

## S3 Appendix

### Invasion conditions

Cover the other parts of the characteristic polynomial here. Waiting for Sally's proof!

A rare neo-Y or neo-W will spread from a given ancestral equilibrium when the leading eigenvalue,  $\lambda$ , of the Jacobian matrix derived from the eight mutant recursion equations (given by ??c,d,g,h), evaluated at the ancestral equilibrium, is greater than one. However, because a neo-Y (neo-W) is always in males (females) and is epistatically dominant to the ancestral sex-determining locus, we need only two recursion equations (e.g., tracking the change in the frequency of neo-Y-A and neo-Y-a gametes from males) and thus the leading eigenvalue is the largest solution the polynomial  $\lambda^2 + b\lambda + c = 0$  as described in the text (Table ??).

The general conditions for the invasion of a neo-sex-determining allele are given in the main text, in terms of the growth rates of the mutant haplotypes in the absence of recombination ( $\lambda_{mi}$ ) and the rate that recombination destroys them ( $\chi_{mi}$ ). For tight linkage between the ancestral sex-determining locus and the selected locus we can calculate these terms explicitly (see below). For weak selection we can take a Taylor series of the leading eigenvalue. The leading eigenvalue,  $\lambda$ , for any  $k$ , is given up to order  $\epsilon^2$  by equation (??).

#### Tight linkage between A and X ( $r \approx 0$ )

Here, we explore the conditions under which a neo-W invades an XY system assuming that the A locus is initially in tight linkage with the ancestral sex-determining region ( $r \approx 0$ ). We disregard neo-Y mutations, which never spread given that the ancestral population is at a stable equilibrium (see supplementary *Mathematica* notebook for proof).

Starting with the simpler equilibrium ( $B$ ), the terms of that determine the leading eigenvalue are

$$\lambda_{mA} = [w_A^\delta(1 + \alpha_\Delta^\delta)]^{-1} \frac{w_A^\varphi}{w_A^\varphi} \frac{[w_A^\delta(1 + \alpha_\Delta^\delta)w_{AA}^\varphi + w_a^\delta(1 - \alpha_\Delta^\delta)w_{Aa}^\varphi(1 + \alpha_\Delta^\varphi)]}{2w_{AA}^\varphi} \quad (\text{S3.1a})$$

$$\lambda_{ma} = [w_A^\delta(1 + \alpha_\Delta^\delta)]^{-1} \frac{w_a^\varphi}{w_A^\varphi} \frac{[w_A^\delta(1 + \alpha_\Delta^\delta)w_{Aa}^\varphi(1 - \alpha_\Delta^\varphi) + w_a^\delta(1 - \alpha_\Delta^\delta)w_{aa}^\varphi]}{2w_{AA}^\varphi} \quad (\text{S3.1b})$$

$$\chi_{mA} = \frac{1}{2} [w_A^\delta(1 + \alpha_\Delta^\delta)]^{-1} \frac{w_A^\varphi}{w_A^\varphi} \frac{[w_a^\delta(1 - \alpha_\Delta^\delta)w_{Aa}^\varphi(1 + \alpha_\Delta^\varphi)]}{w_{AA}^\varphi} \frac{R}{2} \quad (\text{S3.1c})$$

$$\chi_{ma} = \frac{1}{2} [w_A^\delta(1 + \alpha_\Delta^\delta)]^{-1} \frac{w_a^\varphi}{w_A^\varphi} \frac{[w_A^\delta(1 + \alpha_\Delta^\delta)w_{Aa}^\varphi(1 - \alpha_\Delta^\varphi)]}{w_{AA}^\varphi} \frac{R}{2} \quad (\text{S3.1d})$$

Haploid selection impacts the spread of neo-W haplotypes in three ways. Firstly, the zygotic sex ratio becomes male biased,  $\zeta > 1/2$ , when the  $a$  allele (which is fixed on the Y) is favoured during competition among male gametes or by meiotic drive in males. Specifically, at equilibrium ( $B$ ), female zygote frequency is  $1 - \zeta = w_A^\delta(1 + \alpha_\Delta^\delta)/(2\bar{w}_H^\delta)$  where  $2\bar{w}_H^\delta = [w_a^\delta(1 - \alpha_\Delta^\delta) + w_A^\delta(1 + \alpha_\Delta^\delta)]$  has been canceled out in equations (??) to leave the term  $[w_A^\delta(1 + \alpha_\Delta^\delta)]^{-1}$ . Male biased sex ratios facilitate the spread of a neo-W because neo-W alleles cause the zygotes that carry them to develop as the rarer, female, sex.

