Local Moran Process on Graphs

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We study the evolutionary dynamics of a spatial Moran process on graphs. We develop and apply a numerical routine to study a few specific spatial Moran processes which are chosen to model the effects of local spatial structure with increasing generality. After confirming the validity of our results for the homogeneous Moran process and a local spatial Moran process where the matrix W satisfies the isothermal theorem, we study the case of a spatially inhomogeneous Moran process with local spatial structure that is described by a graph which changes in time and is not isothermal. We also include the effects of mutations in the local Moran models we study here. Our numerical routine can be further generalized to more and more realistically model the effects of local spatial structure in population evolutionary dynamics.

I. INTRODUCTION

In studying evolutionary dynamics we are interested in understanding the frequency distribution of the alternative alleles that a gene can take in a population that is evolving under natural selection, random drift, mutation and migration. When the population of interest is finite, its evolutionary dynamics can no longer be described by deterministic differential equations but require a stochastic formulation. Two of the most common models used to study stochastic evolutionary dynamics in finite populations are the Wright-Fisher model [1] [2] and the Moran model [3]. In their simplest formulations, the Wright-Fisher and Moran models assume a well-mixed homogeneous population where all individuals are in equivalent positions, but these models have also been extended to studying evolutionary dynamics on directed graphs [4] to model the effects of non-homogeneous population structure on dynamics. In this case a stochastic matrix W_{ij} determines the probability that the offspring of individual i replaces individual j, with $i, j = 1, 2, ..., N$. Following these studies, we study the Moran process on graphs in a numerical routine which we develop and apply to a few specific spatial Moran processes which are chosen to model local evolution with increasing generality.

The models we consider are constructed to more realistically capture the effect of local spatial structure in certain evolutionary environments where it may be important, for example among animals interacting in an ecosystem or the spread of ideas in a social network of humans [5].

II. THE MODEL

The basic process we study, before considering further generalizations in Sections V and VI, is similar to that of [4]. We have an $M \times M$ spatial grid where each position is occupied by one of two types of individuals, A and B. Thus we consider a population of fixed size $N = M^2$. We start with a single mutant of type A in a population where all other individuals are type B. At each time step a random individual is chosen for reproduction, where individuals of type A have a relative fitness r (and type B individuals have fitness 1), and a random individual is chosen for replacement, such that the probability of a particular individual being replaced is given, at each time step, by a *transfer matrix* $S_{\mu\nu}$, where $\mu, \nu = 1, 2, ..., M$. Our algorithm iterates until the population consists of either all A or all B individuals.

Note that because here we are interested in modeling spatial inhomogeneities in population structure we find it easier to work with this transfer matrix $S_{\mu\nu}$ rather than the usual matrix W_{ij} with $i, j = 1, 2, ..., N = M^2$. Doing so will prove most useful in Section V.

We illustrate the difference between these two matrices S and W in context while illustrating our model: for concreteness, consider a 4×4 spatial grid populated with individuals of type A or B (illustrated in Equation 1), such that the population size is $N = 4 \times 4 = 16$.

$$\text{Grid}_{\mu\nu}(t_n) = \begin{pmatrix} \text{B} & \text{B} & \text{B} & \text{B} \\ \text{B} & \text{B} & \text{B} & \text{B} \\ \text{B} & \text{A} & \text{B} & \text{B} \\ \text{B} & \text{B} & \text{B} & \text{B} \end{pmatrix} \tag{1}$$

Suppose that at time step t_n the individual at position $(\mu, \nu) = (3, 2)$ is chosen for reproduction (indicated by a box in Equation 2); at time step t_n the transfer matrix $S_{\mu\nu}$ is defined locally relative to the individual chosen for reproduction and represents the probabilities that individuals at the positions local to $(\mu, \nu) = (3, 2)$ are chosen for replacement.

$$S_{\mu\nu}(t_n) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/5 & 0 & 0 \\ \boxed{1/5} & \boxed{1/5} & 1/5 & 0 \\ 0 & 1/5 & 0 & 0 \end{pmatrix} \tag{2}$$

Note that at each time step the probabilities in $S_{\mu\nu}$ must sum to 1. Suppose also that at time step t_n the individual at position $(\mu, \nu) = (3, 1)$ is chosen for replacement (indicated by a circle in Equation 2). Then at the start of time step t_{n+1} the population content of our grid is:

$$\text{Grid}_{\mu\nu}(t_n) = \begin{pmatrix} \text{B} & \text{B} & \text{B} & \text{B} \\ \text{B} & \text{B} & \text{B} & \text{B} \\ \text{A} & \text{A} & \text{B} & \text{B} \\ \text{B} & \text{B} & \text{B} & \text{B} \end{pmatrix} \tag{3}$$

Now, suppose at time step t_{n+1} the individual at position $(2, 4)$ is chosen for reproduction (again indicated by a box in Equation 4). And suppose that at time t_{n+1} our transfer matrix takes the form:

$$S_{\mu\nu}(t_n) = \begin{pmatrix} 0 & 0 & 0 & 1/5 \\ 1/5 & 0 & 1/5 & \boxed{1/5} \\ 0 & 0 & 0 & 1/5 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \qquad (4)$$

Note that, as illustrated in Equation 4, we use periodic boundary conditions when defining our transfer matrix $S_{\mu\nu}$.

