Invasion rate versus diversity in population dynamics with catastrophes. Supplemental Material

MODEL

We use an extension of a simple birth-death-innovation process [1], adding the effect of large-scale events (catastrophes) to the three classical processes of the neutral BDIM, where the individuals belong to different types. In this model, a birth event increases the number of individuals in a certain type by 1. A death event decreases the number of individuals in a certain type by 1. A constant fraction of all birth events leads to the creation of new types of size 1 through mutations. A catastrophe event deletes an entire type from the system. In order to equilibrate the total population size, we assume that the death rate is proportional to the total population size, as in the standard nutrient restricted logistic model. The current model has a limited total capacity that can be set to be arbitrarily large. However, beyond that, it has no limit on the size of each type (see Fig. **??** for an illustration of the model).

The catastrophe rate is equal for all types (i.e. the probability that a type would be extinct in a catastrophe is not affected by its size). We denote the size of each type, k, as the number of individuals in this type and N_k, the number of types of this size. The moments of the distribution are $m_j = \sum_k k^j N_k$, $j = 0, 1, 2$, where j is the moment's order. Using this definition, m_0 is the overall number of types and m_1 is the overall number of individuals in the population. The four processes above can be computed using the following reactions: 1) Birth of an individual occurs at a rate of α. 2) Death of an individual occurs at a rate of $\frac{m_1}{\bar{N}}$, $\bar{N}$ being the population size in equilibrium in the absence of catastrophes (up to a time scaling of α). 3) The fraction of mutations out of all birth events is μ. 4) Catastrophe occurs at a rate of γ. α, γ, $\bar{N}$ and μ are free parameters. We can derive the master equations resulting from the four processes above (up to a time scaling).

$$\begin{cases} \dfrac{dN_1}{dt} = m_1 \left[\mu\alpha - \alpha(1-\mu)\dfrac{N_1}{m_1} \right. \\ \qquad\qquad \left. + \dfrac{1}{\bar{N}}\left(-N_1 + 2N_2\right) - \dfrac{\gamma N_1}{m_0} \right] \\ \dfrac{dN_k}{dt} = m_1 \left[\dfrac{\alpha(1-\mu)}{m_1}\left((k-1)N_{k-1} - kN_k\right) \right. \quad \text{for } k > 1 \\ \qquad\qquad \left. + \dfrac{1}{\bar{N}}\left(-kN_k + (k+1)N_{k+1}\right) - \dfrac{\gamma N_k}{m_0} \right] \end{cases} \tag{1}$$

We use moment closure to describe the dynamic of our system. Moments satisfy the following equations:

$$\begin{cases} \dfrac{dm_0}{dt} = m_1 \left[\mu\alpha - \dfrac{N_1}{\bar{N}} - \gamma \right] \\ \dfrac{dm_1}{dt} = m_1 \left[\alpha - \dfrac{m_1}{\bar{N}} - \gamma\dfrac{m_1}{m_0} \right] \\ \dfrac{dm_2}{dt} = m_1 \left[\alpha + \dfrac{m_1}{\bar{N}} + m_2 \left[\dfrac{2\alpha(1-\mu)}{m_1} - \dfrac{2}{\bar{N}} - \dfrac{\gamma}{m_0} \right] \right] \end{cases} \tag{2}$$

When in equilibrium, the eqution for the total population size m_1 yields $\frac{\alpha}{m_1} = \frac{1}{\bar{N}} + \frac{\gamma}{m_0}$. in the absence of catastrophe, $m_1 = \alpha\bar{N}$.

TIME TO EXTINCTION

Expected times to extinction

We introduced T_k as the average time to extinction for a type of initial size k and obtain Eq. 3, where time is discretized with time steps $\frac{1}{m_1}$. We solved this system with a matrix inversion and used numerical estimates for m_0 and m_1 obtained from simulations reaching steady state, for each value of γ. Analytical estimates of m_0 and m_1 would indeed require an assumption on the type size distribution (as mentioned in [1]), which yields accurate, but still slightly imprecise estimates. To avoid that, we, therefore, performed simulations for each parameter combination and computed the average estimate of m_0 and m_1 in equilibrium. A boundary condition with a maximum type size N sufficiently large was imposed for computational purposes. Since the probabilities are very small, the boundary condition only needs to be double the maximum studied size to obtain stable results (see Fig. 1).

