

Autopolyploid establishment through polygenic adaptation

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Abstract

We define the infinitesimal model of quantitative genetics (*sensu* Barton et al. (2017)) for the inheritance of an additive quantitative trait in a mixed-ploidy population consisting of diploid, triploid and autotetraploid individuals producing haploid and diploid gametes. We implement efficient simulation methods and use these to study the quantitative genetics of mixed-ploidy populations and the establishment of autotetraploids in a new habitat. We show that in the absence of migration from the source population, autotetraploids are more likely to found a successful population than diploids under a very broad range of conditions, but that this is unlikely to sufficiently counter the scarcity of tetraploid founders when the source is predominantly diploid. [...]

Introduction

Many plant species exhibit ploidy variation (Levin, 2002; Soltis et al., 2007; Rice et al., 2015), and many of these *mixed-ploidy* species have populations in which different cytotypes coexist or form contact zones (Kolář et al., 2017). How such mixed-ploidy populations emerge and are maintained has proven somewhat challenging to understand.

Consider for instance a randomly mating diploid population. Under the commonly accepted view that polyploids mostly emerge through the union of unreduced gametes (Bretagnolle and Thompson, 1995; Herben et al., 2016; Kreiner et al., 2017b), a new tetraploid individual originating by a chance encounter of two unreduced diploid gametes (an event occurring at an appreciable rate; Kreiner et al. (2017a)) is highly unlikely to establish a stable tetraploid subpopulation, as most of its gametes will end up in unfit hybrids of odd ploidy level (triploid block, Ramsey and Schemske (1998); Köhler et al. (2010); Brown et al. (2024)). This negative frequency dependence effect is commonly referred to as *minority cytotype exclusion* (MCE), after Levin (1975). It is well-appreciated that, due to MCE, in a large random mating mixed-ploidy population dominated by diploids, the rate of unreduced gamete formation needs to be extraordinarily high for tetraploids to establish (Felber and Bever (1997), see also section S2.1).

Hence, to explain the widespread occurrence of mixed-ploidy populations, additional factors besides the continuous formation of polyploids through the union of unreduced gametes need to be considered. Firstly, chance establishment of tetraploids through drift

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could occur. Indeed, the problem is somewhat analogous to the spread of underdominant chromosomal rearrangements, where local establishment through genetic drift and subsequent spreading in a subdivided population through local extinction and recolonization dynamics has been suggested as a plausible model (Lande, 1985). However, MCE is quite strong in randomly mating mixed-ploidy populations, and the population size has to be very small for local tetraploid establishment to occur at an appreciable rate (Rausch and Morgan (2005), see also section S2.2). Secondly, any form of prezygotic isolation between cytotypes could promote establishment of polyploid cytotypes by alleviating MCE. Particularly relevant are assortative mating by cytotype (for instance through phenological differences across cytotypes, or differences in pollinators; Kolář et al. (2017)), self-fertilization (Rausch and Morgan, 2005; Novikova et al., 2023), and localized dispersal (Baack, 2005; Kolář et al., 2017). Finally, selection may be invoked to explain the establishment of polyploids. Tetraploids may have higher relative fitness than their diploid counterparts due to reduced inbreeding depression (Ronfort, 1999), or due to being better adapted to (changing) environmental conditions (Van de Peer et al., 2021).

None of these factors is likely to explain by itself the establishment of polyploids, and the consensus in the field appears to be that some mix of the above is required to explain the occurrence of mixed-ploidy populations in nature (Kolář et al., 2017; Mortier et al., 2024). In particular, polyploids are thought to establish mainly in novel, unoccupied habitats where they evade MCE (for instance at range edges, or after local extinction due to environmental change). If they are able to colonize such habitats at an appreciable rate, they must somehow be better adapted to local conditions, or more able to adapt to those conditions despite inbreeding and migration from the source population while the population is still small, compared to diploids. Indeed, when the source population is dominated by diploids, the probability that a migrant individual is tetraploid will be very small ($O(u^2)$ if u is the probability that a diploid in the source population produces an unreduced gamete in meiosis), so that tetraploids need a substantial advantage during colonization if they are to establish before diploids do.

While there have been substantial modeling efforts aimed at understanding autotetraploid establishment within diploid populations (e.g. Levin (1975); Felber (1991); Felber and Bever (1997); Rausch and Morgan (2005); Oswald and Nuismer (2011); Clo et al. (2022); Griswold (2021)), the problem of polyploid establishment in a novel habitat which presents some adaptive challenge remains largely unaddressed, despite its centrality to verbal arguments about the establishment of polyploids in natural populations (Kolář et al., 2017; Van de Peer et al., 2021; Clo, 2022b).

