# Stochastic Dynamics through Hierarchically Embedded Markov Chains

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Studying dynamical phenomena in finite populations often involves Markov processes of significant mathematical and/or computational complexity, which rapidly becomes prohibitive with increasing population size or an increasing number of individual configuration states. Here, we develop a framework that allows us to define a hierarchy of approximations to the stationary distribution of general systems that can be described as discrete Markov processes with time invariant transition probabilities and (possibly) a large number of states. This results in an efficient method for studying social and biological communities in the presence of stochastic effects—such as mutations in evolutionary dynamics and a random exploration of choices in social systems—including situations where the dynamics encompasses the existence of stable polymorphic configurations, thus overcoming the limitations of existing methods. The present formalism is shown to be general in scope, widely applicable, and of relevance to a variety of interdisciplinary problems.

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Many complex time-dependent processes, from the evolution of cooperation [1] to genetic drift and evolution of ecosystems [2], flocking behavior [3], voter dynamics [4], disease spread [5], diffusion of innovations [6], consensus formation [7], and peer influence [8], have been modeled by stochastic Markov processes. The nonlinear nature of the dynamics often precludes a full analysis, even under continuous approximations, in which case (quasi)stationary distributions of the Markov chain still provide insightful information [9–11]. However, with an increasing number of states, determining these distributions leads to chains of a prohibitive size (see below). As a result, the so-called small mutation approximation (SMA) was introduced, defining a minimal (embedded) Markov chain whose solution estimates the limiting stationary distribution of the population [9].

To reveal the savings obtained under the SMA, let us consider a population of size $Z$ where each individual adopts one of $S$ different strategies (states), $\sigma_1, \sigma_2, \ldots, \sigma_S$. The (mean-field) population configurations are characterized by the number of individuals adopting each strategy, with $\{i_1, i_2, \ldots, i_S\}$ adding up to $|s| = \binom{Z+S-1}{S-1}$ possible configurations, requiring us to solve a Markov chain of that size. The complexity obtained for large finite $S$ turns the complete analysis unfeasible, even for a small $Z$. In the absence of mutations, this stochastic process has $S$ absorbing states, the so-called monomorphic [9,12,13] configurations, in which all individuals play the same strategy. Starting at a given monomorphic configuration, the population will remain there until a mutation happens that flips the state of one individual. This new behavior either spreads, leading to another monomorphic configuration, or goes extinct, leading to the starting configuration. If mutations are rare, the time scales of selection (fast) and mutation (slow) become separated. This allows us to define an embedded Markov chain consisting only of $S$ monomorphic configurations. The transition matrix is given by the fixation probability of a single mutant in a homogeneous population of resident individuals [14]. Thus, under the SMA the (embedded) configuration space has a size $S$ and all transitions are computed through processes involving only two states at a time.

The SMA has been employed with success in different areas of research [10,12,15], its validity requiring the mutation probability $\mu$ to be small [16], depending on the population size and the underlying dynamics of the system. Thus, many time-dependent processes of interest cannot be described in the SMA [15,17].

Here, we develop a new framework leading to a hierarchy of approximations to the stationary distribution of a general population Markov process. At each level, our framework involves implementing the following process: (1) Choose an (ideally) small set of configurations of interest (COIs), thus separating the set of all possible configurations $s = \{s_1, s_2, \ldots, s_{|s|}\}$ into two disjoint sets—$A = \{a_1, a_2, \ldots, a_{|A|}\}$, the COIs, and $B = \{b_1, b_2, \ldots, b_{|B|}\}$, the neglected configurations (NCs)—such that $|s| = |A| + |B|$ and $|A| \ll |B|$. The goal is to infer the full dynamics considering only the COIs. The stable fixed points constitute ideal choices to include in the COIs. If they cannot be determined analytically or numerically, one may use a sample of the state space. Both cases are illustrated below. The hierarchical nature of the approximation stems from the location of the COIs in the state space (the simplex): $Hn$ corresponds to when all points in the COIs belong to hyperfaces of dimension at most $n$. In this case, the approximation is of the order $n$ in the exploration parameter, $\mu$ (typically, mutation), restricting the phase space

 

to those configurations accessible through $n$ cumulative transitions in $\mu$, starting at the vertices. (2) Calculate the transition probabilities among the COIs, $\rho_{a_i \to a_j}$, from the known one-step transitions between the states $s_i$ and $s_j$, $T_{s_i s_j}$. The probability of reaching a COI, $a_j$, starting from one of the NCs, $b_n$, can be computed through an absorbing Markov chain and reads $P_{b_n a_j} = \sum_{\{b_m\}} T_{b_n b_m} P_{b_m a_j} + T_{b_n a_j}$. Thus, for nonadjacent COIs, $\rho_{a_i a_j} = \sum_{\{b_n\}} T_{a_i b_n} P_{b_n a_j}$, allowing the computation of an unnormalized stationary distribution, $p$, over the COIs through $p = \boldsymbol{\rho}^T p$. (3) $p$ reflects the relative time spent in each COI, yet it ignores the prevalence in the COIs relative to the NCs. Thus, a renormalization is in order to allocate the right strength to each point in the COIs. We write the distribution over the whole phase space as $P(x) \propto \sum_{i=1}^{|A|} p(a_i) f_i(x)/f_i(a_i)$, where $f_i$ represents locally defined distributions that characterize $P(x)$ around each COI. This way, we associate with each COI the moments of the distribution around it, reflecting its shape around these configurations. This can be achieved by using local information and/or the remaining COIs.

Whenever analytical approaches are not available, the complexity of $Hn$ is dominated by the computation of $\rho$, involving the inversion of a matrix of size $\approx Z^n/n!$, still much smaller than the original Markov chain for any $n < s-1$ (see the original chain size above). Below, we provide an efficient alternative for $H1$.

Let us illustrate the method with some examples. We consider a one-dimensional system ($S = 2$) to motivate our first-order approximation ($H1$) and the limitations of the SMA ($H0$). Specifically, consider the evolutionary dynamics of a population of size $Z$ where individuals are either **C** or **D** and they interact with all others via a two-person game that posits a social dilemma of cooperation, with the associated payoff matrix

$$\begin{array}{c} \\ C \\ D \end{array} \begin{array}{c} \begin{array}{cc} C & D \end{array} \\ \begin{bmatrix} 1 & f \\ 1+g & 0 \end{bmatrix} \end{array},$$

with $\{f, g\} \in [-1, 1]$ [18]. The states $s_i$ are defined by the number $i$ of **C** individuals ($Z - i$ are **D** individuals). Time evolution proceeds via a discrete-time *birth-death* process [19], characterized by the probabilities that, in each time step, the number of individuals adopting strategy **C** changes by $\pm 1$ or 0. We employ a stochastic imitation process inspired in the Fermi distribution of statistical physics [20], allowing the analytical computation of the transition probabilities: $T_i^{\pm} \equiv T_{(i \to i \pm 1)} = (1-\mu)[i(Z-i)/Z(Z-1)]\{1/[1+e^{\mp\beta[f_C(i)-f_D(i)]}]\} + \mu\{[(Z-i)/Z]\delta_{(1,\pm 1)} + (i/Z)\delta_{(-1,\pm 1)}\}$, where $f_C$ ($f_D$) is the average payoff of a **C** (**D**), and the inverse temperature, $\beta \geq 0$, mimics the intensity of natural selection [19], to which we added a mutation probability $\mu$ that accounts for the possibility of (unanticipated) random exploration of strategies, an important process in social and cultural evolution [21].

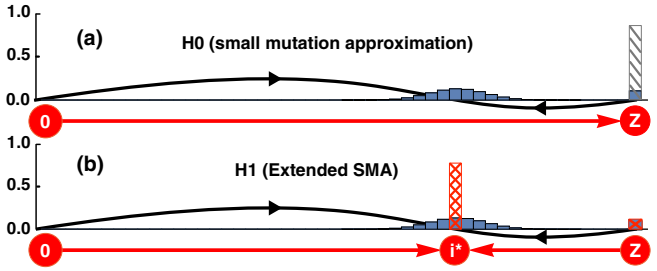


FIG. 1. Stationary distributions associated with a coexistence game ($f = 0.7$, $g = 0.3$). The gradient of selection is represented by the black curves, whereas the exact stationary distribution, computed for $\mu = 10^{-10}$, is depicted by the solid (blue) bars. Two levels of approximation are considered: (i) zeroth order, $H0$ or SMA (the dashed gray bars) and (ii) first order, $H1$ (the crossed red bars). In (a), we compare the exact solution with $H0$ (SMA). In $H0$, the COIs include only the configurations $i = 0$ and $i = Z$, and the most probable transitions between the COIs—indicated by the red arrows—suggest why the full strength is concentrated at $i = Z$. Clearly, $\mu = 10^{-10}$ in a population of size $Z = 50$ is not small enough to bring the exact result into the SMA domain of validity. In (b), the crossed red bars represent the stationary distribution yielded by $H1$, where $i^*$ was added to the COIs. The other parameters are $Z = 50$, $\beta = 10$.