$$\begin{cases} T_1 = 1 + \dfrac{\alpha(1-\mu)}{m_1}T_2 + \left[1 - \dfrac{\alpha(1-\mu)}{m_1} - \left(\dfrac{\alpha}{m_1} - \dfrac{\gamma}{m_0}\right) \right] T_1 \\ T_k = 1 + k\dfrac{\alpha(1-\mu)}{m_1}T_{k+1} + k\left(\dfrac{\alpha}{m_1} - \dfrac{\gamma}{m_0}\right)T_{k-1} \\ \qquad + \left[1 - k\dfrac{\alpha(1-\mu)}{m_1} - k\left(\dfrac{\alpha}{m_1} - \dfrac{\gamma}{m_0}\right) - \dfrac{\gamma}{m_0} \right] T_k. \end{cases} \tag{3}$$

$$a = \dfrac{\alpha(1-\mu)}{m_1},\ b = \dfrac{\alpha}{m_1} - \dfrac{\gamma}{m_0},\ c = \dfrac{\gamma}{m_0}, \tag{4}$$

$$\begin{cases} 1 = [a + b + c]T_1 - aT_2 \\ 1 = -kbT_{k-1} + [k(a+b) + c]T_k - akT_{k+1} \\ 1 = -NbT_{N-1} + [Nb + c]T_N, \end{cases} \tag{5}$$

1 is the vector of ones. $\mathbb{T} = (T_1, ..., T_N)$. We define the following matrix:

$$\mathbb{M} = \begin{bmatrix} a+b+c & -a & 0 & \cdots & 0 & 0 \\ -2b & 2(a+b)+c & -2a & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & -Nb & Nb+c \end{bmatrix}$$

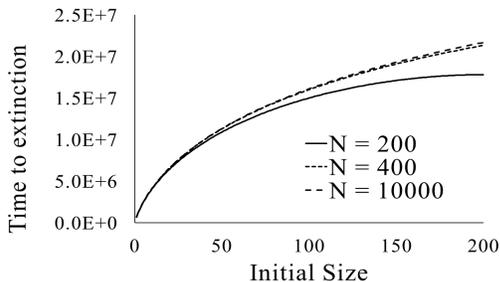$$\mathbb{T} = \mathbb{M}^{-1} \cdot \mathbf{1}. \tag{6}$$

FIG. 1. We compute analytical times to extinction for types with initial size up to 200. If the boundary condition is $N = 400$, results are already stable and equal to those obtained if $N = 10000$.

Times to extinction in a non-linear model with balancing selection

In order to show that catastrophes can reproduce negative frequency dependent selection, we used a model similar to the non-linear model of Karev et. al [2]. To our previous approach for the expected times to extinction, we removed the catastrophe term and added a fixed birth rate a to create balancing selection. We solved this system numerically just as in our model. The values used for m_0 and m_1 were estimated assuming equilibrium.

$$\begin{cases} T_1 = 1 + \dfrac{\alpha(1-\mu)}{m_1}T_2 + \left[1 - \dfrac{\alpha(1-\mu)}{m_1} - \dfrac{1}{\bar{\bar{N}}}\right]T_1 \\ T_k = 1 + \dfrac{\alpha(k+a)(1-\mu)}{m_1}T_{k+1} + \dfrac{k}{\bar{N}}T_{k-1} \\ \quad + \left[1 - \dfrac{\alpha(k+a)(1-\mu)}{m_1} - \dfrac{k}{\bar{N}}\right]T_k, \end{cases} \tag{7}$$

SIMULATIONS

Process Initialization

We consider a discrete-time model. We start by choosing an initial set of types for which the sizes are computed randomly according to a Ewens scale-free distribution [3]. For the simulations, we apply a cut-off by imposing an initial maximum type size. This number has to be sufficiently large.

TABLE I. Simulations parameters

Parameter	Name	Value
α	Birth rate	1
$\bar{N}$	Population size	7.5×10^5
γ	Catastrophe rate	10^{-6} to 10^{-2}
μ	Mutation rate	10^{-2}
T	Total number of time steps	10^8

For the sake of efficiency, all the initial types (and thereafter all types) are plugged into a tree, in order to keep track of each type size. Each leaf corresponds to a type and the number associated with this entry is the type size. The value of each internal node in the tree is the sum of his two sons; the tree root being the size of the total population m_1. A second tree is also created, identical to the first one, except that the values in the leaves are 0 or 1. This tree will record whether a type exists or is extinct and will be used for the catastrophes; the tree root being the total number of types m_0 (see Fig. 2). This configuration enables us to access each type in $O(\log(m_i))$. Those trees have to be sufficiently large to welcome new types. Finally, we also have a vector of creation times for all existing types so that when a type disappears, we can compute its time to extinction.
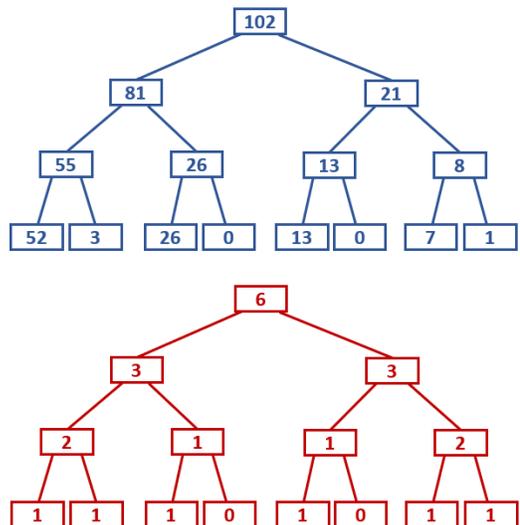

FIG. 2. Trees recording type sizes (blue tree) and whether types exist or not (red tree). Each node is the sum of its two leaves.