Here we develop a model for the establishment of a mixed-ploidy population in a novel, unoccupied habitat based on Barton and Etheridge (2018). In order to establish in the novel habitat, the population has to adapt to local environmental conditions. We assume fitness is determined by directional selection on a single polygenic trait which can be interpreted as log fitness at low density in the new habitat. As in Barton and Etheridge (2018), we assume the trait follows the infinitesimal model (*sensu* Barton et al. (2017), i.e. the ‘Gaussian descendants’ infinitesimal model (Turelli, 2017)). We extend the infinitesimal model, and the approach for exact simulation of trait evolution under the infinitesimal model, to mixed-ploidy populations. We then use simulations to study tetraploid establishment, both from single migrants and under continuous migration from a predominantly diploid source population, examining the effects of autopolyploid genetics, maladaptive migration, selfing and assortative mating on the probability that

Table 1: Glossary of the main notation used in the main text.

notation	description
N	total population size
N_k	population size of the k -ploid cytotype
π_k	equilibrium frequency of the k -ploid cytotype
u	probability of unreduced gamete formation ($u = u_{22} = u_{32} = 1 - u_{42}$)
v	probability that a triploid produces a haploid/diploid gamete ($v = u_{31} = u_{32}$)
m	expected number of migrants per generation arriving in the new habitat
z_i	trait value of individual i
c_i	ploidy level of individual i
g_i	ploidy level of gamete produced by individual i in a particular cross
V	segregation variance in the reference diploid population
$V_{i,k}$	gametic segregation variance associated with the production of a k -ploid gamete by individual i
\mathcal{V}_k	genetic variance associated with a haploid genome in the k -ploid reference population (i.e. a k -ploid non-inbred population at HWLE)
β_k	scaling factor for allelic effects in k -ploids
F_i	inbreeding coefficient in individual i
Φ_{ij}	coancestry coefficient for individuals i and j
α_k	probability that the two genes at a locus in a diploid gamete formed by a k -ploid individual descend from the same parental gene copy
γ	strength of directional selection in the new habitat
θ	trait value beyond which the growth rate becomes positive in the new habitat
w_{ij}	fitness of parental pair (i, j)
w_{ij}^{kl}	expected fitness of offspring from parental pair (i, j) when i contributes a k -ploid gamete and j contributes a l -ploid gamete
σ_k	selfing rate in k -ploids
ρ_k	probability of assortative mating in k -ploids

autotetraploids establish in the novel habitat.

Model and Methods

Mixed-ploidy population model

We consider a mixed-ploidy population of size N consisting of N_2 diploid, N_3 triploid and $N_4 = N - N_2 - N_3$ tetraploid individuals. We assume an individual of ploidy level k forms haploid and diploid gametes with proportions u_{k1} and u_{k2} , as well as a proportion $1 - u_{k1} - u_{k2}$ inviable (e.g. aneuploid or polyploid) gametes. The (relative) fecundity of a k -ploid individual is hence $u_{k1} + u_{k2}$. Unless stated otherwise, we will assume

$$\begin{pmatrix} u_{21} & u_{22} \\ u_{31} & u_{32} \\ u_{41} & u_{42} \end{pmatrix} = \begin{pmatrix} 1 - u & u \\ v & v \\ 0 & 1 - u \end{pmatrix} \quad (1)$$

where u is referred to as the proportion of unreduced gametes, and $2v$ is the proportion of euploid gametes produced by a triploid individual.

When two individuals mate, we assume they produce gametes according to their ploidy level (eq. (1)), which randomly combine to produce offspring (which may be inviable if one

of the contributing gametes is inviable). Intrinsic fitness disadvantages associated with particular zygotic ploidy levels or cross types (e.g. modeling phenomena such as ‘triploid block’) can be straightforwardly included at this level. An analysis of a deterministic model (i.e. where $N \rightarrow \infty$) for the cytotype dynamics and equilibrium cytotype composition under random mating is included in section S2.1 (see also Felber and Bever (1997); Kauai et al. (2024)). The stochastic version for finite and constant N is analyzed briefly in section S2.2.

Infinitesimal model

The basic infinitesimal model. Consider a population which expresses a quantitative trait determined by a large number of additive loci of small effect. The infinitesimal model approximates the inheritance of such a trait by assuming that the trait value Z_{ij} of a random offspring from parents with trait values z_i and z_j follows a Gaussian distribution with mean equal to the midparent value and variance which is independent of the mean:

$$Z_{ij} \sim \mathcal{N}\left(\frac{z_i + z_j}{2}, V_{ij}\right) \quad (2)$$

Here, V_{ij} is referred to as the *segregation variance* in family (i, j) . This is the variation generated among offspring from the same parental pair due to random Mendelian segregation in meiosis. This approximation can be justified as arising from the limit where the number of loci determining the trait tends to infinity (Barton et al., 2017).

An alternative, and for our purposes useful, way to characterize the model is to write $Z_{ij} = Y_i + Y_j$, where Y_i and Y_j are independent Gaussian random variables $Y_i \sim \mathcal{N}\left(\frac{z_i}{2}, V_i\right)$ (and similarly for Y_j). We refer to Y_i as the (random) *gametic value* of individual i , and to V_i as the *gametic segregation variance* of individual i . This formulation is helpful in that it highlights that Mendelian segregation occurs independently in both parents when gametes are produced, which then combine additively to determine the offspring trait value. This model applies readily to an autopolyploid population expressing a trait with infinitesimal genetics. For instance, when an autotetraploid produces a diploid gamete, it will pass on half its trait value to the gamete on average, with a variance determined by the details of tetraploid meiosis (which are not, in general, identical to those of diploid meiosis, see below).