Now note that rather than defining the transfer matrices $S_{\mu\nu}$ at times t_n and t_{n+1} illustrated in Equations 2 and 4, we could have equivalently defined the W_{ij} matrix to operate at both t_n and t_{n+1}:

$$W_{10,10} = W_{10,11} = W_{10,9} = W_{10,6} = W_{10,14} = 1/5 \quad (5)$$
$$W_{8,8} = W_{8,5} = W_{8,7} = W_{8,4} = W_{8,12} = 1/5 \qquad (6)$$
$$W_{i,j} = 0 \text{ for all other combinations } i, j \qquad (7)$$

where the indices (μ, ν) and (i, j) of the matrices S and W are related via:

$$i = (\mu - 1) M + \nu \qquad (8)$$

Working with the transfer matrix defined at each time step $S_{\mu\nu}(t)$ allows us to intuitively visualize spatial structure in the models we consider, and we will see that explicitly working with $S_{\mu\nu}(t)$ will allow us to study the case where individuals in a population are replaced with random probabilities defined locally to the individual chosen for reproduction in a way that changes at each time step, so as to more realistically model relevant local stochastic evolutionary dynamic processes.

III. "WELL-MIXED" HOMOGENEOUS MORAN PROCESS

The most simple Moran process makes the assumption that the population is "well-mixed", such that upon replacement there is no inhomogeneous spatial dependence. This homogeneous Moran process corresponds to the special case that the probability for any individual in the population to be replaced is given by $W_{ij} = 1/N$ for all (i, j), or equivalently, $S_{\mu\nu}(t) = 1/N$ for all (μ, ν) and t.

As shown in [5], for a stochastic birth-death process on a one-dimensional discrete state space $i = 1, 2, ..., N$, in which in each stochastic event the state variable i can either remain unchanged or move to $i - 1$ or $i + 1$, the probability of fixation of mutant A in a homogeneous population of type B is given by:

$$\rho_A = \frac{1}{1 + \sum_{j=1}^{N-1} \prod_{k=1}^{j} \gamma_k} \qquad (9)$$

where

$$\gamma_k = \frac{P_{i,i-1}}{P_{i,i+1}} \qquad (10)$$

where $P_{i,j}$ represents the probability of a transition from i to j (that starting from having i individuals of type A the population transitions to having j individuals of type A at a given time step).

To model random drift with constant selection individuals of type A are assigned fitness values r relative to individuals of type B with fitness 1. If $r > 1$ selection favors A; if $r < 1$ selection favors B; if $r = 1$ we recover the case of neutral drift.

In the homogeneous Moran process we obtain the transition probabilities:

$$P_{i,i-1} = \frac{N - i}{ri + N - i} \frac{i}{N} \qquad (11)$$
$$P_{i,i+1} = \frac{ri}{ri + N - i} \frac{N - i}{N} \qquad (12)$$
$$P_{i,i} = 1 - P_{i,i+1} - P_{i,i-1} \qquad (13)$$

which gives:

$$\gamma_i \equiv \frac{P_{i,i-1}}{P_{i,i+1}} = \frac{1}{r} \qquad (14)$$

which yields the familiar expression for the probability of fixation of A:

$$\rho_A = \frac{1 - 1/r}{1 - 1/r^N}. \qquad (15)$$

As a consistency check of our numerical routine, we introduce a single mutant A with relative fitness r in a population of individuals of type B and run our routine with $W_{ij} = 1/N$ for all (i, j) (or equivalently, $S_{\mu\nu}(t) = 1/N$ for all (μ, ν) and t), recording the probability of fixation of A over many trials for various values of r. Our results are shown with blue data in Figure 1 and are shown to agree with the analytical results of Equation 15 (shown with a red line in Figure 1).

IV. LOCAL ISOTHERMAL MORAN PROCESS

Now we would like to use our numerical routine to study the spatial Moran process away from the "well-mixed" case above. As a first step to doing so, we study the case of the local Moran process where the spatial structure is such that we can still calculate ρ_A according to Equation 15; that is, we study the case where W_{ij} satisfies the isothermal theorem.