Naturally, different assumptions regarding the time evolution of the population will result in different expressions for the transition probabilities, but the method remains valid for any population Markov chain.

In Fig. 1(a) we show results for a coexistence game, known as the snowdrift game in physics and economics [22], the hawk-dove game in evolutionary biology [23], and the chicken game in other contexts [24]. The full stationary distribution is depicted by the blue histogram bars. There are two monomorphic states, associated with configurations in which all individuals are either **D** ($i = 0$) or **C** ($i = Z$). The existence of a probability attractor at $i^* = 0.7Z = 35$ reflects the coexistence dynamics. $H0$ (SMA) leads to the dashed gray bar in Fig. 1(a). The solid line represents the so-called gradient of selection, given by $G(i) = T_i^+ - T_i^-$. Clearly, SMA leads to a distribution that differs substantially from the full distribution. Indeed, Fig. 2(a) shows that the existence of an interior attractor means that, to get a good agreement between the SMA and the full distribution, $\mu$ must be less that $10^{-13}$—leading to $\mu$ values unreasonably small, both in biological and social contexts. Importantly, as $\mu$ increases, the SMA quickly fails to account for the changes introduced in the stationary distribution by nonzero mutations.

Figure 1(b), in turn, shows the result of employing $H1$. The first step consists of adding the attractor $i^*$ to the COIs already including $i = 0$ and $i = Z$. This additional point is trivial to find [19]. The second step implies calculation of the probabilities $\rho_{a_i \to a_j}$ within the COIs, merely requiring a repartition of the terms already computed in $H0$, bringing no additional overhead to the computation. Indeed, an ordering

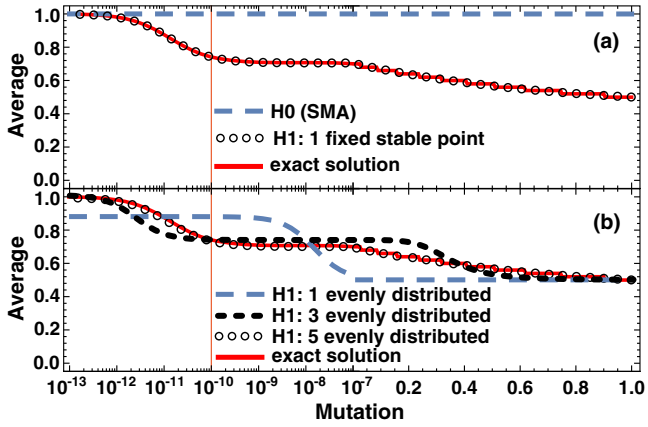


FIG. 2. Same system as Fig. 1. (a) We compare the results of $H0$ and $H1$ with the exact solution. (b) We add one, three, and five homogeneously distributed points to the $H0$ COIs, assuming a flat distribution around each COI. With five equidistant points, we reproduce the full distribution, disregarding any information about the dynamics and its fixed points. The vertical line indicates the value of $\mu$ employed in Fig. 1.

can be defined over configurations in $A$ such that transition probabilities from $a_i$ to $a_{(i\pm1)}$ are written as $\rho^{\pm}_{a_i} \equiv \rho_{a_i \to a_{(i\pm1)}}$. These correspond to the probability of having a one-step transition in the direction of $a_{(i\pm1)}$ and then being absorbed by it, resulting in $\rho^{\pm}_{a_i} = T^{\pm}_{a_i}[1+\sum_{j=a_i\pm1}^{a_{i\pm1}\mp1}\prod_{k=a_i\pm1}^{j}(T^{\mp}_k/T^{\pm}_k)]^{-1}$ [see the Supplemental Material (SM) [25] for additional details].

With $\rho^{\pm}_{a_i}$, the unnormalized stationary distribution over configurations in $A$, $p(a_i)$, is calculated through an eigenvector search [26]. The histogram shown with crossed red bars in Fig. 1(b) results from a proper renormalization of $p(a_i)$ via the implementation of step 3 above. Indeed, as $a_2$ is a probability attractor, it should carry an associated strength that mimics the weight of the full stationary distribution (the solid blue bars) in its vicinity. The natural choice (and the one we propose and adopt throughout) is to derive this renormalization factor from a normal distribution whose expected value is equal to (the value of the process at) $a_2$ and whose variance can be calculated from the Kramers-Moyal expansion of the associated master equation [19]. We may therefore write the distribution as

$$P(i) \approx \alpha^{-1}[p(a_1)\delta_{ia_1} + Z\sqrt{2\pi\sigma^2}\,p(a_2)\delta_{ia_2} + p(a_3)\delta_{ia_3}],$$

where $\alpha = p(a_1) + Z\sqrt{2\pi\sigma^2}\,p(a_2) + p(a_3)$, and $\sigma^2$ can be derived from the transition probabilities $T^+_x$ and $T^-_x$ around $a_2/Z$ as $\sigma^2 = F/|J|$, with $J = d(T^+_x - T^-_x)/dx|_{x=a_2}$ and $F = (T^+_{a_2} + T^-_{a_2})/(2Z)$. In the SM [25] we prove these results and discuss the validity and accuracy of these estimates.

Whenever the game at stake is not one of coexistence but, instead, one of coordination [22,27]—thus characterized by the occurrence of a probability repeller instead of an attractor—our approach remains unchanged, as detailed in the SM [25].

The choice of the COIs (and hierarchy order $n$) dictates the complexity and accuracy of the whole procedure, as the problem is reduced from solving a chain of size $\sim Z^{s-1}$ to one of size $\sim Z^n$, $n < s$. Any choice of COIs optimizing the trade-off between complexity and accuracy will depend on the specifics of each model, such as the characteristic mutation rate, number, and position of fixed points and their basins of attraction. In general, choosing as COIs the stable fixed points of the gradient of selection provides the most natural choice to minimize the size of the embedded chain that leads to an accurate approximation. These fixed points are often easy to find by resorting to numerical methods whose complexity scales linearly with $|s| \sim Z^n$ [28].

Nonetheless, our framework can still be applied whenever the fixed points are unknown. In Fig. 2(b) we provide results analogous to Fig. 2(a) by defining the COIs in the simplest possible way: a homogeneous grid including one, three, or five intermediate configurations. Clearly, depending on the problem, other methods (such as importance sampling) may be employed to improve the choice of COIs.

In terms of accuracy, $H0$ (SMA) leads to the smallest COI set, accurate for $\mu \to 0$. At $H1$, one enlarges the set $A$, including in the COIs points located along the edges of the simplex. A comparison of Figs. 2(a) and 2(b) shows that including the fixed points in the COIs minimizes its size for a given order. Whenever an increase in the order leads to a mismatch between the results, we identify the region of validity of the previous orders. This mismatch occurs whenever a stable fixed point is present at the newly included dimension and exploration rates allow the system to reach them. In turn, this means that, if there are no internal fixed points above a given order $n$, this order will suffice to describe the system for any exploration rates. Indeed, order $Hn$ will be exact to the extent that the probability of reaching dimension $m > n$ from $n$ ($\propto \mu^{(m-n)}$) is much lower than the probability of going back (model dependent). As we increase $\mu$, retaining accuracy will require increasing the hierarchy level.

It is worth pointing out at this stage that, already at $H1$, one is able to study explicitly the role of mutations, whose occurrence is ubiquitous in, e.g., (noisy) social systems [29]. Indeed, whereas in the SMA ($H0$) mutation is a tool to enforce that the embedded Markov chain is irreducible, in our case nothing prevents mutations from occurring *at par* with the selection process.