Note that in a finite population, the segregation variance will decay over time as the population becomes more inbred. Indeed, Mendelian segregation generates less variation among the gametes produced by individual i when that individual is more inbred, as segregation at homozygous loci does not generate any variation. When F_i is the inbreeding coefficient relative to some ancestral reference population with gametic segregation variance V (i.e. the probability that two genes at a locus in individual i sampled without replacement are identical by descent), the gametic segregation variance of individual i will be $V_i = (1 - F_i)V$. This holds for both diploids and tetraploids (section S2.5.1, also Moody et al. (1993)).

Scaling of traits across ploidy levels. If we would somewhat naively assume that the allelic effects underlying an additive quantitative trait are identical across ploidy levels, a tetraploid offspring from a cross between two diploids would yield, on average, a trait value which is the sum of the parental trait values, with a distribution that depends on the variance generated by the process producing unreduced gametes. This

is not likely to reflect biological reality: tetraploids do not tend to have, for instance, twice the size of their diploid progenitors on average. Similarly, the genetic variance at Hardy-Weinberg and linkage equilibrium (HWLE) in tetraploids will be twice that of their diploid counterparts under such assumptions, which is similarly unrealistic (Clo, 2022a).

In order to account for this, we introduce a scaling factor β_k , accounting for the effects of polyploidization *per se* on trait expression in k -ploids. To introduce and interpret this parameter, we consider an L -locus additive model, with two alleles (0 and 1) at each locus. For a k -ploid individual, let $X_{i,j}$ be the allele at homolog j of locus i . We assume the trait value is determined by

$$z = \sum_{i=1}^L \sum_{j=1}^k a_{i,k} X_{i,j} \quad (3)$$

Where $a_{i,k}$ is the allelic effect of the 1 allele at locus i in k -ploids. The genetic variance at HWLE in k -ploids ($\tilde{V}_{z,k}$) will then be

$$\tilde{V}_{z,k} = k \sum_{i=1}^L a_{i,k}^2 p_i q_i = k \mathcal{V}_k \quad (4)$$

where we refer to \mathcal{V}_k as the variance associated with a haploid genome in k -ploids at HWLE. Note that we also have $\tilde{V}_{z,2} = 2\mathcal{V}_2 = 2V$ (Barton et al., 2017), where V is the segregation variance in the diploid population. If we now assume $a_{i,k} = \beta_k a_{i,2}$, i.e. allelic effects in k -ploids are as in diploids, but scaled by a factor β_k . This implies that

$$\frac{\tilde{V}_{z,k}}{\tilde{V}_{z,2}} = \frac{k \mathcal{V}_k}{2 \mathcal{V}_2} = \frac{k}{2} \beta_k^2 \quad (5)$$

and hence also that $\mathcal{V}_k = \beta_k^2 \mathcal{V}_2 = \beta_k^2 V$. These relations will also hold in the infinitesimal limit where $a_{i,2} \rightarrow 0$ as $L \rightarrow \infty$.

Mixed-ploidy infinitesimal model. We can extend the infinitesimal model to the mixed-ploidy case, assuming that the gametic value, on the diploid trait scale, associated with a k -ploid gamete ($k \in \{1, 2\}$) from individual i of ploidy level $c_i \in \{2, 3, 4\}$ is a Gaussian random variable $Y_{i,k}$ with distribution

$$Y_{i,k} \sim \mathcal{N}\left(\frac{k}{c_i} \frac{z_i}{\beta_{c_i}}, V_{i,k}\right)$$

where $V_{i,k}$ is the gametic segregation variance associated with the production of a k -ploid gamete by individual i . The trait value of an individual originating from the union of a k -ploid gamete of individual i and an l -ploid gamete from individual j is then

$$Z_{ij}^{kl} = \beta_{k+l} (Y_{i,k} + Y_{j,l})$$

i.e., Z_{ij}^{kl} is a Gaussian random variate with distribution

$$Z_{ij}^{kl} \sim \mathcal{N}\left(\beta_{k+l} \left(\frac{k}{c_i} \frac{z_i}{\beta_{c_i}} + \frac{l}{c_j} \frac{z_j}{\beta_{c_j}}\right), \beta_{k+l}^2 (V_{i,k} + V_{j,l})\right) \quad (6)$$

Table 2: Gametic segregation variance for haploid and diploid gametes produced by the three cytotypes in the mixed-ploidy model. F_i is the inbreeding coefficient of individual i (producing the gamete), whereas α_k is the probability that a diploid gamete from a k -ploid individual receives two copies of the same parental gene. Note that we have $\alpha_3 \leq 1/4$ and $\alpha_4 \leq 1/6$.

cytotype	haploid gamete variance	diploid gamete variance
diploid	$\frac{1}{2}(1 - F_i)V$	$2\alpha_2(1 - F_i)V$
triploid	$\frac{2}{3}(1 - F_i)V$	$\frac{2}{3}(1 + 3\alpha_3)(1 - F_i)V$
tetraploid	—	$(1 + 2\alpha_4)(1 - F_i)V$

For the production of diploid gametes by a k -ploid individual, the segregation variance depends not only on the segregation variance in the base population (V) and the inbreeding coefficient (F), but also on the detailed assumptions on how these aberrant meiotic processes occur. Importantly however, these details only affect the gametic segregation variance through the quantity α_k , which is the probability that a k -ploid transmits two copies of the same homolog to a diploid gamete. Note that α_4 , the probability that a diploid gamete of a tetraploid individual carries two copies of the same homolog, is the probability of *double reduction* (e.g. Lynch and Walsh (1998) p.57), and is upper bounded by $1/6$ (Stift et al., 2008). The value of α_2 depends on the relative frequency of unreduced gamete formation through so-called *first* and *second division restitution* (Bretagnolle and Thompson, 1995; De Storme and Geelen, 2013). We summarize the expressions for the gametic segregation variance in table 2. Detailed derivations can be found in section S2.6.