Data Processing

As described above, at every time step, the total number of individuals, m_1, is calculated and the death rate is set to be $\delta = \frac{m_1}{N}$. Once δ is determined, α, δ and γ are normalized by their sum, and then an event is chosen randomly according to these probabilities. This event can either be a birth, a death or a catastrophe. In case the event is a birth, it can either occur in an existing type or be a mutation.

For a birth, an individual is chosen randomly in the entire population and its type size will increase by 1 (blue tree). If it is a mutation, a new one-member type is created. A leaf in the red tree that was previously empty is now set to 1 along with the corresponding leaf in the blue tree. The creation time for this type is also recorded.

For a death, we also randomly pick an individual in the population and its type size will be reduced by 1 in the blue tree. In case the type size goes to 0, the corresponding leaf in the red tree will also be set to 0 and it would be considered as an extinction.

In the event of a catastrophe, resulting in the extinction of an entire type, a type is randomly chosen in the red tree and its value set to 0 along with the corresponding leaf in the blue tree. When extinction occurs, the time to extinction of this type is recorded along with the initial size of the extinct type.

CATASTROPHES MODELS

In our baseline model, we assumed that a catastrophe can hit each type with equal probability, independently of their size, and that the entire type would be deleted through this catastrophe. We derived from our model that there exists a transition between "negative invasion rate" and "positive. invasion rate". We also showed that in the later, diversity would decrease. Finally, we also simulated the entry rate to illustrate this transition. For $\mu = 0.01$, $\alpha = 1$, $m_0 \approx 3000$ and $m_1 \approx 75000$ this transition occurs at a rate $\gamma = \frac{\alpha \mu m_0}{m_1} = 0.0004$. To assess the robustness of our results and prove that they do not actually depend on how catastrophes were computed, we checked the existence of this transition for different catastrophe models. Instead of having the entire type deleted, we implemented simulations where only a

fraction (random or fixed) of the type would be eradicated. A fixed fraction of 0.5 or a random fraction corresponds to a probability $p_0 = \frac{\alpha}{m_1} - \frac{\gamma}{2m_0}$ in our GW model. The transition occurs for $\gamma = \frac{2\alpha\mu m_0}{m_1} = 0.0008$. We also simulated catastrophes with a rate proportional to the total population size, which corresponds to a probability $p_0 = \frac{\alpha}{m_1} - \frac{\gamma m_1}{m_0 N}$ and a transition for $\gamma = \frac{m_0}{m_1}\frac{\mu}{1-\mu} \approx 0.0004$. In each of those cases, we still observe a clear transition in the entry rate and diversity as shown in Fig. 3. We also simulated the case where the catastrophes rate is proportional to type sizes, but this case does not exhibit a transition since catastrophes simply add a death effect and do not create a bias (data not shown).
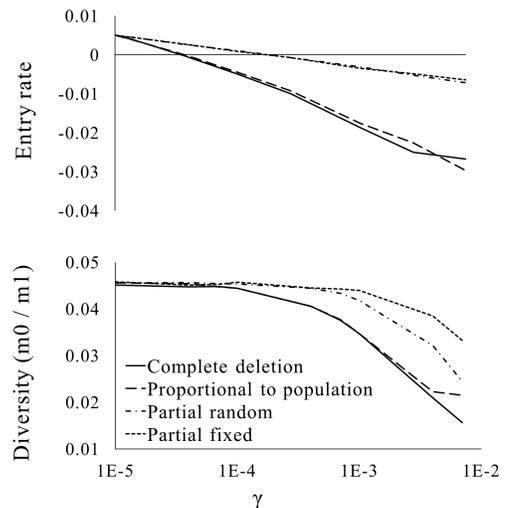

FIG. 3. Entry rate and diversity as a function of γ for the different models of catastrophe. In all models the entry rate decreases and becomes negative and the diversity decreases with the entry rate.

[1] N. Dori, H. Behar, H. Brot and, Y. Louzoun, Phys. Rev. E **98**, 012416 (2018)
[2] G. Karev, Y. Wolf and, E. Koonin, Bioinformatics **19**, 1889 (2003)
[3] W. Ewens, Theor. Popul. Biol. **3**, 87 (1972)