Secondly, haploid selection in females selects on neo-W haplotypes directly. At equilibrium ( $B$ ), the fitness of female gametes under the ancestral sex-determining system is  $w_A^\varphi$  such that the relative fitnesses of neo-W- $A$  and neo-W- $a$  haplotypes during female gametic competition are  $w_A^\varphi/w_A^\varphi$  and  $w_a^\varphi/w_A^\varphi$  (see terms in equation ??). Meiotic drive in females will also change the proportion of gametes that carry the  $A$  versus  $a$  alleles, which will be produced by heterozygous females in proportions  $(1 + \alpha_\Delta^\varphi)/2$  and  $(1 - \alpha_\Delta^\varphi)/2$ , respectively. These terms are only associated with heterozygous females, i.e., they are found alongside  $w_{Aa}^\varphi$ .

Thirdly, haploid selection in males affects the diploid genotypes of females by altering the allele frequencies in the male gametes that female gametes pair with. At equilibrium ( $B$ ), neo-W female gametes will mate with X- $A$  male ga-

metes with probability  $w_A^\delta(1 + \alpha_\Delta^\delta)/(2\bar{w}_H^\delta)$  and Y-*a* male gametes with probability  $w_a^\delta(1 - \alpha_\Delta^\delta)/(2\bar{w}_H^\delta)$ , where the  $2\bar{w}_H^\delta$  terms have been canceled in equation (??) (as mentioned above). Thus, for example, neo-W-*A* haplotypes are found in *AA* female diploids with probability  $w_A^\delta(1 + \alpha_\Delta^\delta)/(2\bar{w}_H^\delta)$  (first term in square brackets in the numerator of equation ??a) and in *Aa* female diploids with probability  $w_a^\delta(1 - \alpha_\Delta^\delta)/(2\bar{w}_H^\delta)$  (see equation ??c and the second term in square brackets in the numerator of equation ??a).

The other terms in equations (??) are more easily interpreted if we assume that there is no haploid selection in either sex, in which case  $\lambda_{mA} = (w_{AA}^\varphi + w_{Aa}^\varphi)/2w_{AA}^\varphi$  and  $\lambda_{ma} = (w_{aa}^\varphi + w_{Aa}^\varphi)/2w_{AA}^\varphi$ . Neither haplotype can spread under purely sexually-antagonistic selection, where *A* is directionally favoured in females ( $w_{AA}^\varphi > w_{Aa}^\varphi > w_{aa}^\varphi$ ) and *a* is directionally favoured in males ( $w_{AA}^\delta > w_{Aa}^\delta > w_{aa}^\delta$ ). Essentially, the X is then already as specialized as possible for the female beneficial allele (*A* is fixed on the X), and the neo-W often makes daughters with the Y-*a* haplotype, increasing the flow of *a* alleles into females, which reduces the fitness of those females.

If selection doesn't uniformly favour *A* in females, however, neo-W-*A* haplotypes and/or neo-W-*a* haplotypes can spread ( $\lambda_{mA} > 1$  and/or  $\lambda_{ma} > 1$ ). A neo-W-*A* haplotype can spread ( $\lambda_{mA} > 1$ ) when  $w_{Aa}^\varphi > w_{AA}^\varphi$ , despite the fact that a neo-W brings Y-*a* haplotypes into females. In this case the *a* allele is favoured by selection in females despite *A* being fixed on the X. For this equilibrium to be stable (i.e., to keep *A* fixed on the X), X-*a* cannot be overly favoured in females and X-*A* must be sufficiently favoured in males (for example, by overdominance in males). Specifically, from the stability conditions for equilibrium (B), we must have  $w_{Aa}^\varphi < 2w_{AA}^\varphi$  and  $w_{Aa}^\delta / [(w_{aa}^\delta + w_{Aa}^\delta)/2] > w_{Aa}^\varphi / w_{AA}^\varphi$ .