Recursions for inbreeding coefficients We can simulate the mixed-ploidy infinitesimal model for a finite population through a straightforward extension of the approach outlined in Barton et al. (2017), provided we can efficiently track inbreeding and coancestry coefficients across the different ploidy levels. Denoting the parents of individual i by k and l , the recursion for the inbreeding coefficients in the mixed-ploidy case becomes

$$\begin{aligned}
F_i &= \Phi_{kl} & \text{if } c_i = 2 \\
F_i &= \frac{1}{3}(F_k^* + 2\Phi_{kl}) & \text{if } c_i = 3, g_k = 2, g_l = 1 \\
F_i &= \frac{1}{3}(F_l^* + 2\Phi_{kl}) & \text{if } c_i = 3, g_k = 1, g_l = 2 \\
F_i &= \frac{1}{6}(F_k^* + F_l^* + 4\Phi_{kl}) & \text{if } c_i = 4
\end{aligned} \tag{7}$$

where $F_k^* = \alpha_{c_k} + (1 - \alpha_{c_k})F_k$ (section S2.5.1). The recursion for the coancestry coefficients in is given by

$$\begin{aligned}
\Phi_{ii} &= \frac{1}{c_i}(1 + (c_i - 1)F_i) \\
\Phi_{ij} &= \sum_k \sum_l P_{ik}P_{jl}\Phi_{kl} & i \neq j
\end{aligned} \tag{8}$$

where the sums are over individuals in the parental population, and where $P_{ik} \in \{0, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, 1\}$ is the probability that a gene copy in i is derived from parent k .

Establishment model

Our model for the establishment of a population in an initially unoccupied habitat is based on Barton and Etheridge (2018). We assume a large non-inbred ‘mainland’ population at HWLE and cytotype equilibrium, with $\mathbb{E}[z] = 0$ irrespective of the cytotype. In generation t , $M(t)$ migrant individuals arrive on an island (the new habitat) joining $N^*(t)$ resident individuals, where $M(t)$ is Poisson distributed with mean m . The migrant individuals are assumed to be unrelated to the resident individuals. After migration in generation t , the $N(t) = N^*(t) + M(t)$ individuals reproduce sexually, and the offspring thus produced survives until the next generation with a probability determined by their trait value. In the basic model, random selfing is allowed (but see below for a model with self-incompatibility). We assume the trait is under directional selection, with fitness is $w(z) = e^{\gamma(z-\theta)}$, where γ is the intensity of directional selection and θ is the trait value for which the growth rate of the population becomes positive.

Again following Barton and Etheridge (2018), we simulate the model by first calculating the fitness of each parental pair (i, j) , which is the expected fitness of offspring of this pair

$$w_{ij} = \sum_{k=1}^2 \sum_{l=1}^2 w_{ij}^{kl} = \sum_{k=1}^2 \sum_{l=1}^2 u_{c_i,k} u_{c_j,l} \mathbb{E} \left[e^{\gamma(Z_{ij}^{kl} - \theta)} \right] \quad (9)$$

The expectation on the right hand side can be calculated from eq. (6) using the moment-generating function of the Gaussian. Having calculated the w_{ij} , the number of offspring surviving into the next generation is calculated as $N^*(t+1) = \sum_{i,j} w_{ij}/N(t)$. Next, $N^*(t+1)$ offspring individuals are sampled by sampling parental pairs and gametes proportional to w_{ij}^{kl} , and sampling a trait value in accordance with eq. (6).

Self-fertilization and assortative mating

We model partial self-fertilization by assuming that a proportion σ_{c_i} of the ovules of individual i with ploidy level c_i are fertilized by self-pollen, while the remaining proportion $1 - \sigma_{c_i}$ are fertilized by randomly sampled pollen (which may be self-pollen with probability $1/N$). That is, the expected number of offspring from individual i as mother surviving after selection is

$$\mathbb{E}[w_i] = \sigma_{c_i} w_{ii} + (1 - \sigma_{c_i}) \left[\frac{1}{N} \sum_{j=1}^N w_{ij} \right] \quad (10)$$

We hence assume no pollen limitation (all outcrossing ovules are fertilized), and no pollen discounting (the probability of being a father is unaffected by an individual’s selfing rate). When modeling self-incompatibility, we assume there is no intrinsic disadvantage to self-incompatibility, except when there is only a single individual in the population, i.e.

$$\mathbb{E}[w_i] = \begin{cases} \frac{1}{N-1} \sum_{j \neq i} w_{ij} & \text{if } N > 1 \\ 0 & \text{if } N = 1 \end{cases} \quad (11)$$

