

Supplementary Information: Evolution of in-group favoritism

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I. MODEL

Consider a population of asexual haploid individuals. Initially there are N total individuals, randomly assigned into M groups. For simplicity, let us suppose that each individual's group identity is visible to everyone else and can be recognized perfectly. Let $G_i \in \{1, \dots, M\}$ denote the group identity of an individual i . The behavioral (conditional) strategy of the individual i can be described by a pair of variables (p_i, q_i) , $0 \leq p_i, q_i \leq 1$. Herein p_i and q_i represent the individual i 's preferences towards in-group members and out-group members respectively.

In this work, we focus our study on individual helping behavior, a widely discussed example of cooperative behaviors. An individual using strategy (p, q) cooperates with the in-group with probability p while cooperating with the out-group with probability q . In-group favoritism means $p > q$, namely, preferential treatment to in-group members. In our model, the ratio of benefit to cost, b/c , is fixed for all individuals. This means that any pairwise helping behavior has the same synergistic effect per unit cost. It is noteworthy that our model can be easily extended to study any type of game interactions with continuous mixed strategies (p, q) . Individuals can even play different games within and between groups. In the theoretical analysis we provide a general framework for studying such "in-group/out-group" evolutionary processes.

We consider well-mixed populations where individuals are equally likely to interact with everyone else. Such pairwise all-to-all interactions, however, are weighted and differentiated by the similarity/difference of bilateral group affiliations. Furthermore, the game is only one shot, and there is no high-order social norm at work. At each evolutionary update event, an individual's total payoff P_i , accrued through pairwise interactions with all others once, determines its reproductive fitness. We express the *effective payoff* as an exponential function of the total payoff, *i.e.*, $f_i = \exp(\beta P_i)$, where β is the intensity of selection [1].

In this paper, we study two models: one is focused on the evolutionary dynamics in homogeneous populations consisting of in-group cooperators (p, q) and defectors $(0, 0)$; the other is focused on the emergence of in-group favoritism in heterogeneous populations with continuous individual strategies (p_i, q_i) distributed over the unit square, $[0, 1]^2$. We detail both models in the following.

A. Basic model of two discrete strategies

In this model, we study the competition between in-group cooperators (p, q) and unconditional defectors $(0, 0)$. We adopt a frequency-dependent Moran process (i.e., birth-death process) for the evolutionary dynamics [2, 3]. At each time step t , an individual i is selected for reproduction proportional to its *effective payoff* f_i . One offspring is being reproduced that replaces another individual randomly selected from the entire population (including the parent itself). Thus the population size N is constant over time. The newborn inherits the parent's strategy with probability $1 - u$; otherwise, with probability u it mutates to a random strategy, either (p, q) or $(0, 0)$. Migration occurs right after the reproduction phase. With probability v the newborn migrates to a randomly chosen group out of the total M groups. Otherwise, it stays within the parent's group with probability $1 - v$. Because of this asynchronous updating, there are overlapping generations. Here we describe reproduction in terms of genetic evolution. An alternative description of cultural learning (e.g., imitation dynamics) is quite straightforward. In addition to agent-based simulations, we shall provide an analytical condition for strategy (p, q) to be favored over $(0, 0)$ by selection in the long term mutation-selection equilibrium.

B. Coevolutionary model of continuous strategies

We also consider stochastic evolutionary dynamics of individual preferences (p_i, q_i) in heterogeneous populations. Initially, each individual's strategy is drawn from a uniform distribution over the unit square. The game interactions are the same as stated above. The population system is updated according to the frequency-dependent Moran process. At each time step, an individual is chosen to reproduce proportional to its *effective payoff* f_i . Its offspring replaces another randomly chosen individual from the population (including its parent). Reproduction is, however, subject to mutation. Individual migration between groups can be seen as some kind of mutation process of group memberships, which is independent of the strategy mutation events. With probability v , migration of the newborn occurs; the offspring randomly chooses to affiliate with one of the total M groups. Otherwise, it stays within the parent's group with probability $1 - v$.

The offspring inherits the parent's strategy (p_i, q_i) with probability $1 - u$. Otherwise, it adopts a novel strategy with probability u . Here we consider both local and global mutation models. In the local mutation model, the offspring's strategy is drawn from a Gaussian distribution with the

parental value as mean and with a small standard deviation ($= 0.01$ in our case). In the simulations, we use a truncated Gaussian distribution within 2 standard deviations away from the mean value, and guarantee that all (p_i, q_i) values are constrained in the unit square. We also study the global mutation model, in which the strategy of a mutated offspring is uniformly and randomly drawn from the unit square.

C. Methods

For weak selection ($\beta \ll 1$), we can analytically calculate the evolutionary dynamics using coalescent theory [4–8]. For strong selection (large β values), we have to instead rely on extensive computer simulations.