Consider now a population in which $Z$ individuals may adopt (be in) one of three possible strategies (states) ($\sigma_k$, $k = 1, 2, 3$). This higher dimension problem may call for higher order approximations, as we discuss next. Each configuration $s_{\mathbf{i}} = (i_1, i_2)$ is one in which $i_1$ ($i_2$) individuals have the strategy $\sigma_1$ ($\sigma_2$) (and $Z - i_1 - i_2$ have the strategy $\sigma_3$). Both $G$ and the stationary distribution can be represented using the two-dimensional simplex portrayed in Fig. 3. We consider the evolutionary dynamics of a three-strategy game

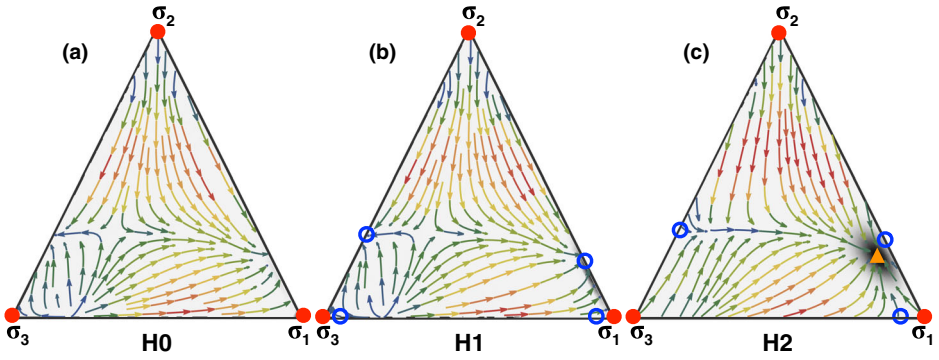


FIG. 3. COIs at different levels of the hierarchical approximation. The arrows represent the most likely direction of evolution of the system (the gradient of selection, $G$, with warm colors representing larger magnitudes), whereas the background gray shading represents the stationary distribution (darker areas correspond to states with higher probability). As mutation increases, the population explores configurations deviating gradually from the vertices. For the dynamics and parameters specified below, this trend starts (a) at $\mu = 10^{-4}$, exploration of the phase space extending mostly along the edges (b) up to $\mu = 10^{-2}$, to finally explore the interior of the simplex for higher values of $\mu$ [$\mu = 10^{-1}$ in (c)]. The probabilities of updates from strategies $\sigma_i$ to $\sigma_j$ are given by $T_{(\sigma_i \to \sigma_j)} = [Z/(Z-1)]x_i x_j(1-\mu)(1+e^{(\Delta f_{(\sigma_i \sigma_j)})})^{-1} + x_i(\mu/d)$, with $\Delta f_{\sigma_i \sigma_j} = \beta_{ijx}(x_1 - x_1^*) + \beta_{ijy}(x_2 - x_2^*)$, with $x_i$ being the frequency of strategy $\sigma_j$ and $d$ the number of accessible strategies, given the restriction of the phase space considered. The parameters are $Z = 50$, $\beta_{12x} = 2$, $\beta_{12y} = \beta_{13x} = 10$, $\beta_{23y} = -10$, $\beta_{13y} = \beta_{23x} = 0$, $x_1^* = 2/10$, and $x_2^* = 3/10$.

(see the caption to Fig. 3), characterized by an interior saddle point, while exhibiting both coexistence and coordination dynamics along the edges of the simplex, a problem reminiscent of the evolutionary dynamics of multiple myeloma cancer cells [30,31]. Under $H0$ (SMA), the COIs include the three monomorphic configurations [vertices of the triangles and the red solid circles in Fig. 3(a)], confining the evolutionary trajectories to the edges of the simplex. Under $H1$, the COIs now include additional configurations along the edges, as illustrated by the blue

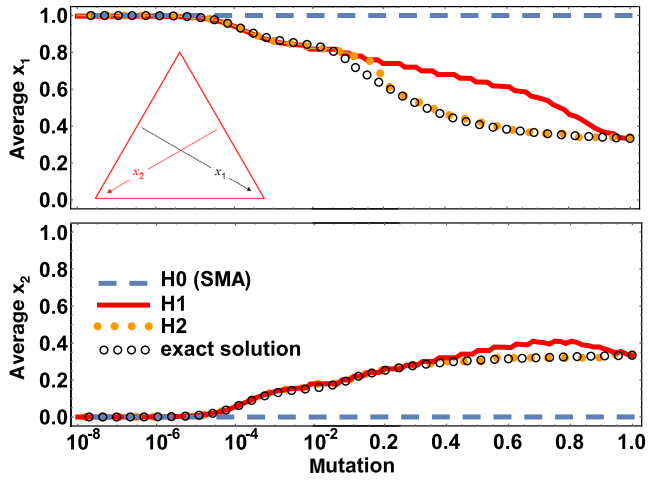


FIG. 4. We plot the average of the stationary distributions as a function of mutation probability for the system depicted in Fig. 3, and at different levels of the hierarchical approximation. At the $H0$ level (SMA), accurate average values are obtained whenever $\mu < 10^{-5}$. As mutation increases, the polymorphic configurations attract higher probabilities, requiring the inclusion of COIs along the edges of the simplex ($H1$) and in its interior ($H2$)—see the text for details.

open circles in Fig. 3(b). Importantly, the criteria adopted in choosing these COIs follow straightforwardly from the one-dimensional cases already discussed, given the constraints that apply to the trajectories at this level of approximation.

At level $H2$, we add to the COIs one configuration in the interior of the simplex (in which three strategies are present), identified by the (interior) solid orange triangle in Fig. 3(c). The results obtained are shown in Fig. 4, where we compare the exact solution (the black open circles) with the results provided by successive orders of approximation, for a wide range of mutation values. As expected, $H0$ (SMA) is unable to provide an overall accurate description of the stationary distribution. As $\mu$ increases, the stable fixed points move away from the vertices, first along the edges, a feature which is nicely captured at the level of $H1$, and subsequently to the interior of the simplex, requiring one to move to $H2$.

Notably, both $H1$ and $H2$ provide accurate results for the average distribution. This, for a large $\mu$, is an artifact of averaging, as the variance of the distribution will be different. Indeed, $H1$ imposes a dynamics along the edges, whereas $H2$ allows exploration of the interior of the simplex.

In summary, as is well known in many areas of science, a judicious choice of COIs proves instrumental in minimizing the workload necessary to reach a good description of a system. In this Letter we show how this concept applies to nonlinear population dynamics where individuals may be equipped with complex physical, biological, or social repertoires. In dealing with population Markov chains, we establish an approximation order associated with the dimensionality of the simplex points to be included as COIs, an approach that allows the explicit inclusion of mutations in the dynamics, leading to, among other features, an explicit

dependence of the weight and location of the fixed points on $\mu$. Although reminiscent of the approach of Freidlin and Wentzell [32], these features of our framework make it different and especially well suited to treat not so large deviations, mostly when mutations induce deviations with time scales comparable to those of the dynamical process, having a direct impact on $G$, as well as on higher moments. By dramatically reducing the complexity of the multidimensional Markov processes we aim to describe, the present framework allows one to retain analytical and/or numerical tractability, being general in scope, and thus of a potential applicability in a wide variety of problems that transcend pure physics applications.

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# Stochastic dynamics through hierarchically embedded Markov chains Supplemental Material

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Here we elaborate on the method introduced in the main text, which can be used to calculate a hierarchy of approximations to the stationary distribution of a Markov chain by means of simpler embedded chains that comprise a reduced number of configuration (configurations of interest, CoI). The granularity of this procedure can be tuned by moving up or down in the hierarchy, allowing to choose between accuracy and computational ease and to opt for the approximation level that concedes a proper validity given the phenomena being modeled.

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## CONTENTS



## I. ON THE SCOPE OF THE METHOD

The examples used in the main text belong to evolutionary game theory, which provides a very convenient framework to explore the approximation procedure that we propose given that, on one hand, different games lead to very different phase-space dynamics, while on the other hand a single parameter – mutation – controls the probability of jumping between the different topologically distinct regions in phase space. More precisely, mutation allows the system to move from the vertices to the edges of the phase space simplex, as well as from the edges to the faces, and so on. In this sense, it is natural that the simplest (and, in our notation, the 0th-order) estimate of the stationary distribution at the vertices was coined as the small mutation approximation (SMA).