We model assortative mating by ploidy level in a similar way, assuming that a fraction ρ_{c_i} of the ovules of individual i are fertilized by pollen sampled from the c_i -ploid portion of the population, while a fraction $1 - \rho_{c_i}$ is fertilized by pollen randomly sampled from

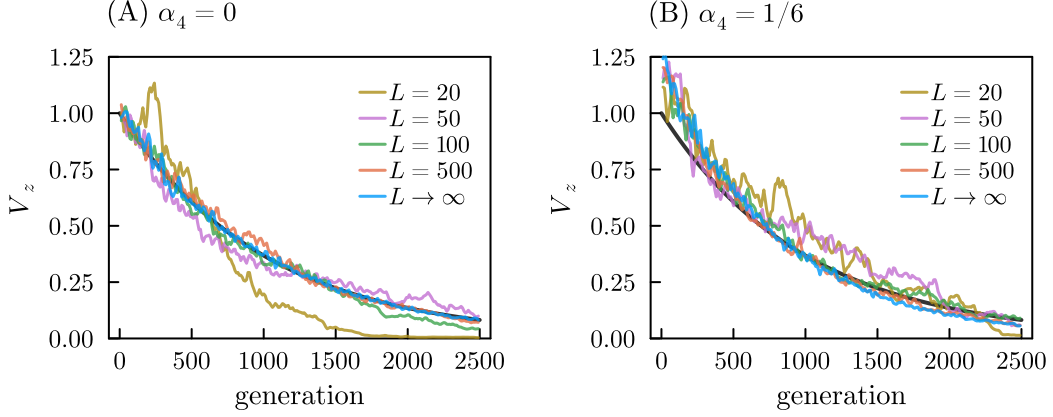


Figure 1: The infinitesimal model in autotetraploids. Comparisons are shown for the decay of the genetic variance (V_z) due to inbreeding in exact simulations of the infinitesimal model in autotetraploids against individual-based simulations of autotetraploid populations with L unlinked additive loci determining the quantitative trait. (A) Simulations of a model without double reduction ($\alpha_4 = 0$). (B) Simulations of a model with maximal double reduction ($\alpha_4 = 1/6$) (for all loci in the finite L simulations). We show window-smoothed values for visual clarity, with observed genetic variances averaged in windows of 20 generations every 10 generations. The black line marks $e^{-t/4N}$. We assume $N = 250$ and $V_z(0) = 1$.

the entire population.

$$\mathbb{E}[w_i] = \rho_{c_i} \frac{1}{N_{c_i}} \sum_{j=1}^N \delta_{c_i, c_j} w_{ij} + (1 - \rho_{c_i}) \left[\frac{1}{N} \sum_{j=1}^N w_{ij} \right] \quad (12)$$

Implementation and availability

Individual-based simulations for the mixed-ploidy infinitesimal model were implemented in Julia (Bezanson et al., 2017). Documented code and simulation notebooks are available at <https://github.com/arzwa/InfGenetics>.

Results

Autotetraploid and mixed-ploidy infinitesimal model

We evaluate the accuracy of the autotetraploid infinitesimal model as an approximation to the evolution of a quantitative trait determined by L additive loci. We find that the infinitesimal model with inbreeding generally yields accurate predictions for the evolution of the genetic variance when the number of loci is sufficiently large ($L \geq 100$, say, figs. 1 and S1). Furthermore, we confirm that, in the absence of double reduction, the decay in genetic variance due to inbreeding after a time t is well-predicted by $e^{-t/4N}$ (fig. 1A), as expected from the results of Arnold et al. (2012). As predicted, double reduction leads to an immediate increase in genetic variance, but leads to accelerated inbreeding, causing faster loss of genetic variance in the long-term (figs. 1 and S1). As noted by Arnold et al. (2012), the loss of genetic variation in the presence of double reduction cannot, however, be described by a single long-term effective population size.

Simulations for the mixed-ploidy model further confirm the correctness of our infinitesimal approximation and highlight the importance of assumptions regarding the scaling of

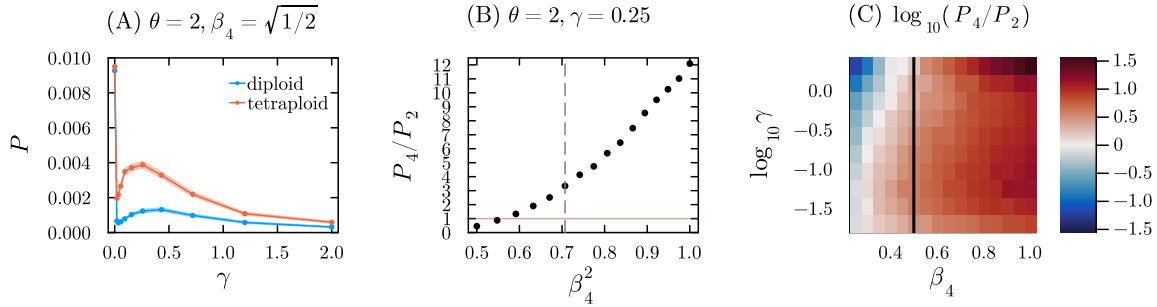


Figure 2: (A) Probability of establishment from a single diploid or tetraploid individual with trait value $z = 0$ for increasing selection intensity γ . We assume $m = 0$ and $u = 0$, i.e. there is no migration, and no unreduced gametes are produced. The trait is scaled in tetraploids so as to yield the same genetic variance at HWLE ($\beta_4 = \sqrt{1/2}$) (B) Probability of a tetraploid individual with trait value $z = 0$ successfully founding a population (P_4), relative to the probability for a diploid individual with the same trait value (P_2). The vertical dashed line marks $\beta_4 = \sqrt{1/2}$, for which the variance at HWLE is identical between diploids and autotetraploids. (C) Probability of tetraploid establishment relative to the probability of diploid establishment (on a \log_{10} scale) across a range of values for γ and β_4 . The vertical line again marks $\beta_4 = \sqrt{1/2}$. All results are estimated from 500,000 replicate simulations and assume $\theta = 2$.