In our simulations, at each time step, we first calculate each individual’s fitness according to the current population composition, and then update the population (including migration and mutation events) as aforementioned. This updating process is repeated for a sufficiently long period. The frequency of strategies is averaged over more than 10^6 time steps per individual. We focus our investigation on the resulting stationary distribution of strategies in the long-run mutation-selection dynamics.

In the basic model, our analysis is focused on the critical b/c ratio, above which in-group cooperators (p, q) are more abundant than defectors $(0, 0)$. To do this, we fix the benefit of cooperation $b = 1$ and vary c . We simulate the evolutionary process for a series of c values from less to more than the theoretical threshold, with equal interval 0.01 in between. In theory, the equilibrium frequency of cooperators (y -axis) decreases linearly with increasing c values (x -axis) under weak selection. At a certain c cooperators become less abundant than defectors. Because of the stochasticity in finite-sized populations, we need to do linear regression to the data points obtained by simulations. The intersection of the best linear fitting line and the horizontal neutral line (at $1/2$) gives the critical b/c determined by numerical simulations.

In the coevolutionary model, there are infinitely many continuous strategies. In order to practically determine stationary distributions of strategies, we virtually discretize the strategy space by chopping it into a grid of size 50×50 . At each evolutionary update, we count the number of individual strategies falling into each grid cell. Averaging these quantities over more than 10^9 time steps, we obtain desirable statistics of the stationary distribution by simulations. It should be noted that under this discrete setting, the average frequency of all strategies is $1/2500 = 4 \times 10^{-4}$.

II. ANALYTICAL THEORY

Here we present an analytical theory of our models in the limit of weak selection. For generality, let us consider competition of n strategies ($n \geq 2$) in the mutation-selection dynamics. Let $\mathbf{A} = \{a_{ij}\}$ be the $n \times n$ payoff matrix, where a_{ij} is the payoff of an i -th strategy playing against a j -th strategy. Denote by x_i the frequency of i strategy ($i = 1, 2, \dots, n$), $\sum_{j=1}^n x_j = 1$. For notational simplicity, let us now assume that the average total number of interactions between strategy i and j is given by I_{ij} . Then the payoff of an individual playing strategy k is $P_k = \sum_j a_{kj} I_{kj} / (x_k N)$. The fitness (*i.e.*, effective payoff) of an individual k is given by $f_k = \exp(\beta P_k)$. The total population fitness is $\sum_k N x_k f_k$, where N is the population size. Evolutionary updating occurs according to a frequency-dependent Moran process [3, 8]. In an update event, the average change of x_k due to selection can be written as:

$$\Delta x_k^{\text{sel}} = x_k \left(\frac{f_k}{\sum_j N x_j f_j} + 1 - \frac{1}{N} \right) - x_k. \quad (1)$$

For weak selection, the above equation can be linearized in the leading order of β :

$$\Delta x_k^{\text{sel}} = \frac{\beta}{N} x_k \left(\sum_j a_{kj} I_{kj} / (x_k N) - \sum_i \sum_j x_i a_{ij} I_{ij} / (x_i N) \right) + \mathcal{O}(\beta). \quad (2)$$

Averaging above change over all possible population states, we can obtain the expected change in the stationary state in the leading order of β (from now on let us omit higher order of β):

$$\langle \Delta x_k^{\text{sel}} \rangle = \frac{\beta}{N^2} \left(\sum_j \langle a_{kj} I_{kj} \rangle - \sum_i \sum_j \langle x_k a_{ij} I_{ij} \rangle \right). \quad (3)$$

According to the perturbation theory developed in Refs. [6–8], in the limit of weak selection the average $\langle \cdot \rangle$ can be taken over the stationary population state in the neutral evolution where $\beta = 0$.

On the other hand, the average change of x_k due to strategy mutation is given by $[(1 - x_k)/n - x_k(n - 1)/n]/N = (1/n - x_k)/N$. Thus the total expected change Δx_k^{tot} in the mutation-selection equilibrium is:

$$\langle \Delta x_k^{\text{tot}} \rangle = (1 - u) \langle \Delta x_k^{\text{sel}} \rangle + \frac{u}{N} \langle \left(\frac{1}{n} - x_k \right) \rangle = 0. \quad (4)$$

It follows that the stationary frequency $\langle x_k \rangle$ is given by:

$$\langle x_k \rangle = \frac{1}{n} + \frac{\beta(1 - u)}{Nu} \left(\sum_j \langle a_{kj} I_{kj} \rangle - \sum_i \sum_j \langle x_k a_{ij} I_{ij} \rangle \right). \quad (5)$$