Despite our arguments being built on evolutionary models, we believe the scope of the method reaches far beyond that and can be applied to a broader class of problems, of potential interest in several branches of science. In fact, the method we propose allows one to estimate the stationary distribution of a generic discrete Markov process through a corresponding embedded Markov chain whose states are selected (starting) from the hyperfaces of smallest dimension of the original phase-space (or simplex) and moving inward, to successively higher dimensional hyperfaces. The approximation is hierarchical as one may tune the recursion level of the state-space reduction, starting from the vertices (0th-order), to the edges (1st-order), faces (2nd-order) and so on. This means that it can be adapted to the needs and features of different problems.

## II. TRANSITION PROBABILITIES BETWEEN CoI ($\rho$) IN AN ARBITRARY MARKOV CHAIN

Let us start by laying down the general framework for an arbitrary chain, defining the transition probabilities

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between the selected CoI using the transitions stemming from the full chain. To begin with, it is worth noting that in any finite chain, the configurations can be counted and ordered. Thus, we consider a finite set of configurations $\{s_1, s_2, \ldots, s_{|A|+|B|}\}$ that, as clarified below, can be divided in those of interest (CoI, here belonging to set A) and those to be neglected (set B). A time-homogeneous Markov process happens over this set such that the system moves from configuration $s_k$ to configuration $s_l$, in each step, with a time invariant probability $T_{s_k \to s_l}$ (or $T_{s_k s_l}$ in matrix notation) independent of the configurations it occupied in all previous times.

The goal now is to reduce the number of considered configurations to those of interest (CoI), $A = \{a_1, \ldots, a_{|A|}\}$, and calculate the transition probabilities between each of these selected configurations, $\rho_{a_i \to a_j}$ (or $\rho_{a_i a_j}$). For this we also need the one-step transition probabilities $T_{b_n b_m}$ between neglected configurations in $B = \{b_1, \ldots, b_{|B|}\}$, the one-step transitions between neglected configurations and CoI, $T_{b_n a_i}$, and vice-versa for $T_{a_i b_n}$ and, also, the transitions between neglected configurations and CoI, which we call $P_{b_n \to a_j}$ (or $P_{b_n a_j}$). Thus, we can write that

$$\rho_{a_i a_j} = \sum_{\{b_n\}} T_{a_i b_n} P_{b_n a_j} + T_{a_i a_j} \text{ and} \tag{1}$$

$$P_{b_n a_j} = \sum_{\{b_m\}} T_{b_n b_m} P_{b_m a_j} + T_{b_n a_j}. \tag{2}$$

If we conveniently order the configurations, placing the neglected configurations first and then the CoI, we can make use of matrix notation and algebra. We may write

$$\mathbf{T} = [T_{kl}] = \begin{bmatrix} \mathbf{Q} & \mathbf{R} \\ \mathbf{U} & \mathbf{V} \end{bmatrix}, T_{kl} \equiv T_{s_k s_l} \tag{3}$$

with $Q_{mn} = T_{b_m b_n}$ representing one-step transitions between neglected configurations, $R_{mi} = T_{b_m a_i}$ representing one-step transitions from neglected configurations to CoI, $U_{im} = T_{a_i b_m}$ representing one-step transitions from CoI to neglected configurations and $V_{ij} = T_{a_i a_j}$ representing one-step transitions between CoI. Notice that if there are no adjacent CoI, $\mathbf{V} = 0$. This turns Eqs.(1,2) into

$$\rho = \mathbf{UP} + \mathbf{V} \text{ and} \tag{4}$$

$$\mathbf{P} = \mathbf{QP} + \mathbf{R}. \tag{5}$$

Finally, we can write for the transitions between CoI

$$\rho = \mathbf{U}(1 - \mathbf{Q})^{-1}\mathbf{R} + \mathbf{V}. \tag{6}$$

Notice, however, that the calculation of these transitions involves a matrix inversion, which, if calculated numerically, may be ill-conditioned.

Nonetheless, when considering a one dimensional chain – which turns out to be the cornerstone of our 1st-order approximation – this expression becomes fairly simple and exempts the numerical inversion of matrices or the eigenvector search. After presenting the general framework, we devote a whole a section (VII) to explore this scenario.

## III. USING $\rho$ TO COMPUTE STATIONARY DISTRIBUTIONS OVER CoI AND THE NECESSITY OF ESTIMATING THE REMAINING DISTRIBUTION

Let us distinguish between the general process we defined, with transition probability between configurations $s_k$ and $s_l$, $T_{s_k s_l}$, and the process that happens only over the set of CoI that one gets from using $\rho$ as its transition matrix. Because we calculate transitions between CoI, $\rho$, from the microscopic transitions between all states, $T_{s_k s_l}$, the two processes must be related. Let us figure out that relation.

Consider the full Markov chain with transition probability between configurations $s_k$ and $s_l$, $T_{s_k s_l}$. We have seen that we can write $\mathbf{T}$ as in Eq.(3) and, thus, according to the Master Equation [1], the stationary distribution of the system can be obtained as the vector $\mathbf{p} = \{\mathbf{p}_b, \mathbf{p}_a\}$ whose sum of the entries is 1 and is given by

$$\begin{bmatrix} \mathbf{p}_b \\ \mathbf{p}_a \end{bmatrix} = \begin{bmatrix} \mathbf{Q} & \mathbf{R} \\ \mathbf{U} & \mathbf{V} \end{bmatrix}^T \begin{bmatrix} \mathbf{p}_b \\ \mathbf{p}_a \end{bmatrix}. \tag{7}$$

Solving Eq.(7) by substitution we get that, apart from normalization, the probability of finding the system in the subset of configurations $a_i$, $\mathbf{p}_a$, is given by

$$\mathbf{p}_a = \rho^{\mathbf{T}} \mathbf{p}_a. \tag{8}$$

This equation for $\mathbf{p}_a$ is exactly the equation of the stationary distribution of the process concerning only the CoI and $\rho$ as its transition matrix, and this defines the relation between the two processes.

This result shows that the transitions $\rho$, computed in the previous section as Eq.(6), when used as transition matrices for the calculation of the stationary distribution, turn out to give the probability of finding the full system in each CoI apart from a normalization constant, which depends on the neglected configurations. Consequently, i) the ratios between the probabilities of being in each CoI can be easily computed as the ratios of the unnormalized $\mathbf{p}_a$ obtained in Eq.(8). Moreover, ii) correct normalization of $\mathbf{p}_a$ requires, at least, an estimate of the distribution over the neglected configurations.

These points formally clarify our arguments. i) clarifies why using the SMA – or, in general, an approximation level lower in hierarchy compared to the dimensionality of the system – is important, as in this way we already collect crucial information on the process; ii), in turn,

calls for our comprehension of the shape of the distribution around the CoI. That is precisely what we discuss next.

## IV. RENORMALIZATION PROCEDURE

Let us assume that we have $|A|$ CoI, $a_i$, of which $S$ correspond to vertex configurations (also called monomorphic, see Section VI), and $|A|-S$ to internal stable fixed points. We can write a continuous stationary probability density for the state variable, $\mathbf{x} = \{x_1, \ldots, x_{S-1}\}$, which we call $P(\mathbf{x})$. As shown already, we are able to compute $p(a_i)$, the non-normalized stationary distribution over configurations in $A$ computed from the eigenvector of $\rho$, in Eq.(6). Since the probability of being in a CoI $a_i$ is $\alpha^{-1}p(a_i)$, where $\alpha^{-1}$ is a normalization constant over the entire phase-space, and given that this configuration has a range of $1/Z$ in each of the $S-1$ independent directions, the probability density at that point must be $\alpha^{-1}Z^{S-1}p(a_i)$. In other words, $P(a_i/Z) = \alpha^{-1}Z^{S-1}p(a_i)$, for $i = 1, \ldots, |A|$. A simple way of collecting this information is by writing

$$P(\mathbf{x})\,\alpha/Z^{S-1} = \sum_{i=1}^{|A|} p(a_i)\,\frac{f_i(\mathbf{x})}{f_i(a_i/Z)}. \tag{9}$$

The $f_i(\mathbf{x})$ functions are normalized probability densities that are non-zero in the neighborhood of $\mathbf{x} = a_i/Z$, $D[a_i]$, and their shape allows one to compute $\alpha$. The choice of $D[a_i]$ should take into account the decay of the function near $a_i$, such that includes most of its probability, and the union of all $D[a_i]$ should be the whole phase space. In general, the boundary of $D[a_i]$ should estimate the minimum of the PDF, moving away from $a_i$. However, if the functions decay fast enough, in a way that their tails do not intersect, one can set all $D[a_i]$ to the whole phase-space, avoiding the computation of cumulative distribution functions.