allelic effects across ploidy levels (β parameters, fig. S2). Although inbreeding is slower in autotetraploids than in diploids for the same population size, the tetraploid fraction of a diploid-dominated mixed-ploidy population will have an equal or higher average inbreeding coefficient (fig. S3). This is because in such a population, triploid and tetraploid individuals mostly arise from gametes formed by diploid individuals or polyploid individuals with very recent diploid ancestry (about $1 + u + 2v$ generations ago for tetraploids, and $1 + \frac{2}{3}(u + 2v)$ generations ago for triploids, see section S2.3), so that the polyploid subpopulations will show an average relatedness similar to that of the diploid population and not evolve as an isolated higher-ploidy population would. A nonzero probability of producing IBD diploid gametes ($\alpha_k > 0$) will then further increase the inbreeding coefficient in the tetraploid and triploid fraction of the population relative to their diploid progenitors (fig. S3). Therefore, as long as diploids dominate, the effect of harboring some fraction of the gene pool in polyploid individuals on the rate of inbreeding is negligible, and we find that the evolution of the inbreeding coefficient over time is well predicted by $1 - e^{-t/2N_e}$, where the inbreeding-effective population size is, to first order in u , given by $(1 - 2u)N$ (section S2.4).

Establishment from a single individual

Having established the validity of the mixed-ploidy infinitesimal model, we now use it to study the establishment of polyploids in a marginal habitat to which migrants from a mixed-ploidy source population are maladapted.

We first consider the establishment of a population from a single migrant individual with trait value $z_0 = 0$. We assume $u = 0$ and compare the probability of establishment when the migrant is diploid vs. tetraploid (fig. 2). As noted by Barton and Etheridge (2018), the establishment probability (for a given cytotype) depends essentially on two dimensionless parameters, $\gamma\sqrt{2V}$ and $\theta/\sqrt{2V}$, corresponding to the intensity of selection and the degree of maladaptation, respectively. We shall scale our results accordingly, assuming $2V = 1$ throughout, and shall assume $\theta = 2$, i.e. adaptation has to increase the

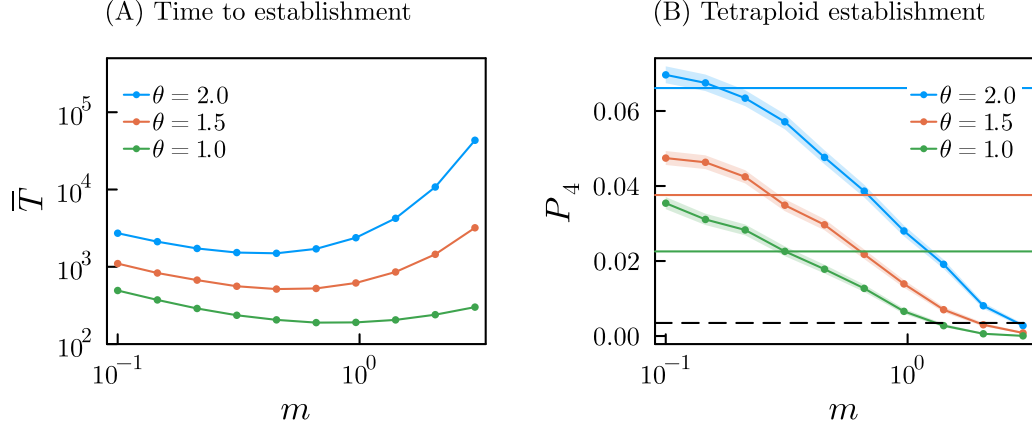


Figure 3: Establishment with recurrent migration. (A) Expected time until a population is established in the novel habitat for increasing rates of migration and different degrees of maladaptation (\bar{z}_s , the mean trait value in the source population). (B) Proportion of simulation replicates in which tetraploids established. The dashed horizontal line marks the proportion of tetraploid migrants (i.e. the proportion of tetraploids at equilibrium in the source population). The solid horizontal lines mark $\frac{p_4\pi_4}{(p_4\pi_4+p_2\pi_2)}$, where p_2 and p_4 are the establishment probabilities for a single diploid and a single tetraploid individual in the absence of migration (as in fig. 2, but with unreduced gamete formation included). All results are based on 10,000 replicate simulations. We assume $\gamma = 0.25$, $\theta = 1.5$ and $u = v = 0.05$.

trait value by two standard deviations relative to achieve a positive growth rate.

