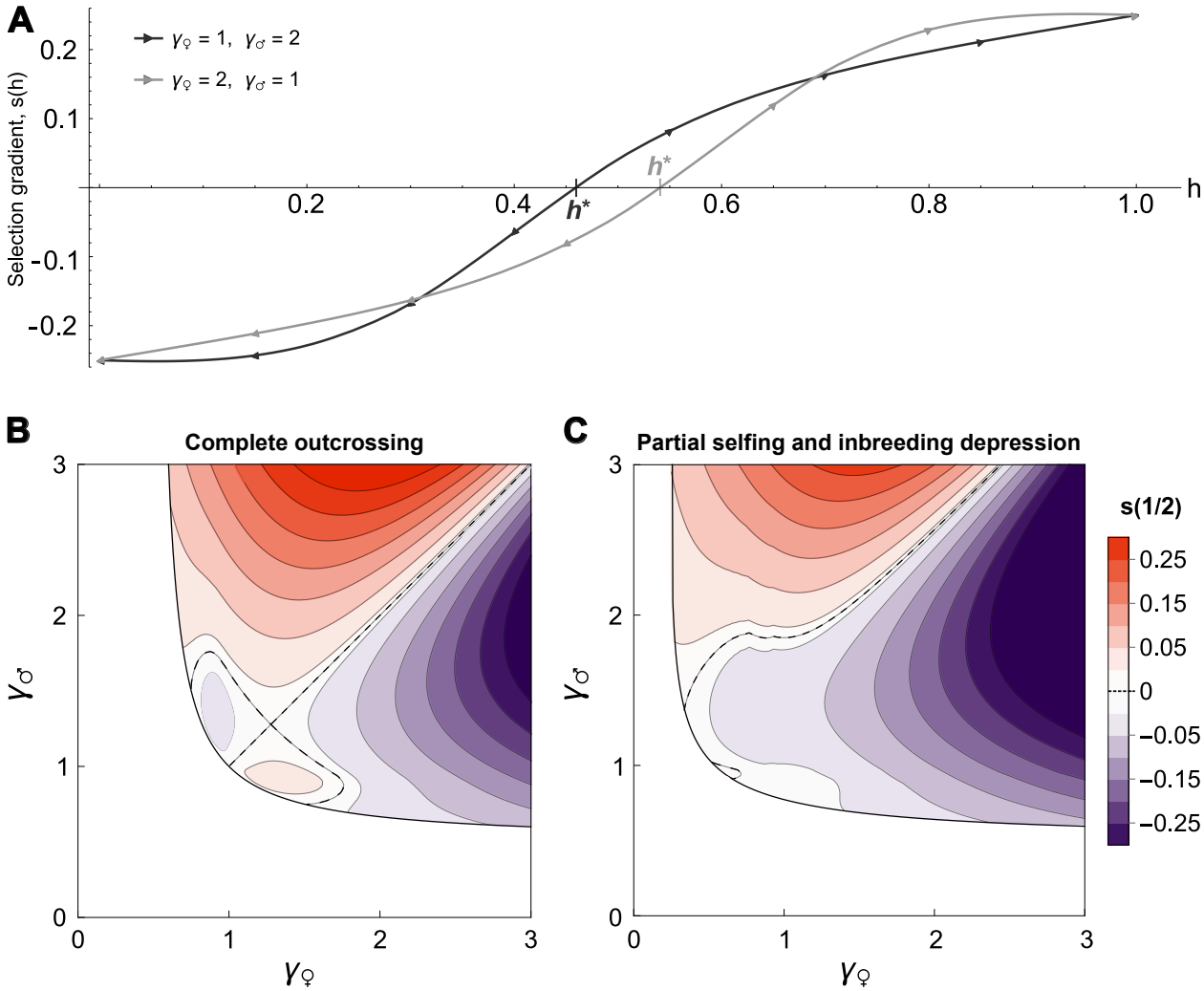

Figure 4: The nature of selection on dominance at a sex-determining locus. A Selection gradient $s(h)$ acting on the dominance h of the female allele $x_{♀} = 1$ over the male allele $x_{♂} = 0$ for two cases leading to dioecy (Appendix C.2.4 for how to compute this gradient). The selection gradient $s(h)$ 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 gray 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.