In order to further simplify the procedure, let us compute the weight of each peak, $w_{a_i} = \int\limits_{D[a_i]} P(\mathbf{x})\,d\mathbf{x}$, and then use it as the probability of being in configuration $a_i$.

Taking the weights of each peak as the value of the distribution in that CoI and setting the remaining states as unoccupied, we may write a discrete counterpart as

$$P(s) = \alpha^{-1}\sum_i p(a_i)\,\frac{Z^{S-1}}{f_i(a_i/Z)}\delta_{sa_i}. \tag{10}$$

We are left with computing a normalized function $f_i$ in a single point that reflects the shape of the distribution around the CoI. Bellow we deduce the expressions for different functions in different dimensionalities.

## V. PDF SOLUTION NEAR AN INTERNAL STABLE FIXED POINT

Now that we have laid down the general framework, we can start making some assumption in order to produce some closed form formulas.

Let us estimate the shape of the probability distribution function (PDF) near an attractor that corresponds to a stable fixed point in the infinite dynamics and show that it can be approximated by a Gaussian function. To this end, let us keep considering a general phase space of arbitrary dimension. The system moves from configuration $s_k$ to configuration $s_l$, in each step, with a probability $T_{s_k s_l}$. In general this corresponds to an $S-1$ dimensional process with the same properties.

The evolution of the PDF of the process $\mathbf{x} = \mathbf{i}/Z$, $p(\mathbf{x}, t)$, is given by the Master Equation [1] below.

$$p(\mathbf{x}, t+\tau) - p(\mathbf{x}, t) = \sum_{\boldsymbol{\delta}} \left( p(\mathbf{x}+\boldsymbol{\delta}, t)\, T^{-\boldsymbol{\delta}}(\mathbf{x}+\boldsymbol{\delta}) - p(\mathbf{x}, t)\, T^{\boldsymbol{\delta}}(\mathbf{x}) \right), \tag{11}$$

where $T^{\boldsymbol{\delta}}(\mathbf{x}) \equiv T_{\mathbf{Zx},\mathbf{Z}(\mathbf{x}+\boldsymbol{\delta})}$. This, in turn, can be expanded in power series in $\boldsymbol{\delta} \sim 1/Z$ to give

$$\begin{aligned}\frac{\partial p}{\partial t}(\mathbf{x}, t) = &-\sum_k \frac{\partial}{\partial x_k}\left( D_k^{(1)}(\mathbf{x})\, p(\mathbf{x}, t) \right) \\ &+\sum_k \sum_{k'} \frac{\partial^2}{\partial x_k \partial x_{k'}}\left( D_{kk'}^{(2)}(\mathbf{x})\, p(\mathbf{x}, t) \right) \\ &+ \ldots \end{aligned} \tag{12}$$

where

$$\begin{aligned} D_k^{(1)}(\mathbf{x}) &= T^{k+}(\mathbf{x}) - T^{k-}(\mathbf{x}), \text{with} \\ T^{k\pm}(\mathbf{x}) &\equiv \sum_{\boldsymbol{\delta}:\delta_k = \pm 1/Z} T^{\boldsymbol{\delta}}(\mathbf{x}) \end{aligned} \tag{13}$$

and

$$D_{kk}^{(2)}(\mathbf{x}) = \frac{1}{2Z}\left( T^{k+}(\mathbf{x}) + T^{k-}(\mathbf{x}) \right) \tag{14}$$

$$D_{kk}^{(2)}(\mathbf{x}) = -\frac{1}{2Z}\left( T^{k\to k'}(\mathbf{x}) + T^{k'\to k}(\mathbf{x}) \right), k \neq k' \tag{15}$$

Here, $T^{t\to t'}$corresponds to a transition with $\boldsymbol{\delta} = \{0,\ldots,0,\delta_t=-1,0,\ldots,0,\delta_t=+1,0,\ldots,0\}$.

If we neglect the remaining terms of the expansion, we get a Fokker-Planck equation, in which the term $D_t^{(1)}$ corresponds to the drift, or gradient of selection, giving us the most likely direction of evolution of the system, whereas the $D_{tt'}^{(2)}$ term accounts for diffusion [2]. Thus, it is natural that the system spends a lot a time around the attractive roots of $D^{(1)}$ as long as diffusion is not too high. As a rough approximation, we linearize the gradient of selection, $\mathbf{D}^{(1)}(\mathbf{x}) = \mathbf{J}(\mathbf{x}-\mathbf{x}^*)$, with $\mathbf{J}$ the Jacobian matrix of $\mathbf{D}^{(1)}(\mathbf{x})$ at $\mathbf{x}^*$ and set $\mathbf{D}^{(2)}(\mathbf{x}) = \mathbf{D}^{(2)}(\mathbf{x}^*) = \mathbf{D}$ as a constant. Using the gradient, $\boldsymbol{\nabla} = \left(\partial_{x_1},\ldots,\partial_{x_{S-1}}\right)$, and Hessian, $\mathbf{H}$, operators, we can write

$$\frac{\partial p}{\partial t}(\mathbf{x},t) = -\nabla.\left(\mathbf{J}(\mathbf{x}-\mathbf{x}^*)\,p(\mathbf{x},t)\right) + \mathrm{Tr}\left(\mathbf{H}(p(\mathbf{x},t))\mathbf{D}\right) \tag{16}$$

which corresponds to a multidimensional Ornstein-Uhlenbeck process, whose stationary solution is a multivariate normal distribution [1]. This gaussian should, then, be plugged into Eq.(9) or Eq.(10) as the appropriate $f$ function.

Bellow we explicitly show the equations and solutions of the normal distribution for 1D and 2D cases as a function of the transition probabilities, as well as the particular expression for the population dynamics models we used in the main text.

### A. One dimensional case (two strategies)

The equation for a linear drift or gradient of selection, $D^{(1)}(x) = J(x-x^*)$, and constant diffusion $D$ is

$$0 = -\frac{d}{dx}\left(J(x-x^*)\,p(x)\right) + D\frac{d^2p}{dx^2}(x),\ p(x) = \mathrm{Normal}\left(x;\langle x\rangle = x^*, \sigma_x^2 = -D/J\right), \tag{17}$$

where $x^*$ is such that $T^+(x^*) - T^-(x^*) = 0$, $J = d\left(T^+(x) - T^-(x)\right)/dx|_{x=x^*}$ and $D = \left(T^+(x^*) + T^-(x^*)\right)/(2Z)$. For a pairwise Fermi update rule [3, 4], we can write

$$T^+(x) - T^-(x) = (1-\mu)\frac{Z}{Z-1}x(1-x)\tanh\frac{\beta\Delta f_{12}}{2} + \mu(1-2x), \tag{18}$$

$$T^+(x) + T^-(x) = (1-\mu)\frac{Z}{Z-1}x(1-x) + \mu, \tag{19}$$

with $\Delta f_{12}$ representing the fitness difference driving the update of players of trait 1 in relation to trait 2. This completely defines the parameters of the Gaussion function for any given $\Delta f_{12}$. For this particular 1D scenario, the expression of the variance is fairly simple:

$$\sigma_x^2 = \frac{1}{2}\left(1 - \frac{1-\mu}{\mu}\frac{Z}{Z-1}\frac{\left(\frac{1}{2}-x^*\right)\sinh\beta\Delta f_{12}(x^*) + x^*(1-x^*)\frac{\beta\Delta f'_{12}(x^*)}{2}}{1+\cosh\beta\Delta f_{12}(x^*)}\right)^{-1} \tag{20}$$