We find that reduced inbreeding in tetraploids substantially increases the establishment probability. Indeed, in the case where allelic effects are scaled across ploidy levels to yield the same equilibrium genetic variance ($\beta = \sqrt{1/2}$, so that polyploid migrants are not more likely to have high fitness than diploid migrants), the establishment probability for tetraploids can be almost five times as high as in diploids depending on the selection gradient (fig. 2A). As the segregation variance and initial trait value are the same across these simulations, this is a consequence of the reduced rate of inbreeding, which slows down the exhaustion of the genetic variance carried by the initial migrant individual.

While the probability of establishment becomes lower as the strength of selection becomes large, the establishment probability does not decrease monotonically with γ , i.e. as selection becomes very weak, the establishment probability also decreases. This happens because, although the probability of surviving the first couple of generations becomes higher when selection is weaker, adaptation (i.e. increase in the trait mean) will be slower, and the risk that genetic variation is exhausted due to inbreeding before the population is able to reach a consistently positive growth rate is increased as a result.

Evidently, the scaling of the genetic variance across ploidy levels has a profound effect on the establishment probability, but only when β is close to 0.5 (i.e. individual alleles have almost half the effect size in tetraploids compared to diploids) is the benefit of the slower rate of inbreeding in tetraploids canceled (fig. 2B,C).

Establishment under recurrent migration

We next consider establishment in the new habitat when there is a continuous influx of migrants (at rate m) coming from a large, noninbred and predominantly diploid source population at cytotype equilibrium. In this setting, establishment is certain to happen

eventually, and we are interested in the probability that a tetraploid population establishes before a diploid one does, as well as the effects of maladaptive gene flow and MCE (which both increase with increasing migration rate) on the time until establishment.

We hypothesized that two counteracting processes affect the probability of autotetraploid establishment in this scenario. On the one hand, increased migration will increase the probability that an otherwise likely successful tetraploid migrant suffers from MCE in the early generations while the population size is low, because migrants are likely to be diploid. On the other hand, tetraploids are strongly reproductively isolated from a typical migrant, so that they are less prone to maladaptive swamping. Hence, conditional on evading MCE, they should be able to adapt to the new habitat at a rate which is not strongly affected by the migration rate. This contrasts with diploids, which interbreed freely with maladapted migrants, resulting in a pulling back of the trait mean towards that of the source population.

As expected, we find that the time to establishment (of a population of either ploidy level) first decreases with increasing migration as a result of a larger influx of potentially successful migrants, but later increases with increasing migration as a result of swamping by gene flow (fig. 3A). The probability that a tetraploid population establishes decreases monotonically with increasing migration and is considerably larger than the probability that a migrant individual is tetraploid over a large part of the parameter range (fig. 3B). Together, this suggests that the negative effects of MCE generally outweigh the benefits that come from reproductive isolation as migration increases.

Loss of self-incompatibility and assortative mating

When polyploidization disrupts an existing SI system, we expect that tetraploids suffer less from MCE as some portion of their ovules are now assured to be fertilized by diploid gametes. At the same time, we expect that accelerated inbreeding in selfing tetraploids diminishes the adaptive advantage of tetraploids we found above. As shown in fig. 4, we find that when polyploidization is associated with the loss of a SI system, tetraploids have a strongly increased establishment probability. This is the case even when the selfing rate σ in tetraploids is zero (in which case, under our modeling assumptions, there is only random selfing, i.e. the *realized* selfing rate in tetraploids is $1/N$). Besides reducing MCE, selfing is also expected to simultaneously reduce the effects of maladaptive gene flow, and we indeed find that when the selfing rate is sufficiently high (≥ 0.4 in fig. 4), the relative establishment probability of tetraploids increases with increasing migration rate. In this regime, the increased strength of MCE due to increased migration is compensated by the stronger maladaptive gene flow experienced by diploids.

Another prezygotic isolating mechanism that has often been considered relevant for explaining tetraploid establishment is assortative mating by ploidy level, where ovules from a tetraploid are more likely to be fertilized by pollen coming from a tetraploid – irrespective of the trait values of these individuals. Clearly, assortative mating increases the probability of tetraploid establishment (fig. 5), although not as strongly as the loss of an SI system does. Again, we find that for some parameter values (roughly $\rho \geq 0.4$), assortative mating may be strong enough so that tetraploid establishment increases with increasing migration rates, suggesting that tetraploids evade maladaptive gene flow sufficiently to overcome MCE.