We say natural selection favors strategy k if its abundance is greater than $1/n$ in the stationary state. We thus obtain the condition for strategy k to be favored by natural selection is

$$\sum_j \langle a_{kj} I_{kj} \rangle - \sum_i \sum_j \langle x_k a_{ij} I_{ij} \rangle > 0. \quad (6)$$

Following prior work [8, 9], we can simplify the calculations by the symmetry condition. As for the case of neutral evolution, different strategies act like different colors of individuals, index permutations do not bring in any changes. Accordingly we need to consider only five cases: $i = j = k$, $i = j \neq k$, $i = k \neq j$, $j = k \neq i$, and $i \neq j \neq k \neq i$. After some algebra, and introducing the notations $\overline{a_{k*}} = \sum_j a_{kj}/n$, $\overline{a_{*k}} = \sum_j a_{jk}/n$, $\overline{a_{**}} = \sum_j a_{jj}/n$, and $\bar{a} = \sum_i \sum_j a_{ij}/n^2$, we can greatly simplify the condition (6) as:

$$\lambda_1(a_{kk} - \overline{a_{**}}) + \lambda_2(\overline{a_{k*}} - \overline{a_{*k}}) + \lambda_3(\overline{a_{k*}} - \bar{a}) > 0, \quad (7)$$

where, up to the same positive constant factor, these λ 's are proportional to:

$$\lambda_1 \propto \langle x_k I_{ii} \rangle - \langle x_k I_{ij} \rangle, \quad (8)$$

$$\lambda_2 \propto \langle x_k I_{jk} \rangle - \langle x_k I_{ij} \rangle, \quad (9)$$

$$\lambda_3 \propto n \langle x_k I_{ij} \rangle. \quad (10)$$

We should note that the condition (7) generally holds for a wide class of evolutionary processes under weak selection, and that the λ formula (8)–(10) hold for evolutionary processes where individuals globally compete to reproduce offspring and either the birth rate or the death rate is constant (that is, the total payoff from the game can only affect either the birth rate or the death rate, but not both) [9]. Tarnita *et al.* also prove that the ratios of these λ_i values (that is, λ_1/λ_2 and λ_3/λ_2 for $\lambda_2 \neq 0$) do not depend on the number of strategies n [9].

A. In-group/out-group evolutionary dynamics

In the present model, the payoff of strategy k , (p_k, q_k) playing against strategy l , (p_l, q_l) , depends not only on their strategy, but also on the similarity/difference of their group memberships. We therefore must distinguish two dividing cases: individuals using strategy k and l belong to the same group, or they are from different groups. We can write the payoff matrix \mathbf{A} as $\delta(G_i, G_j) a_{ij}^i + [1 - \delta(G_i, G_j)] a_{ij}^o$, where $G_i \in \{1, 2, \dots, M\}$ is the group identity, and $\delta(G_i, G_j) = 1$ if $G_i = G_j$, otherwise being zero. The superscripts ‘i’ and ‘o’ denote in-group and out-group game

interactions respectively. In this way we can separate the payoff matrix \mathbf{A} and the associated λ_i parameters into two parts:

$$\begin{aligned}\lambda_1^i &\propto \langle x_k I_{ii} \delta(G_i, G_i) \rangle - \langle x_k I_{ij} \delta(G_i, G_j) \rangle, \\ \lambda_2^i &\propto \langle x_k I_{jk} \delta(G_j, G_k) \rangle - \langle x_k I_{ij} \delta(G_i, G_j) \rangle, \\ \lambda_3^i &\propto n \langle x_k I_{ij} \delta(G_i, G_j) \rangle,\end{aligned}\tag{11}$$

which are associated with the payoff matrix $\mathbf{A}^i = \{a_{ij}^i\}$, and

$$\begin{aligned}\lambda_1^o &\propto \langle x_k I_{ii} [1 - \delta(G_i, G_i)] \rangle - \langle x_k I_{ij} [1 - \delta(G_i, G_j)] \rangle, \\ \lambda_2^o &\propto \langle x_k I_{jk} [1 - \delta(G_j, G_k)] \rangle - \langle x_k I_{ij} [1 - \delta(G_i, G_j)] \rangle \\ \lambda_3^o &\propto n \langle x_k I_{ij} [1 - \delta(G_i, G_j)] \rangle,\end{aligned}\tag{12}$$

which are associated with the payoff matrix $\mathbf{A}^o = \{a_{ij}^o\}$.