Still considering  $w_{Aa}^\varphi > w_{AA}^\varphi$ , the neo-W can also spread alongside the *a* allele ( $\lambda_{ma} > 1$ ) if  $w_{aa}^\varphi$  is large enough such that  $(w_{Aa}^\varphi + w_{aa}^\varphi)/2 > w_{AA}^\varphi$ . This can occur with overdominance or directional selection for *a* in females (Figure ??B,C). In this case, *a* is favoured in females (comparing *Aa* to *AA* genotypes in females) but *A* is fixed on the X due to selection in males. The neo-W-*a* haplotype can spread

because it produces females with higher fitness  $Aa$  and  $aa$  genotypes.

Similar equations can be derived for equilibrium (A) by substituting the equilibrium allele frequencies into Table ??

$$\lambda_{mA} = \frac{a}{b} [w_{AA}^{\varphi} w_{Aa}^{\delta} w_A^{\delta} (1 + \alpha_{\Delta}^{\delta}) \phi + w_{Aa}^{\varphi} (1 + \alpha_{\Delta}^{\varphi}) w_a^{\delta} c] / (2w_a^{\varphi}) \quad (\text{S3.2a})$$

$$\lambda_{ma} = \frac{a}{b} [w_{Aa}^{\varphi} (1 - \alpha_{\Delta}^{\varphi}) w_{Aa}^{\delta} w_A^{\delta} (1 + \alpha_{\Delta}^{\delta}) \phi + w_{aa}^{\varphi} w_a^{\delta} c] / (2w_A^{\varphi}) \quad (\text{S3.2b})$$

$$\chi_{mA} = \frac{a}{b} \frac{R}{2} [w_{Aa}^{\varphi} (1 + \alpha_{\Delta}^{\varphi}) w_a^{\delta} c] / w_a^{\varphi} \quad (\text{S3.2c})$$

$$\chi_{ma} = \frac{a}{b} \frac{R}{2} [w_{Aa}^{\varphi} (1 - \alpha_{\Delta}^{\varphi}) w_{Aa}^{\delta} w_A^{\delta} (1 + \alpha_{\Delta}^{\delta}) \phi] / w_A^{\varphi} \quad (\text{S3.2d})$$

where

$$a = w_a^{\varphi} \phi + w_A^{\varphi} \psi \quad (\text{S3.3a})$$

$$b = w_{AA}^{\varphi} [w_{Aa}^{\delta} w_A^{\delta} (1 + \alpha_{\Delta}^{\delta})] \phi^2 + w_{Aa}^{\varphi} [w_{Aa}^{\delta} w_A^{\delta} (1 + \alpha_{\Delta}^{\delta}) + w_{aa}^{\delta} w_a^{\delta}] \psi \phi + w_{aa}^{\varphi} (w_{aa}^{\delta} w_a^{\delta}) \psi^2 \quad (\text{S3.3b})$$

$$c = w_{Aa}^{\delta} (1 - \alpha_{\Delta}^{\delta}) \phi + 2w_{aa}^{\delta} \psi \quad (\text{S3.3c})$$

As with equilibrium (B), haploid selection again modifies invasion fitnesses by altering the sex ratio and the diploid genotypes of females and directly selecting upon female gametes. The only difference is that resident XX females are no longer always homozygote  $AA$  and males are no longer always heterozygote  $Aa$ . Thus the effect of haploid selection in males is reduced, as is the difference in fitness between neo-W haplotypes and resident X haplotypes, as both can be on any diploid or haploid background.

The other terms are easier to interpret in the absence of haploid selection. For instance, without haploid selection, the neo-W- $A$  haplotype spreads ( $\lambda_{mA} > 1$ ) if and only if

$$2(w_{Aa}^{\varphi} - w_{aa}^{\varphi})w_{aa}^{\delta}\psi^2 > (w_{AA}^{\varphi} - w_{Aa}^{\varphi})w_{Aa}^{\delta}\phi(\phi - \psi) \quad (\text{S3.4})$$

where  $\phi - \psi = w_{AA}^{\varphi}w_{Aa}^{\delta} - w_{aa}^{\varphi}w_{aa}^{\delta}$  and both  $\phi$  and  $\psi$  are positive when equilibrium (A) is stable. In contrast to equilibrium (B), a neo-W haplotype can spread under purely sexually-antagonistic selection ( $w_{aa}^{\varphi} < w_{Aa}^{\varphi} < w_{AA}^{\varphi}$  and  $w_{AA}^{\delta} < w_{Aa}^{\delta} < w_{aa}^{\delta}$ ). The neo-W-A can spread as long as it becomes associated with females that bear more A alleles than observed at equilibrium (A).