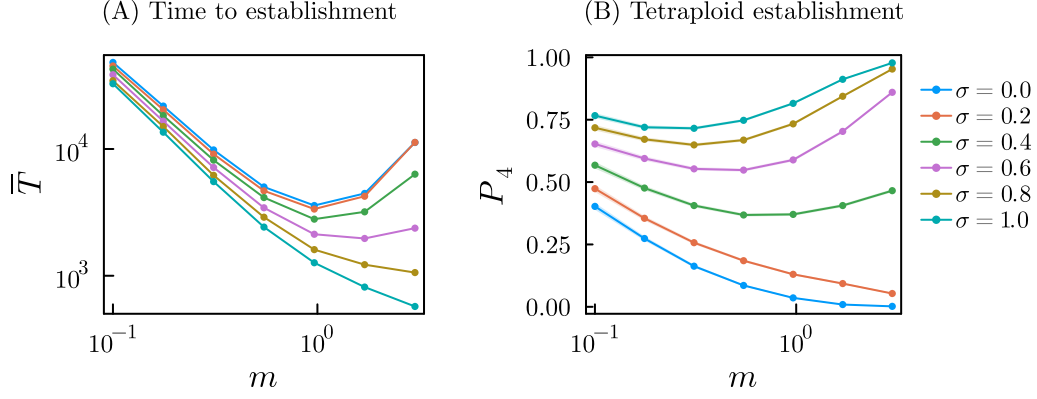


Figure 4: Establishment with recurrent migration and loss of self-incompatibility in polyploids (diploids are assumed to be self-incompatible). (A) Expected time until a population is established in the novel habitat for increasing rates of migration and different self-fertilization rates in polyploids. Triploids and tetraploids have the same selfing rate. Diploids are assumed to be self-incompatible. Note that $\sigma = 0.0$ refers to random self-fertilization (i.e. self-fertilization with probability $1/N$). (B) Proportion of simulation replicates in which tetraploids established. All results are based on 25,000 replicate simulations. We assume $\gamma = 0.25$, $\theta = 1.5$ and $u = v = 0.05$.

Discussion

Despite a sizeable literature on the topic, the question whether the establishment of autopolyploids requires particular fitness advantages associated with polyploidy or not has remained rather unclear and a topic of considerable speculation. The observation that polyploid populations tend to inhabit more extreme habitats or occur at range margins of their diploid progenitors has been interpreted as supporting the hypothesis that polyploids may be more tolerant to extreme environmental conditions.

In a recent study, Griswold (2021) also investigated the effects of maladaptive gene flow on polyploid establishment in a peripheral habitat, focusing however on the case where fitness is determined by a single biallelic locus rather than a polygenic trait. The author found that autotetraploids can establish when adaptation in the peripheral habitat is conferred by recessive alleles, when inbreeding depression in tetraploids is lower than in diploids, and when maladaptive gene flow is due to pollen dispersal, rather than seed dispersal.

We have ignored the effects of dominance throughout. Polyploids are expected to accumulate a larger mutation load when deleterious variation is recessive due to less efficient purging, and this may yield increased inbreeding depression. These effects have been studied in the context of range expansions (Booker and Schrider, 2024). However, this applies only to polyploids that have been established for a long time. In our case, polyploids are always recently descended from diploid ancestors, so they will not have accumulated more deleterious recessives than their diploid counterparts. As inbreeding is slower in tetraploids, we should hence have reduced inbreeding depression in tetraploids, since they have the same deleterious load as diploids but it is less expressed (when recessive). There should therefore be an immediate benefit to polyploidy (reduced inbreeding depression), which is however associated with a long term disadvantage because eventually the established polyploid will start to accumulate a higher load due to less efficient purging.

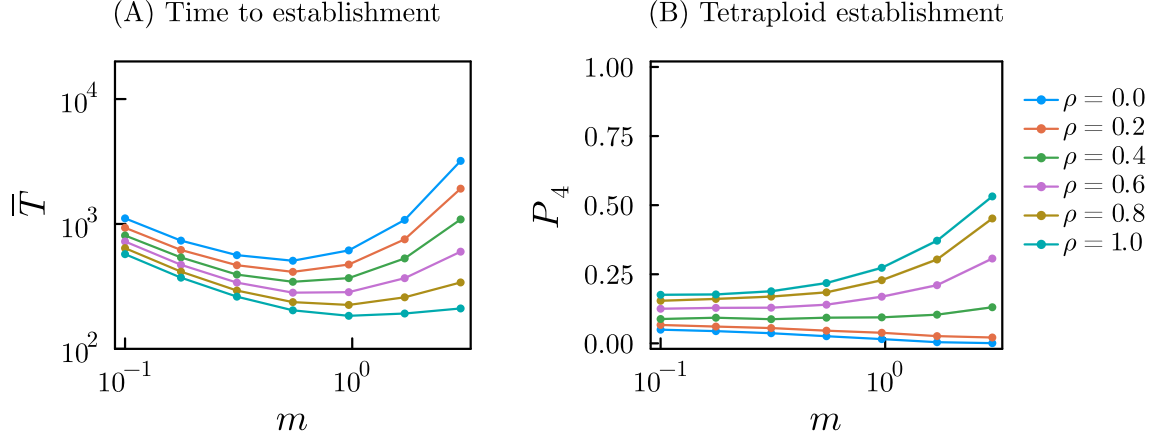


Figure 5: Establishment with recurrent migration and assortative mating by cytotype. (A) Expected time until a population is established in the novel habitat for increasing rates of migration and different probabilities of assortative mating ($\rho_k = \rho$ for $k = 2, 3, 4$, where ρ_k is the probability that an ovule from a k -ploid mother is pollinated by a k -ploid father). (B) Proportion of simulation replicates in which tetraploids established. All results are based on 25,000 replicate simulations. We assume $\gamma = 0.25$ and $u = v = 0.05$.

(Novikova et al., 2023)

Acknowledgements

I thank Christelle Fraïsse for employment, encouragement and feedback. I acknowledge funding from the Research Foundation – Flanders (FWO, Junior Postdoctoral Fellowship 1272625N).

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