Then the condition in Inequality (7) can be extended to such ‘‘in-group/out-group’’ evolutionary processes with six structural coefficients. The strategy (p_k, q_k) for the in-group and the out-group games is favored by selection, if and only if:

$$\lambda_1^i (a_{kk}^i - \bar{a}_{**}^i) + \lambda_2^i (\bar{a}_{k*}^i - \bar{a}_{*k}^i) + \lambda_3^i (\bar{a}_{k*}^i - \bar{a}^i) + \lambda_1^o (a_{kk}^o - \bar{a}_{**}^o) + \lambda_2^o (\bar{a}_{k*}^o - \bar{a}_{*k}^o) + \lambda_3^o (\bar{a}_{k*}^o - \bar{a}^o) > 0.\tag{13}$$

We remark here that there is one population structure, but the structure itself implies two different games, one for in-group interactions and the other for out-group interactions, leading to two sets of structural coefficients (three each).

Let us further interpret these λ parameters. To this end, let x_i^l be the abundance of strategy i in group l , $\sum_{l=1}^M x_i^l = x_i$, and let x_*^l be the abundance of individuals in group l , $x_*^l = \sum_{k=1}^n x_k^l$. Alternatively, we can see x_i^l as the probability of finding strategy i in group l . For convenience, let us denote $I_{ij} \delta(G_i, G_j)$ by I_{ij}^i , the average number of in-group interactions between strategy i and strategy j . And denote $I_{ij} [1 - \delta(G_i, G_j)]$ by I_{ij}^o , the average number of out-group interactions between strategy i and strategy j . It follows that:

$$I_{ij}^i = N^2 \sum_{l=1}^M x_i^l x_j^l,\tag{14}$$

$$I_{ij}^o = N^2 \sum_{l=1}^M \sum_{r=1, r \neq l}^M x_i^l x_j^r.\tag{15}$$

It should be noted that due to symmetry the average number of interactions between the same strategy should be doubly counted. That is how we obtain the above equations. Henceforth we omit

the common factor N^2 for conciseness. Moreover, we can drop the sums in the above equations and rewrite $I_{ij}^i \propto x_i^l x_j^l$ and $I_{ij}^o \propto x_i^l x_j^r$. The former means the probability of finding two strategies i and j in the same group, while the latter means the probability of finding two strategies i and j in different groups. Substituting these quantities into Eqs.(11) (12), we have

$$\lambda_1^i \propto \langle x_k x_i^l x_i^l \rangle - \langle x_k x_i^l x_j^l \rangle, \quad (16)$$

$$\lambda_2^i \propto \langle x_k x_k^l x_j^l \rangle - \langle x_k x_i^l x_j^l \rangle, \quad (17)$$

$$\lambda_3^i \propto n \langle x_k x_i^l x_j^l \rangle, \quad (18)$$

and

$$\lambda_1^o \propto \langle x_k x_i^l x_i^r \rangle - \langle x_k x_i^l x_j^r \rangle, \quad (19)$$

$$\lambda_2^o \propto \langle x_k x_k^l x_j^r \rangle - \langle x_k x_i^l x_j^r \rangle \quad (20)$$

$$\lambda_3^o \propto n \langle x_k x_i^l x_j^r \rangle. \quad (21)$$

We interpret these correlations as follows. Let us randomly pick up three different individuals. The average $\langle x_k x_i^l x_i^l \rangle$ (resp. $\langle x_k x_i^l x_i^r \rangle$) is the expected probability that two of them are in the same group (resp. different groups) and have the same strategy, while the third one has a different strategy; the average $\langle x_k x_k^l x_j^l \rangle$ (resp. $\langle x_k x_i^l x_j^l \rangle$) is the expected probability that two of them are from the same group (resp. different groups), and all three have different strategies; $\langle x_k x_k^l x_j^l \rangle$ (resp. $\langle x_k x_i^l x_j^r \rangle$) is the probability that the first two of them have the same strategy, different from the third one's, and the latter two are in the same group (resp. different groups). To avoid double counting, we must bear in mind that, for example, the actual value of $\langle x_k x_i^l x_i^l \rangle$ should be divided by $n(n-1)$. We will come back to this issue in the subsequent calculations.

We should note that the averages of these triplet correlations result from counting individuals with replacement, while here they are interpreted/computed by sampling three different individuals. Taking this difference into account only brings in a correction term of order $1/N$ [6, 7], which can be safely neglected when population size N is large.

B. Correlations at neutrality

We can analytically calculate these triplet correlations using the coalescent theory described in Refs. [5–8]. It is convenient to compute in the continuous time limit, τ , by rescaling the discrete time $\tau = 2t/N^2$. In this new time scale, we need to rescale the mutation probability u and the

migration probability ν as well. Thus for the Moran process, we obtain the rates $\mu = Nu$ and $\nu = N\nu$ respectively. The key idea of coalescent theory is tracing two individual lineages back in time. After some certain steps, we can always find their most recent common ancestor. Intuitively, these two lineages “coalesce” backward in some time τ_2 , where τ_2 is called the coalescent time. The coalescent time density of τ_2 is given by