### B. Two-dimensional case (three strategies)

In a population with three strategies, $\mathbf{x} = (x_1, x_2)$ is the configuration of a population with a fraction of individuals $x_1$ with strategy 1 and $x_2$ individuals with strategy 2 ($1-x_1-x_2$ is the fraction of individuals with strategy 3). Setting $\mathbf{y} = \mathbf{x} - \mathbf{x}^*$, with $\mathbf{x}^*$ such that $T^{1+}(\mathbf{x}^*) - T^{1-}(\mathbf{x}^*) = 0 \wedge T^{2+}(\mathbf{x}^*) - T^{2-}(\mathbf{x}^*) = 0$, the equation for a linear drift or gradient of selection, $\mathbf{D}^{(1)}(\mathbf{y}) = \mathbf{J}(\mathbf{y})$, and constant diffusion $\mathbf{D}$ is

$$0 = -\frac{\partial}{\partial y_1}(J_{11}y_1 + J_{12}y_2)p(\mathbf{y},t) - \frac{\partial}{\partial y_2}(J_{21}y_1 + J_{22}y_2)p(\mathbf{y},t) + D_{11}\frac{\partial^2 p(\mathbf{y},t)}{\partial y_1^2} + 2D_{12}\frac{\partial^2 p(\mathbf{y},t)}{\partial y_1 \partial y_2} + D_{22}\frac{\partial^2 p(\mathbf{y},t)}{\partial y_2^2},$$

$$p(\mathbf{x},t) = \frac{1}{\sqrt{\pi^2 \det\boldsymbol{\Sigma}}}e^{-(\mathbf{x}-\mathbf{x}^*)^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\mathbf{x}^*)}, \tag{21}$$

with

$$\Sigma_{11} = \left(2D_{12}J_{12}J_{22} - D_{22}J_{12}^2 - D_{11}\left(J_{22}^2 + \det\mathbf{J}\right)\right)\left((\mathrm{tr}\mathbf{J}\det\mathbf{J})2\right) \tag{22}$$

$$\Sigma_{12} = \Sigma_{21} = \left(2D_{12}J_{11}J_{22} - D_{11}J_{21}J_{22} - D_{22}J_{11}J_{12}\right)\left((\mathrm{tr}\mathbf{J}\det\mathbf{J})2\right) \tag{23}$$

$$\Sigma_{22} = \left(2D_{12}J_{21}J_{11} - D_{11}J_{21}^2 - D_{22}(J_{11}^2 + \det\mathbf{J})\right)\left((\mathrm{tr}\mathbf{J}\det\mathbf{J})2\right), \tag{24}$$

where

$$\mathbf{J} = \left[\begin{array}{cc} \partial_{x_1}\left(T^{1+}(\mathbf{x}) - T^{1-}(\mathbf{x})\right) & \partial_{x_2}\left(T^{1+}(\mathbf{x}) - T^{1-}(\mathbf{x})\right) \\ \partial_{x_1}\left(T^{2+}(\mathbf{x}) - T^{2-}(\mathbf{x})\right) & \partial_{x_2}\left(T^{2+}(\mathbf{x}) - T^{2-}(\mathbf{x})\right) \end{array}\right]\Bigg|_{\mathbf{x}=\mathbf{x}^*}, \tag{25}$$

$$\mathbf{D} = \frac{1}{2Z}\left[\begin{array}{cc} T^{1+}(\mathbf{x}^*) + T^{1-}(\mathbf{x}^*) & T^{1\to 2}(\mathbf{x}^*) + T^{2\to 1}(\mathbf{x}^*) \\ T^{1\to 2}(\mathbf{x}^*) + T^{2\to 1}(\mathbf{x}^*) & T^{2+}(\mathbf{x}^*) + T^{2-}(\mathbf{x}^*) \end{array}\right]. \tag{26}$$

Again, for a pairwise Fermi update rule, we can write

$$T^{k+}(\mathbf{x}) - T^{k-}(\mathbf{x}) = (1-\mu)\frac{Z}{Z-1}x_k\sum_{l\neq 1}^{3}\tanh\frac{\beta\Delta f_{kl}}{2}x_l + \frac{\mu}{2}(1-3x_k) \tag{27}$$

$$T^{k+}(\mathbf{x}^*) + T^{k-}(\mathbf{x}^*) = (1-\mu)\frac{Z}{Z-1}x_k^*(1-x_k^*) + \frac{\mu}{2}(1+x_k^*) \tag{28}$$

$$T^{1\to 2}(\mathbf{x}^*) + T^{2\to 1}(\mathbf{x}^*) = (1-\mu)\frac{Z}{Z-1}x_1^*x_2^* + \frac{\mu}{2}(x_1^*+x_2^*), \tag{29}$$

with $\Delta f_{kl}$ representing the fitness difference driving the update of players of trait $k$ in relation to trait $l$. This set of equations completely defines the parameters of the Gaussian for any given set of $\Delta f_{kl}$.

## VI. PDF SOLUTION NEAR MONOMORPHIC CONFIGURATIONS

In the previous section we gave functional forms for the functions that can be used to weight the internal CoI. Now we look at what happens in the boundaries, which can also act as attractors and that is why some of its configurations are usually included in the CoI.

The boundaries are characterized by having at least one absent strategy, while the remaining coexist. Notice that each direction is defined by a pair of interacting strategies. This means that the shape of the function in the directions of the coexisting strategies falls into the previous section, with a reduced number of total strategies, since in those direction the CoI are internal. Thus, we are left with computing the shape of the function in the directions where absent strategies invade others.

Because new strategies can only appear through mutation, and the boundaries are only occupied when mutation is small, the simplest shape we can assume for the distribution around the CoI in the boundary is that it decays immediately to zero, requiring no renormalization, as the range of the function in that direction is $1/Z$ and thus its value is $Z$, canceling out.

However, one might want to improve this estimation. Whenever those CoI act as attractors and mutation is non-zero a tail arises in the distribution, conferring strength to configurations near the CoI. The solution is to study the behavior of the system close to the boundaries, which will depend on the system at hands.

For the sake of completeness, let us be more strict and deduce the behavior of the systems we used in the main text.

Because the configurations corresponding to the vertices only have transitions into the edges, we can start analyzing the 1D case. There, the evolution of the PDF of the process $i$, $p(i,t)$, is given by the appropriate Master Equation (11),

$$p(i,t+\tau) - p(i,t) = \sum_{\delta}\left(p(i+\delta,t)\,T^{-\delta}(x+\delta) - p(i,t)\,T^{\delta}(i)\right), \tag{30}$$

which has an analytical solution $p(i)$, for its stationary distribution when considering a one step process,

$$p(i) = p(0)\prod_{l=0}^{i-1}\frac{T_l^+}{T_{l+1}^-},\ p(0) = \left(1 + \sum_{i=1}^{Z} p(i)\right)^{-1}. \tag{31}$$

Typically, when a configuration from the CoI – in this case a monomorphic configuration – is an attractor, the stationary probability of the adjacent configuration is smaller than that of the CoI. In this case, and assuming that the attractor is state 0, we have that $p(0) > p(1) = p(0) T_0^+/T_1^-$ or $T_0^+ < T_1^-$ or, equivalently, $\mu < T_1^-$, reflecting the balance between mutation and selection of a mutant in a population.

Let us assume a resident (and dominant) strategy $R$ and a mutant strategy $M$. If $i$ is the number of individuals with strategy $R$, the assumption that configuration 0 is an attractor means that the fitness of a mutant in the population is smaller than that of the individuals in the populations by an amount $\Delta f$. For simplicity, let us make it frequency independent (at least in the region where the function decays). With these assumptions we can calculate $p(i)$ and use it to renormalize the probability of being in the considered monomorphic state ($i = 0$).

Assuming a Fermi-update process, we have that $T_i^+ = \frac{Z-i}{Z}\left(\frac{i}{Z-1}\frac{1-\mu}{1+e^{\beta\Delta f}}+\mu\right)$ and $T_i^- = \frac{i}{Z}\left(\frac{Z-i}{Z-1}\frac{1-\mu}{1+e^{-\beta\Delta f}}+\mu\right)$. Using Eq.(12) we obtain a decaying function. Recalling Eq.(10), we need both the value of the function, $p(i)$, at 0 and the cumulative function to guaranty a distribution (with a normalization of one) in the selected range $D[0]$. In this case, the value of the distribution at zero is a hypergeometric function,

$$p(0) = {}_2F_1\left[-Z, \left(1+\mathrm{e}^{-\beta\Delta f}\right)(Z-1)\frac{\mu}{1-\mu}; -\frac{(Z-1)\left(1+\mathrm{e}^{\beta\Delta f}\mu\right)}{1-\mu}; \mathrm{e}^{\beta\Delta f}\right]^{-1}, \tag{32}$$

which can be obtained using Eq.(31) and reads, approximately, $\left(1-\mathrm{e}^{\beta\Delta f}\right)^{-\left(1+\mathrm{e}^{-\beta\Delta f}\right)Z\mu}$. The cumulative function must be used whenever the decay is not fast enough and the function penetrates the domain of other attractors. With the knowledge of the transition to be computed between CoI and the right renormalizations to the distributions, we have shown all the ingredients present in the main text.