The isothermal theorem states that a graph is ρ-equivalent to the homogeneous Moran process if and only if is is isothermal [5]. A graph is said to be isothermal if all its vertices have the same "temperature" T_j for all j, where T_j is defined as:

$$T_j = \sum_{i=1}^{N} W_{ij} \qquad (16)$$

This can be shown to imply the condition that W be doubly-stochastic, with $\sum_j W_{kj} = \sum_j W_{jk} = 1$ for all k [5]. All symmetric graphs $W_{ij} = W_{ji}$ are isothermal, and thus ρ-equivalent to the homogeneous Moran process.

We use our numerical routine to study the local isothermal Moran process where at each time step, for a given individual chosen for reproduction, the transfer matrix $S_{\mu\nu}(t)$ assigns equal probability for replacement to all the nearest adjacent individuals, including the individual itself; that is, taking the example of a 4×4 spatial grid of 16 individuals, the matrix $S_{\mu\nu}(t)$ has the form shown in Equations 2 and 4 relative to the individual chosen for reproduction (indicated by boxes) at each time step. One can compute the corresponding matrix W_{ij} and confirm that it is symmetric $W_{ij} = W_{ji}$, and that this spatially local Moran process is indeed isothermal. We therefore expect it to be ρ-equivalent to the homogeneous Moran process.

Our numerical results for ρ_A for this local isothermal Moran process are shown with green data in Figure 1 and are shown to be in agreement with the analytical results of Equation 15 (shown with a red line) as well as with the numerical results of the homogeneous Moran process of Section III (shown with blue data).

This local isothermal Moran model is a useful way to study local evolutionary dynamics on a graph while making use of the isothermal theorem in such a way that we can still use the results of the homogeneous Moran process to calculate fixation probabilities.

Now we are interested in generalizing our spatial Moran process further.

V. LOCAL INHOMOGENEOUS MORAN PROCESS

So far we have used our numerical routine to study the fixation probability of an A-type mutant introduced into a population of B-type individuals for the well-mixed Moran process and for a local isothermal Moran process. However, both of those models can be studied with simpler and familiar routines. We will now see the usefulness of our routine as we study a more general spatial Moran process which models replacement locally with a graph that is not isothermal and is allowed to change in time.

In this local inhomogeneous model, at each time step, for a given individual chosen for reproduction, the transfer matrix $S_{\mu\nu}(t)$ assigns random probabilities for replacement to all nearest adjacent individuals, including the reproducing individual itself; that is, again taking the example of a 4×4 spatial grid of 16 individuals, if at time t the individual at position $(\mu, \nu) = (3, 2)$ is chosen for reproduction, then the transfer matrix at t may take the form:

$$S_{\mu\nu}(t) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.3776 & 0 & 0 \\ 0.1949 & \boxed{0.0993} & 0.2872 & 0 \\ 0 & 0.041 & 0 & 0 \end{pmatrix}; \quad (17)$$
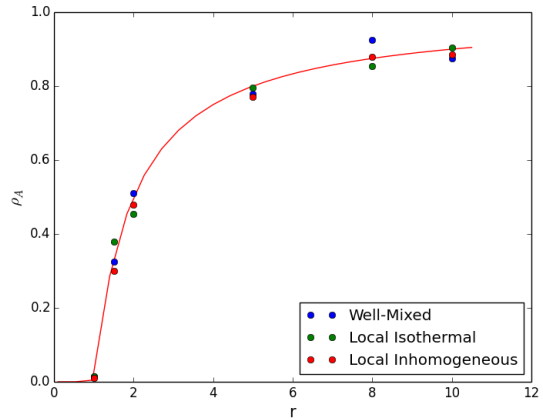

FIG. 1: ρ_A as a function of r for the homogeneous Moran model (blue data), local isothermal Moran model (green data) and local inhomogeneous Moran process (red data) plotted against the analytical result of Equation 15. All data were generated using our numerical routine for an 8×8 spatial grid, and ρ_A was calculated running our routine for 200 trials.

and if at another time t_2 the individual at position $(\mu, \nu) = (2, 4)$ is chosen for reproduction then the transfer matrix at t_2 may take the form:

$$S_{\mu\nu}(t_2) = \begin{pmatrix} 0 & 0 & 0 & 0.1536 \\ 0.0992 & 0 & 0.3501 & \boxed{0.3698} \\ 0 & 0 & 0 & 0.0273 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (18)$$

where all non-zero entries in Equations 17 and 18 are generated randomly and normalized such that they sum to 1 (so the corresponding matrix W is stochastic at all times), and boxes again indicate the position of the individual chosen for reproduction at t.