$$p_2(\tau_2) = e^{-\tau_2}. \quad (22)$$

Similarly, we can obtain the coalescent time density function $p_3(\tau_2, \tau_3)$ for three randomly chosen individuals. In this case, either two of them coalesce first back in time τ_3 , and then this lineage coalesces with the remaining one back in time τ_2 . We have

$$p_3(\tau_2, \tau_3) = 3e^{-3\tau_3}e^{-\tau_2}. \quad (23)$$

We have two identical individuals (*i.e.*, they have the same strategy and are in the same group) immediately after the coalescence of the two chosen lineages. It is worthy of noting that each lineage mutates with rate $Nu/2 = \mu/2$ and the migration along each lineage happens with rate $N\nu/2 = \nu/2$. Furthermore, we can treat individual migration between groups as a kind of ‘group membership’ mutation process, which is independent of behavioral strategy mutation events. If at least one strategy mutation occurs along the two lineages after their coalescence, the two individuals have the same strategy with probability $1/n$. Similarly, if at least one migration event happens along the two lineages after their coalescence, the two individuals are still in the same group with probability $1/M$. Taking these into account, we get the probability that for two randomly chosen individuals, they still have the same strategy (are in the same group) after their coalescent time τ_2 , respectively:

$$s_2(\tau_2) = e^{-\mu\tau_2} + \frac{1 - e^{-\mu\tau_2}}{n}, \quad (24)$$

$$g_2(\tau_2) = e^{-\nu\tau_2} + \frac{1 - e^{-\nu\tau_2}}{M}. \quad (25)$$

To derive the probability $s_3(\tau_2, \tau_3)$ that three randomly chosen individuals all have the same strategy after their coalescent time $\tau_2 + \tau_3$ requires a bit more but similar work. This has already been done in Ref. [8]:

$$s_3(\tau_2, \tau_3) = \frac{1}{n^2} \left[s_2(\tau_2) \left(1 + 3(n-1)e^{-\mu\tau_3} + (n-1)(n-2)e^{-3/2\mu\tau_3} \right) + (1 - s_2(\tau_2)) \left(1 + (n-3)e^{-\mu\tau_3} - (n-2)e^{-3/2\mu\tau_3} \right) \right] \quad (26)$$

Taking into account the order of coalescent events for triplets, we now can calculate the pair/triplet correlations in the following:

$$\langle x_k^l x_k^l \rangle = \frac{1}{n} \int_0^\infty p_2(\tau_2) s_2(\tau_2) g_2(\tau_2) d\tau_2, \quad (27)$$

$$\langle x_k x_k^l x_k^l \rangle = \frac{1}{n} \frac{1}{3} \int_0^\infty \int_0^\infty p_3(\tau_2, \tau_3) s_3(\tau_2, \tau_3) [g_2(\tau_3) + g_2(\tau_2 + \tau_3) + g_2(\tau_2 + \tau_3)] d\tau_2 d\tau_3, \quad (28)$$

$$\begin{aligned} \langle x_k x_k^l x_*^l \rangle &= \frac{1}{n} \frac{1}{3} \int_0^\infty \int_0^\infty p_3(\tau_2, \tau_3) [s_2(\tau_3) g_2(\tau_2 + \tau_3) + s_2(\tau_2 + \tau_3) g_2(\tau_3) \\ &+ s_2(\tau_2 + \tau_3) g_2(\tau_2 + \tau_3)] d\tau_2 d\tau_3. \end{aligned} \quad (29)$$

The factor $1/n$ in the right hand side of above equations accounts for the probability of randomly selecting an individual with strategy k . In the neutral evolution, this probability is given by $1/n$.

By symmetry, we can have other correlations calculated as follows:

$$\langle x_i^l x_j^l \rangle = \frac{1}{n-1} (\langle x_i^l x_*^l \rangle - \langle x_i^l x_i^l \rangle), \quad (30)$$

$$\langle x_k x_k^l x_j^l \rangle = \frac{1}{n-1} (\langle x_k x_k^l x_*^l \rangle - \langle x_k x_k^l x_k^l \rangle), \quad (31)$$

$$\langle x_k x_i^l x_j^l \rangle = \frac{1}{n-2} (\langle x_i^l x_j^l \rangle - 2\langle x_k x_k^l x_j^l \rangle), \quad (32)$$

$$\langle x_k x_i^l x_i^l \rangle = \frac{1}{n-1} (\langle x_i^l x_i^l \rangle - \langle x_k x_k^l x_k^l \rangle), \quad (33)$$

where for the first two quantities we use $x_*^l = x_i^l + \sum_{j \neq i} x_j^l$, for the last two we use $x_k = 1 - \sum_{j \neq k} x_j$. Omitting the intermediate calculation steps, we present the λ terms associated with in-group games:

$$\lambda_1^i \propto \frac{\mu(M(2+\mu)(3+3\mu+2\nu) + \nu(4+3\mu+2\nu))}{Mn^2(2+3\mu+\mu^2)(1+\mu+\nu)(6+3\mu+2\nu)}, \quad (34)$$

$$\begin{aligned} \lambda_2^i &\propto \frac{\mu(M(2+\mu)(3\mu^2 + (3+\nu)^2 + \mu(12+5\nu)))}{Mn^2(2+3\mu+\mu^2)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)} \\ &+ \frac{(\nu(3\mu^3 + 2(2+\nu)(3+\nu)^2 + \mu^2(21+8\nu) + \mu(49+38\nu+7\nu^2)))}{Mn^2(2+3\mu+\mu^2)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)}, \end{aligned} \quad (35)$$

$$\begin{aligned} \lambda_3^i &\propto \frac{\mu^2(M(2+\mu)(9+3\mu^2+7\nu+2\nu^2 + \mu(12+5\nu)))}{Mn^2(2+3\mu+\mu^2)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)} \\ &+ \frac{\mu^2\nu(3\mu^3 + \mu^2(21+8\nu) + \mu(48+37\nu+7\nu^2) + 2(17+20\nu+8\nu^2+\nu^3))}{Mn^2(2+3\mu+\mu^2)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)}. \end{aligned} \quad (36)$$

Analogously, we calculate the λ_i^o associated with out-group interactions as follows. The probability $z_2(\tau_2)$ of two randomly chosen individuals having different groups since their coalescent

time τ_2 is given by:

$$z_2(\tau_2) = \frac{M-1}{M} (1 - e^{-\nu\tau_2}). \quad (37)$$

Then we can calculate the following pair/triplet correlations:

$$\langle x_i^l x_i^r \rangle = \frac{1}{n} \int_0^\infty p_2(\tau_2) s_2(\tau_2) z_2(\tau_2) d\tau_2, \quad (38)$$

$$\langle x_k x_k^l x_k^r \rangle = \frac{1}{n} \frac{1}{3} \int_0^\infty \int_0^\infty p_3(\tau_2, \tau_3) s_3(\tau_2, \tau_3) [z_2(\tau_3) + z_2(\tau_2 + \tau_3) + z_2(\tau_2 + \tau_3)] d\tau_2 d\tau_3, \quad (39)$$

$$\begin{aligned} \langle x_k x_k^l x_k^r \rangle &= \frac{1}{n} \frac{1}{3} \int_0^\infty \int_0^\infty p_3(\tau_2, \tau_3) [s_2(\tau_3) z_2(\tau_2 + \tau_3) + s_2(\tau_2 + \tau_3) z_2(\tau_3) \\ &+ s_2(\tau_2 + \tau_3) z_2(\tau_2 + \tau_3)] d\tau_2 d\tau_3, \end{aligned} \quad (40)$$

$$\langle x_i^l x_j^r \rangle = \frac{1}{n(n-1)} \int_0^\infty p_2(\tau_2) (1 - s_2(\tau_2)) z_2(\tau_2) d\tau_2. \quad (41)$$

We should note that, as mentioned before, the factor $1/[n(n-1)]$ in Eq. (41) takes into account the fact that there are $n(n-1)$ different combinations of the strategy index satisfying $i \neq j$.

We can also have the following correlations calculated by symmetry:

$$\langle x_k x_k^l x_j^r \rangle = \frac{1}{n-1} (\langle x_k x_k^l x_k^r \rangle - \langle x_k x_k^l x_k^r \rangle), \quad (42)$$

$$\langle x_k x_i^l x_j^r \rangle = \frac{1}{n-2} (\langle x_i^l x_j^r \rangle - 2\langle x_k x_k^l x_k^r \rangle), \quad (43)$$

$$\langle x_k x_i^l x_i^r \rangle = \frac{1}{n-1} (\langle x_i^l x_i^r \rangle - \langle x_k x_k^l x_k^r \rangle). \quad (44)$$

We finally arrive at the explicit expressions of λ^o terms for out-group interactions:

$$\lambda_1^o \propto \frac{(M-1)\mu\nu(4+3\mu+2\nu)}{Mn^2(2+3\mu+\mu^2)(1+\mu+\nu)(6+3\mu+2\nu)}, \quad (45)$$

$$\lambda_2^o \propto \frac{(M-1)\mu\nu(3\mu^3+2(2+\nu)(3+\nu)^2+\mu^2(21+8\nu)+\mu(49+\nu(38+7\nu)))}{Mn^2(1+\mu)(2+\mu)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)}, \quad (46)$$

$$\lambda_3^o \propto \frac{(M-1)\mu^2\nu(34+3\mu^3+40\nu+2\nu^2(8+\nu)+\mu(3+\nu)(16+7\nu)+\mu^2(21+8\nu))}{Mn^2(1+\mu)(2+\mu)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)}. \quad (47)$$

We can further simplify these six λ expressions altogether by canceling out their greatest common divisor:

$$\frac{\mu}{Mn^2(2+3\mu+\mu^2)(1+\nu)(1+\mu+\nu)(3+\mu+\nu)(6+3\mu+2\nu)}.$$

Finally we can have the simplified λ expressions as follows.