In general, when there are several strategies in place, this means that, in order to renormalize the probability of the monomorphic states, one needs the fitness of each of the mutants. This fitness should be smaller than that of the resident population and satisfy $T_{\text{mutant}\to\text{resident}} > \frac{\mu}{S-1}$, for all the $S-1$ mutant strategies. If this is not the case, the state will not be an attractor and no renormalization is needed. The same procedure can be used to calculate more accurately the shape of the attractor in any boundary in the direction caused by a single mutation.

## VII. ONE DIMENSIONAL SYSTEMS: TRANSITION PROBABILITIES BETWEEN CoI

As promised, we deduce next the expression for Eq.(6) in a one-dimensional Markov chain.

For a one dimensional one-step Markov chain the phase space, of size $Z+1$, is simply $\{0, 1, \ldots, Z\}$. This phase-space is a single line, corresponding to an edge of a multi-dimensional problem. Because in 1st order only edge points are included, the following treatment corresponds to the 1st order correction to the SMA.

The one dimensional process is characterized by allowing transitions only between adjacent states, contrary to what happens in the general scenario of the previous section and the different notation in the labeling of states is done to reflect that.

Consider $|A|$ non-adjacent ordered CoI $\{a_1, \ldots, a_{|A|}\}$, and, the remaining, $|B| = Z+1-|A|$ neglected configurations $\{b_1, \ldots, b_{|B|}\}$. Once again, the goal is to reduce the Markov chain containing the whole phase space to one containing only the CoI $\{a_i\}$ and calculate the transition probabilities $\rho_{a_i a_j}$ between those configurations as a function of the one-step transition probabilities of the whole 1D chain $T_{kl}$. Notice that the new simpler chain of CoI is also a 1D one-step Markov chain, in the sense that each configuration has two transitions outward, apart from the two boundary configurations that have only one.

Let $T_k^\pm \equiv T_{kk\pm1}$ and $T_k^0 \equiv T_{kk}$, $\rho_{a_i}^\pm \equiv \rho_{a_i a_{(i\pm1)}}$ and $P_b^a \equiv P_{ba}$ (see Fig. 1). In what follows we will use configurations and the value of the process in that configuration interchangeably.

Given two non-adjacent configurations $a_i \equiv L < a_j \equiv R$ (Left and Right), we have

$$\rho_L^+ = T_L^+ P_{L+1}^R, \tag{33}$$

meaning that the probability of moving from $L$ to $R$, requires a (one step) transition to the right from configuration $L$ (to the neglected configuration $L+1$), $T_L^+$, and then eventually going to $R$ from $L+1$, $P_{L+1}^R$. To calculate this term, we write the equations for the probability of being absorbed by $R$ from any intermediate configuration $b \in \{L+1, \ldots, R-1\}$

$$\begin{aligned} P_b^R =& T_b^- P_{b-1}^R (1-\delta_{b\,L+1}) + T_b^0 P_b^R \\ &+ T_b^+ P_{b+1}^R (1-\delta_{b\,R-1}) + \delta_{b\,R-1} T_b^+, \end{aligned} \tag{34}$$

which are known and whose solution is [5]

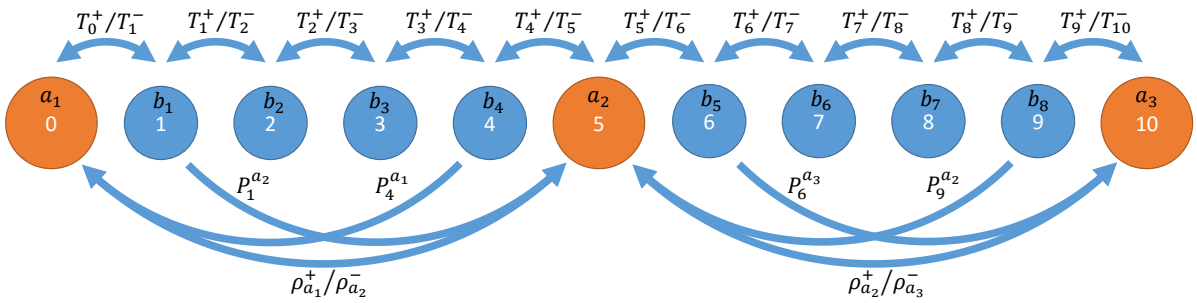


FIG. 1. Illustration of the transition and notation considered in this section. $T$ denotes the one-step transition probabilities between any pair of adjacent configurations, whereas $\rho$ and P denote the long run transition probabilities to configurations in A departing from, respectively, configurations in set $A$ in set $B$.

$$P_{L+1}^{R}=\left(1+\sum_{j=L+1}^{R-1}\prod_{k=L+1}^{j}\frac{T_k^-}{T_k^+}\right)^{-1}. \tag{35}$$

With this we can define $\rho_L^+$ as a function of the one step transitions. Using the same procedure for $\rho^-$ we can finally write

$$\rho_{a_i}^{\pm}=T_{a_i}^{\pm}P_{a_i\pm1}^{a_{(i\pm1)}}=T_{a_i}^{\pm}\left(1+\sum_{j=a_i\pm1}^{a_{(i\pm1)}\mp1}\prod_{k=a_i\pm1}^{j}\frac{T_k^{\mp}}{T_k^{\pm}}\right)^{-1} \tag{36}$$

Now the constraint to non-adjacent CoI can be lifted, in which case we may write $\rho_{a_i}^{\pm}=T_{a_i}^{\pm}$ for adjacent configurations.

## VIII. ONE DIMENSIONAL SYSTEMS: EXAMPLE OF AN INTERNAL STABLE FIXED POINT

Let us continue with the one dimensional case with phase space $\{0,1,\ldots,Z\}$, of size $Z+1$. Let us assume that we have three CoI, the two monomorphic configurations, $a_1=0$ and $a_3=Z$ and a coexistence (stable fixed point) at $a_2$. Following the general procedure, we can write a continuous stationary probability density for the fraction of individuals playing strategy $\sigma_1$, $x=i/Z$, which we call $P(x)$. As shown already, we are able to compute $p(a_i)$, the non-normalized stationary distribution over configurations in $A$ computed from the $\rho_{a_i}^{\pm}$, in Eq.(36). Since the probability of being in configuration $a_i$ is $\alpha^{-1}p(a_i)$, and given that this configuration has a range of $1/Z$, the probability density at that point must be $\alpha^{-1}Zp(a_i)$, where $\alpha^{-1}$ is a normalization constant. In other words, $P(a_i/Z)=\alpha^{-1}Zp(a_i)$, for $i=1,2,3$. A simple way of writing this is

$$P(x)\,\alpha/Z=p(a_1)\frac{f_1(x)}{f_1(a_1/Z)}+p(a_2)\frac{f_2(x)}{f_2(a_2/Z)}+p(a_3)\frac{f_3(x)}{f_3(a_3/Z)}. \tag{37}$$

The $f_i(x)$ functions are normalized probability densities that are non-zero in the neighborhood of $a_i/Z$, $D[a_i]$. The simplest choice for $f_1(x)$ and $f_3(x)$ is to let them reflect the peaking in the monomorphic configurations as a constant with value $Z$ in a range $1/Z$ – see section VI for further refinements – whereas for $f_2(x)$ we consider a Normal distribution, $N(x)$, centered at point $a_2/Z$ with variance $\sigma^2$. This defines an estimate of the distribution. In order to further simplify the procedure, let us compute the weight of each peak, $w_{a_i}=\int\limits_{D[a_i]}P(x)\,dx$, and then use it as the probability of being in configuration $a_i$.

$$w_1=\int_0^{1/Z}\alpha^{-1}Zp(a_0)\frac{1/Z}{1/Z}dx=\alpha^{-1}p(a_1), \tag{38}$$

$$w_2=\int_{1/Z}^{1-1/Z}\alpha^{-1}Zp(a_2)\frac{N(x)}{N(a_2/Z)}dx=\alpha^{-1}Zp(a_2)\sqrt{2\pi\sigma^2}\frac{1}{2}\left(\mathrm{Erf}\left[\frac{a_2/Z-1/Z}{\sqrt{2\sigma^2}}\right]+\mathrm{Erf}\left[\frac{1-a_2/Z-1/Z}{\sqrt{2\sigma^2}}\right]\right), \tag{39}$$

$$w_3=\int_{1-1/Z}^{1}\alpha^{-1}Zp(a_3)\frac{1/Z}{1/Z}dx=\alpha^{-1}p(a_3). \tag{40}$$

where $\sigma^2$ can be derived from the transition probabilities $T_x^+$and $T_x^-$ around $a_2/Z$ as $\sigma^2=F/|J|$ with $J=d\left(T_x^+-T_x^-\right)/dx|_{x=a_2/Z}$ and $F=\left(T_{a_2/Z}^+ + T_{a_2/Z}^-\right)/(2Z)$ (see section V A).