Without haploid selection, the neo-W-a haplotype spreads ( $\lambda_{ma} > 1$ ) if and only if

$$(w_{aa}^{\varphi} + w_{Aa}^{\varphi} - 2w_{AA}^{\varphi})w_{Aa}^{\delta}\phi^2 + (w_{aa}^{\varphi} - w_{Aa}^{\varphi})(w_{Aa}^{\delta} + 2w_{aa}^{\delta})\phi\psi > 0 \quad (\text{S3.5})$$

This condition cannot be met with purely sexually antagonistic selection (as both terms on the left-hand side would then be negative), but it can be met under other circumstances. For example, with overdominance in males there is selection for increased A frequencies on X chromosomes in males, which are always paired with Y-a haplotypes. Directional selection for a in females can then maintain a polymorphism at the A locus on the X. This scenario selects for a modifier that increases recombination between the sex chromosomes (e.g., blue region of Figure 2d in ?) and facilitates the spread of neo-W-a haplotypes, which create more females bearing more a alleles than the ancestral X chromosome does.

### Role of Haploid Selection with Tight Linkage

Haploid selection generally expands the conditions under which neo-W alleles can spread within ancestral systems that have evolved tight linkage between the sex-determining locus and a selected locus ( $r \approx 0$ ). First, haploid selection can allow a polymorphism to be maintained when it would not under diploid selection alone (e.g., with directional selection in diploids). In cases of ploidy-antagonistic selection, where there is a balance between alleles favored in the haploid stage and

the diploid stage, neo-W alleles - even unlinked alleles - can spread (Figure ??). Second, even when diploid selection could itself maintain a polymorphism, haploid selection can increase the conditions under which transitions among sex chromosomes are possible. Of particularly importance, when selection is sexually-antagonistic in diploids ( $s^{\varphi}s^{\delta} < 0$  and  $0 < h^{\delta} < 1$ ), an unlinked neo-W ( $R = 1/2$ ) cannot invade unless there is also haploid selection (see proof in supplementary *Mathematica* file; Figures ?? and ??). More generally, haploid selection alters the conditions under which neo-W chromosomes can spread (compare Figures ??-?? to Figure ??).

Male haploid selection in favour of the  $a$  allele ( $\alpha_{\Delta}^{\delta} < 0$ ,  $w_A^{\delta} < w_a^{\delta}$ ) generates male-biased sex ratios at equilibria (A) and (B), where Y- $a$  is fixed ( $\hat{p}_Y^{\delta} = 0$ ). Male-biased sex-ratios facilitate the spread of neo-W- $A$  and neo-W- $a$  haplotypes (increasing  $\lambda_{mA}$  and  $\lambda_{ma}$ ). Panels A-C in Figures ?? and ?? show that neo-W haplotypes tend to spread for a wider range of parameters when sex ratios are male biased, compared to Figure ?? without haploid selection. By contrast, male haploid selection in favour of the  $A$  allele generates female-biased sex ratios and reduces  $\lambda_{mA}$  and  $\lambda_{ma}$ , as demonstrated by panels D-F in Figures ?? and ??.

Female haploid selection generates direct selection on the neo-W- $A$  and neo-W- $a$  haplotypes as they spread in females. Thus, female haploid selection in favour of the  $a$  allele tends to increase  $\lambda_{ma}$  and decrease  $\lambda_{mA}$ , as shown by panels A-C in Figures ?? and ??). Conversely, female haploid selection in favour of the  $A$  allele increases  $\lambda_{mA}$  and decreases  $\lambda_{ma}$ , see panels D-F in Figures ?? and ??.

Thus, the impact of haploid selection on sex chromosome transitions must be considered as two sides of a coin: it can generate sex ratio biases that drive sex chromosome transitions to equalize the sex ratio, but it can also drive in new sex chromosomes and thereby cause sex ratios to become biased.