

FILE S1

I. Invasion of gene duplicates on Y chromosomes that carry an arbitrary number of linked genes.

Y-linked duplicate genes evolve within the genetic background of the entire Y chromosome, which is likely to contain multiple functional genes, particularly during early stages of sex chromosome evolution. To determine the generality of the single gene duplication scenario in the main text, we developed a second model to examine the evolutionary dynamics of rare, Y-linked duplicates on ancestral chromosomes carrying an arbitrary number (n) of single-copy genes.

Consider a rare, Y-linked duplicate on Y chromosome carrying n single-copy genes. By duplicating one of the n single-copy genes, the individual has $n - 1$ single-copy genes and a single duplicated pair. Though expanding the number of loci greatly increases the number of possible genotypes to follow within the population, subsequent calculations can be simplified by making each gene essential. In other words, fitness drops to zero ($s = 1$) unless each of the n genes has at least one functional copy.

Given this simplification, there are four relevant genotypic classes within the population: (i) individuals with n functional singletons and no duplicates, each at frequency x_n and with fitness $w_n = 1 - sh$; (ii) those with $n + 1$ functional genes ($n - 1$ singleton) at frequency x_{n1} and with fitness $w_{n1} = 1$; (iii) those with $n + 1$ genes ($n - 1$ singleton), of which n are functional, at frequency x_{n0} and with fitness $w_{n0} = 1 - sh$; and (4) a class of sterile individuals, at frequency x_s and with fitness $w_s = 1 - s = 0$, that either lack a functional copy of an essential gene, or carry an abnormal Y chromosome.

In an individual carrying n singletons, the Y chromosome deleterious mutation rate per gamete per generation is $U = nu$, and the distribution of mutations across gametes is reasonably modeled as a Poisson variable with mean of nu . However, given that the diploid, genomic deleterious mutation rate is unlikely to be much greater than one, and Y chromosomes typically represent a tiny fraction of a genome, the number of new mutations should be close to the Bernoulli distribution: $U = nu$ is probability of one mutation, and $1 - U$ represents the probability of zero mutations, per generation. For an individual carrying $n + 1$ total genes, the overall mutational target will be slightly increased, and the Y chromosome mutation rate becomes $U_{dup} = U(n + 1)/n$, per generation. The presence of gene duplicates introduces an opportunity for gene conversion, which as before, are governed by recombination rate (d), crossover (c), and conversion bias (b) parameters.

Following the events order of (i) birth, (ii) selection, (iii) mutation, (iv) recombination, and (v) fertilization, the Y chromosome recursions are:

$$x_{n1}' = \frac{x_{n1}[2Ud(1-c)b + (n-U-Un)(1-dc)]}{[x_{n1} + (x_{n0} + x_n)(1-h)]n} + \frac{x_{n0}(1-h)(1-U)d(1-c)b}{x_{n1} + (x_{n0} + x_n)(1-h)}$$

$$x_{n0}' = \frac{2x_{n1}U(1-d)}{[x_{n1} + (x_{n0} + x_n)(1-h)]n} + \frac{x_{n0}(1-h)(1-U)(1-d)}{x_{n1} + (x_{n0} + x_n)(1-h)}$$

$$x_n' = \frac{x_n(1-h)(1-U)}{x_{n1} + (x_{n0} + x_n)(1-h)}$$

$$x_s' = x_{n1}' + x_{n0}' + x_n'$$

Stability of the equilibrium $x_{n1} = x_{n0} = 0$, $\hat{x}_n = 1 - U = 1 - \hat{x}_s$, and $\bar{w} = (1 - U)(1 - h)$ is governed by the eigenvalue:

$$\lambda = \frac{2Ud(1-c)b + (n-U-Un)(1-dc) + (1-h)(1-U)(1-d)n}{2(1-h)(1-U)n} + \frac{\sqrt{\{2Ud(1-c)b + (n-U-Un)(1-dc) + (1-h)(1-U)(1-d)n\}^2 - 4(n-U-Un)(1-dc)(1-d)(1-h)(1-U)n}}{2(1-h)(1-U)n}$$

When there is no recombination ($d = 0$), a rare gene duplicate is favored by selection when $sh > U/(n - nU)$. Substituting for $U = nu$ yields $sh > u/(1 - nu)$. This result differs slightly from the previous model of a duplicate linked to a single essential gene (the former model predicts that a duplicate invades when $sh > u/(1 - u)$). Multiple Y-linked genes will therefore decrease opportunities for positive selection in favor of new duplicates.

When selection is weak ($sh \approx 0$), recombination can promote selection in favor of the duplicate. For $sh = c = 0$, the Taylor series approximation around $d = 0$ gives a leading eigenvalue of:

$$\lambda = \lambda|_{d=0} + \left. \frac{\partial \lambda}{\partial d} \right|_{d=0} d + O(d^2) \approx 1 + d(2b - 1)$$

which is greater than one for $b > 0.5$, as in the previous model. Numerical simulations of the leading eigenvalue under a broad range of parameter space show that, as before, the opportunity for positive selection for a new duplicate is greater with recombination.