Notice that collapsing the weight of the distribution around the fixed point is particularly useful if one is interested in computing the first moment.

Furthermore, if $0 < a_2/Z \pm 2\sigma < 1$, then $w_2 = \alpha^{-1} Z p(a_2)\sqrt{2\pi\sigma^2}$. Taking the weights of each peak, we may write a discrete counterpart as

$$P(i) = \alpha^{-1}\left(p(a_1)\,\delta_{ia_1} + Z\sqrt{2\pi\sigma^2}p(a_2)\,\delta_{ia_2} + p(a_3)\,\delta_{ia_3}\right) \tag{41}$$

where $\alpha = \left(p(a_1) + Z\sqrt{2\pi\sigma^2}p(a_2) + p(a_3)\right)$.

Indeed, for the average we get

$$\langle i/Z\rangle = \alpha^{-1}\left(\sqrt{2\pi\sigma^2}p(a_2)\,a_2 + p(a_3)\right). \tag{42}$$

Also, one could use Eq.(41) to compute the second moment, but since we already know the variance of the Gaussian, we can use Eq.(37) to get an estimation of the variance of any 1D process with a single fixed point. For $0 < a_2/Z \pm 2\sigma < 1$ the expression is can also be simplified to

$$\mathrm{var}_{i/Z} = \alpha^{-1}\left(\langle i/Z\rangle^2 p(a_1) + \sigma^3 Z\sqrt{2\pi}p(a_2) + (1-\langle i/Z\rangle)^2 p(a_3)\right). \tag{43}$$

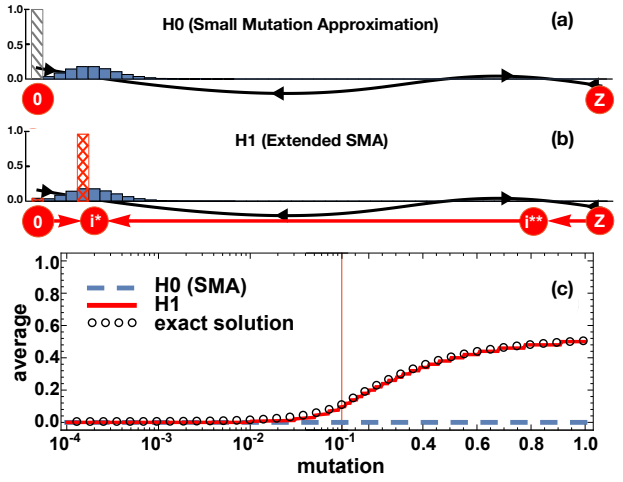


FIG. 2. Stationary distributions resulting from a Coordination game ($f = -0.7$, $g = -0.3$). We use the same notation and conventions as in Fig.1 in the main text.

## IX. ONE DIMENSIONAL SYSTEMS: EXAMPLE OF AN INTERNAL UNSTABLE FIXED POINT

Whenever the game at stake is not one of coexistence (see main text) but, instead, one of coordination, our approach remains unchanged. In Fig.2-a we show results for a coordination game, embodying both payoff and risk-dominant equilibria, of ubiquitous importance in areas as diverse as Economics, Econo-Physics, Biology and Philosophy [6, 7]. In this case, the evolutionary dynamics is characterized by the occurrence of a probability repeller at $i^* = 35$.

Fig.2-c shows that SMA (H0) leads to a much better scenario under coordination than under coexistence, leading to very good results up to $\mu \approx 1/Z$. However, as $\mu$ increases, deviations inevitably occur (Fig.2-a), and SMA fails whenever $\mu > 10^{-0.5}$. In Fig.2-b we show the H1 results after adding two configurations to the CoI. These, again, are trivial to find, being associated with the probability attractors that are roots of $G(i)$ close to the monomorphic states. Naturally, these two roots will depend on $\mu$ and their location should be determined for each value of $\mu$. Once this choice is made, we merely repeat the procedure described and already adopted to produce Figs.1 and 2 in the main text. As Fig.2-c shows, H1 leads to an excellent agreement between the hierarchical approximation and the exact solution.

## X. SUMMARY AND GENERAL PROCEDURE

Our approach attempts to describe the dynamics and steady state solution of the system by following a series of systematic steps:

1. Investigate the existence of stable fixed points, based on the gradient of selection dynamics. Choose the desired order of approximation (order $n$ or $Hn$-approximation), in which at most $n+1$ strategies are present in the population. These configurations, together with the monomorphic configurations, are named configurations of interest (CoI) and compose the set called A, making SMA the H0-approximation.

2. Calculate the transition probabilities $\rho_{a_i a_j}$ between all configurations in A. Then, compute the (unnormalized) stationary distribution given the reduced Markov chain whose configurations and transition probabilities are, respectively, the configurations in A and the transitions just calculated.

3. Build a normalized stationary distribution by renormalizing the stationary distributions calculated in point 2 with a normalization factor deduced either from properly linearizing the system close to those points (presented in the main text and detailed in sections IV, V and VI above) or using the collected information to estimate the distribution over the neglected configurations.

Each of these points encompasses advantages and limitations. Point 1 reflects the limitations of stopping the expansion. Whenever there are stable fixed points more internal than the phase space considered in a given term of the expansion, its validity only holds for lower mutation rates, which was the original problem of the SMA. Nonetheless, we are able to incorporate, without significant increase in computational cost, the ability to take into account fixed points along the edges of the phase space. This evidences the fact that higher order approximations come with a computational cost. It is worth mentioning that, in the expressions deduced, we assume that the distribution near the monomorphic configurations either adopts the shape of a delta function, or a decaying function resulting from frequency independent mutant disadvantage. Moreover, we regard the distribution near the stable fixed points as displaying the symmetry properties of a Gaussian curve, which may not be the case. Ways to improve both matters can be introduced in order to attain results with higher precision, whenever necessary.

In the main text, in order to compute the stationary distribution at different orders of $\mu$ (the mutation parameter), we estimate the behavior of that distribution employing an approximation of the Master Equation as a Fokker-Planck equation near the stable fixed points. As we show above, this consists in using a normal distribution near the stable fixed points and delta – or rapidly decaying – functions on the borders. Naturally, these estimates can be improved by studying, for instance, the discrete version of the equations, or by taking into account the influence of the borders.

Additionally, if analytical tractability is not an issue, when dealing with step 3, one might use Eq.(7) to compute $\mathbf{p_b}$, the distribution over the neglected configurations. Notice that this computation is done over the restricted phase-space of any given order in the hierarchy and, thus, has the same complexity of the computation of the transitions between CoI. In particular, if one inverts $(\mathbf{1}-\mathbf{Q})$ to compute $\rho$, as a consequence of Eq.(6), the bulk of the calculations have already been done in that step and, given that we have already computed $\mathbf{p_a}$, using Eq.(8), we have that

$$\mathbf{p_b} = (\mathbf{1}-\mathbf{Q})^{-\mathbf{1}}\mathbf{U}\mathbf{p_a}. \tag{44}$$

Nonetheless, this approach may not be so easy to do in general, especially for higher orders in $\mu$, which increase the dimensionality of the phase-space taken in consideration.

Finally, it is worth to point out that the accuracy of the numerical implementation of our method is not a closed problem and it will depend on the population model considered. Depending on the complexity of the problem under study, computer simulations can and should be used to assess the validity of the approximation.


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