This local inhomogeneous Moran model explicitly breaks the isothermal property of the model of the previous Section IV; this model clearly breaks spatial symmetry $W_{ij} \neq W_{ji}$ and W changes in time and is not necessarily doubly stochastic $\sum_j W_{jk} \neq 1$. We therefore do not necessarily expect this model to be ρ-equivalent to the homogeneous Moran process.

Our numerical results for ρ_A for this local inhomogeneous Moran process are shown with red data in Figure 1. Perhaps surprisingly, the results are shown to agree as well with the analytical results of Equation 15 as the results of the homogeneous Moran process (blue data) and the local isothermal Moran process (green data).

VI. FURTHER GENERALIZATIONS: MUTATIONS

So far we've presented numerical results for spatial Moran processes which model local stochastic evolutionary dynamics with increasing generality. The numerical
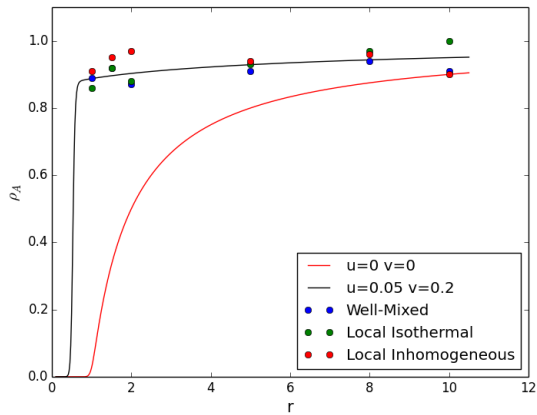
FIG. 2: ρ_A as a function of r for the homogeneous, local isothermal and local inhomogeneous Moran models including mutations, with the mutation probabilities $u = 0.05$ and $v = 0.2$, plotted against the analytical result obtained by plugging Equation 22 into Equation 9 (black line), as well as that of Equation 15 (red line). All data were generated using our numerical routine for a 6×6 spatial grid, and ρ_A was calculated running our routine for 100 trials.

routine we have presented is also easy to further generalize to more and more realistically study spatial effects in evolutionary dynamics. As an example, in this section we'll include mutations in our numerical routine.

We include mutations in our routine by assigning to each reproducing individual in a given time step, if it is type A a probability u of mutating to type B, and if it is type B a probability v of mutating to A. Because we only allow the reproducing individual to mutate we can still study well-defined fixation probabilities if we stop our simulation at the time-step that a mutant fixates or becomes extinct.

In the well-mixed Moran process with mutations included this way we obtain the transition probabilities:

$$P_{i,i-1} = \frac{N-i}{ri+N-i}\left(1-v\right)\frac{i}{N} + \frac{ir}{ir+N-i}u\frac{i}{N} \quad (19)$$

$$P_{i,i+1} = \frac{ri}{ri+N-i}\left(1-u\right)\frac{N-i}{N} + \frac{N-i}{ri+N-i}v\frac{N-i}{N} \quad (20)$$

$$P_{i,i} = 1 - P_{i,i+1} - P_{i,i-1} \quad (21)$$

which gives:

$$\gamma_i \equiv \frac{P_{i,i-1}}{P_{i,i+1}} = \frac{\left(N-i\right)\left(1-v\right)i + i^2 ru}{ir\left(1-u\right)\left(N-i\right) + \left(N-i\right)^2 v} \quad (22)$$

which we can plug into Equation 9 to obtain ρ_A.

Our numerical results for ρ_A for the homogeneous, local isothermal, and inhomogeneous Moran processes we present here, including mutations, are shown in Figure 2.

VII. CONCLUSION

We developed a numerical routine to study the spatial Moran process on graphs and applied it to a few specific spatial Moran processes which are chosen to model local stochastic evolution. We studied the case of a local Moran process where the matrix W_{ij} describing spatial effects is symmetric and satisfies the isothermal theorem, and we verified that such a local isothermal Moran process is ρ-equivalent to the well-mixed Moran process. We then used our numerical routine to study a spatial Moran process in which replacement is modeled locally and randomly such that W changes in time and is stochastic at any time, but is not doubly stochastic and so not isothermal. Interestingly, we found that the result for ρ_A of such a local inhomogeneous Moran process was in agreement with that of the homogeneous and local isothermal Moran processes, despite not satisfying the isothermal condition. This is an interesting result and worth thinking more about in the context of such local random spatial Moran models.

The numerical routine we develop to study local spatial Moran processes here can be further generalized rather easily, as we illustrated by including the effects of mutations. It is worthwhile to continue developing and studying such local Moran processes to more realistically model the evolutionary dynamics of systems in which local spatial structure plays an important role.

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