For in-group interactions,

$$\lambda_1^i \propto (1 + \nu)(3 + \mu + \nu)(M(2 + \mu)(3 + 3\mu + 2\nu) + \nu(4 + 3\mu + 2\nu)), \quad (48)$$

$$\lambda_2^i \propto M(2 + \mu)(9 + 3\mu(4 + \mu) + 6\nu + 5\mu\nu + \nu^2) + \nu(3\mu^3 + 2(2 + \nu)(3 + \nu)^2 + \mu^2(21 + 8\nu) + \mu(49 + \nu(38 + 7\nu))), \quad (49)$$

$$\lambda_3^i \propto \mu \left[M(2 + \mu)(9 + 3\mu(4 + \mu) + 7\nu + 5\mu\nu + 2\nu^2) + \nu(34 + 3\mu^3 + 40\nu + 2\nu^2(8 + \nu) + \mu(3 + \nu)(16 + 7\nu) + \mu^2(21 + 8\nu)) \right]. \quad (50)$$

and for out-group interactions,

$$\lambda_1^o \propto (M - 1)\nu(1 + \nu)(3 + \mu + \nu)(4 + 3\mu + 2\nu), \quad (51)$$

$$\lambda_2^o \propto (M - 1)\nu(3\mu^3 + 2(2 + \nu)(3 + \nu)^2 + \mu^2(21 + 8\nu) + \mu(49 + \nu(38 + 7\nu))), \quad (52)$$

$$\lambda_3^o \propto (M - 1)\mu\nu(34 + 3\mu^3 + 40\nu + 2\nu^2(8 + \nu) + \mu(3 + \nu)(16 + 7\nu) + \mu^2(21 + 8\nu)). \quad (53)$$

We can see that these λ expressions indeed do not depend on the number of strategies, but are jointly determined by the number of groups, the mutation rate, and the migration rate.

III. THEORETICAL RESULTS

Having these six structural coefficients λ 's at hand, we now can readily apply this theoretical framework to analyze in detail the stochastic evolutionary dynamics of in-group favoritism. We would also like to stress the broad applicability of our framework in studying other social behaviors that can be invoked by minimal group construction. Taking an illustrative example, we shall also study the evolution of parochial altruism, where individuals tend to help members of their own groups but also express aggression towards members of different groups.

A. Two discrete strategies

Specifically, let us consider the simple case of two strategies for both the in-group game (A versus B) and the out-group game (A' versus B'). In the following, we derive the condition for strategy (A, A') to be favored over strategy (B, B').

Suppose the payoff matrix \mathbf{A}^i for the in-group game is given by:

$$\begin{array}{c} A \quad B \\ A \quad \begin{pmatrix} a & b \end{pmatrix} \\ B \quad \begin{pmatrix} c & d \end{pmatrix} \end{array} \quad (54)$$

and the payoff matrix \mathbf{A}^o for the out-group game is given by:

$$\begin{array}{c} A' \quad B' \\ A' \quad \begin{pmatrix} a' & b' \end{pmatrix} \\ B' \quad \begin{pmatrix} c' & d' \end{pmatrix} \end{array} \quad (55)$$

If A (A') is a cooperative strategy and B (B') is a defective strategy, then we have $a > d$ ($a' > d'$).

Using Inequality (13), we arrive at the simplified condition for (A, A') to be favored over (B, B') as follows:

$$k_1(a - d) + k_2(b - c) + k'_1(a' - d') + k'_2(b' - c') > 0, \quad (56)$$

where the coefficients k_i 's and k'_i 's are given by:

$$k_1 = \lambda_1^i + \frac{\lambda_3^i}{2}, \quad (57)$$

$$k_2 = \lambda_2^i + \frac{\lambda_3^i}{2}, \quad (58)$$

$$k'_1 = \lambda_1^o + \frac{\lambda_3^o}{2}, \quad (59)$$

$$k'_2 = \lambda_2^o + \frac{\lambda_3^o}{2}. \quad (60)$$

Substituting the λ expressions calculated above and canceling out the common factor, we obtain the explicit expressions for k_i 's and k'_i 's:

$$k_1 = (1 + \mu + \nu)(\nu(2 + \mu + \nu) + M(3 + \mu + 2\nu)), \quad (61)$$

$$k_2 = (3 + \mu + \nu)(M(1 + \mu) + \nu(2 + \mu + \nu)), \quad (62)$$

$$k'_1 = (M - 1)\nu(1 + \mu + \nu)(2 + \mu + \nu), \quad (63)$$

$$k'_2 = (M - 1)\nu(2 + \mu + \nu)(3 + \mu + \nu). \quad (64)$$

For low strategy mutation $\mu \rightarrow 0$ and large number of groups M , we have

$$k_1 = (1 + \nu)[\nu(2 + \nu) + M(3 + 2\nu)]$$

$$k_2 = (3 + \nu)[\nu(2 + \nu) + M]$$

$$\begin{aligned}
k'_1 &= M\nu(1 + \nu)(2 + \nu) \\
k'_2 &= M\nu(2 + \nu)(3 + \nu).
\end{aligned} \tag{65}$$

We see that the in-group game can promote cooperation ($k_1 > k_2$), but the out-group game always opposes cooperation ($k'_1 < k'_2$). Moreover if ν is of order \sqrt{M} (close to its optimum value) then k_1 and k_2 are much smaller than k'_1 and k'_2 .

Now let us focus on cooperative dilemmas and consider the general 2×2 payoff matrix for the pure strategies of cooperation (C) versus defection (D):

$$\begin{array}{cc}
& C & D \\
C & \left(\begin{array}{cc} R & S \end{array} \right) \\
D & \left(\begin{array}{cc} T & P \end{array} \right).
\end{array} \tag{66}$$

We now specifically consider the evolutionary dynamics of two competing strategies in our model: $\mathbf{S}_1 = (p, q)$ and $\mathbf{S}_2 = (0, 0)$. An individual using strategy \mathbf{S}_1 cooperates with probability p and defects otherwise with probability $1 - p$ if the opponent is from the same group (in-group); whereas it cooperates with probability q and defects otherwise with probability $1 - q$ if the opponent is from a different group (out-group). The strategy \mathbf{S}_2 never cooperates. In-group favoritism implies $1 \geq p > q \geq 0$. According to the general condition presented above, we can derive the condition for strategy \mathbf{S}_1 to be favored over \mathbf{S}_2 .

To this end, the payoff matrix for in-group games is

$$\begin{array}{cc}
& \mathbf{S}_1 & \mathbf{S}_2 \\
\mathbf{S}_1 & \left(\begin{array}{cc} p^2R + p(1-p)S + (1-p)pT + (1-p)^2P & pS + (1-p)P \end{array} \right) \\
\mathbf{S}_2 & \left(\begin{array}{cc} pT + (1-p)P & P \end{array} \right).
\end{array} \tag{67}$$

The payoff matrix for out-group games is

$$\begin{array}{cc}
& \mathbf{S}_1 & \mathbf{S}_2 \\
\mathbf{S}_1 & \left(\begin{array}{cc} q^2R + q(1-q)S + (1-q)qT + (1-q)^2P & qS + (1-q)P \end{array} \right) \\
\mathbf{S}_2 & \left(\begin{array}{cc} qT + (1-q)P & P \end{array} \right).
\end{array} \tag{68}$$

Thus we have for in-group games:

$$\begin{aligned}
\overline{a_{11}^i} &= p^2R + p(1-p)S + (1-p)pT + (1-p)^2P, \\
\overline{a_{**}^i} &= \frac{1}{2}[p^2R + p(1-p)S + (1-p)pT + (2-2p+p^2)P], \\
\overline{a_{1*}^i} &= \frac{1}{2}[p^2R + (2p-p^2)S + (1-p)pT + (1-p)(2-p)P], \\
\overline{a_{*1}^i} &= \frac{1}{2}[p^2R + p(1-p)S + (2p-p^2)T + (1-p)(2-p)P], \\
\overline{a^i} &= \frac{1}{4}[p^2R + (2p-p^2)S + (2p-p^2)T + (2-2p+p^2)P].
\end{aligned}$$

And for out-group games:

$$a_{11}^o = q^2R + q(1-q)S + (1-q)qT + (1-q)^2P,$$

$$\overline{a_{**}^o} = \frac{1}{2}[q^2R + q(1-q)S + (1-q)qT + (2-2q+q^2)P],$$

$$\overline{a_{1*}^o} = \frac{1}{2}[q^2R + (2q-q^2)S + (1-q)qT + (1-q)(2-q)P],$$

$$\overline{a_{*1}^o} = \frac{1}{2}[q^2R + q(1-q)S + (2q-q^2)T + (1-q)(2-q)P],$$

$$\overline{a^o} = \frac{1}{4}[q^2R + (2q-q^2)S + (2q-q^2)T + (2-2q+q^2)P].$$

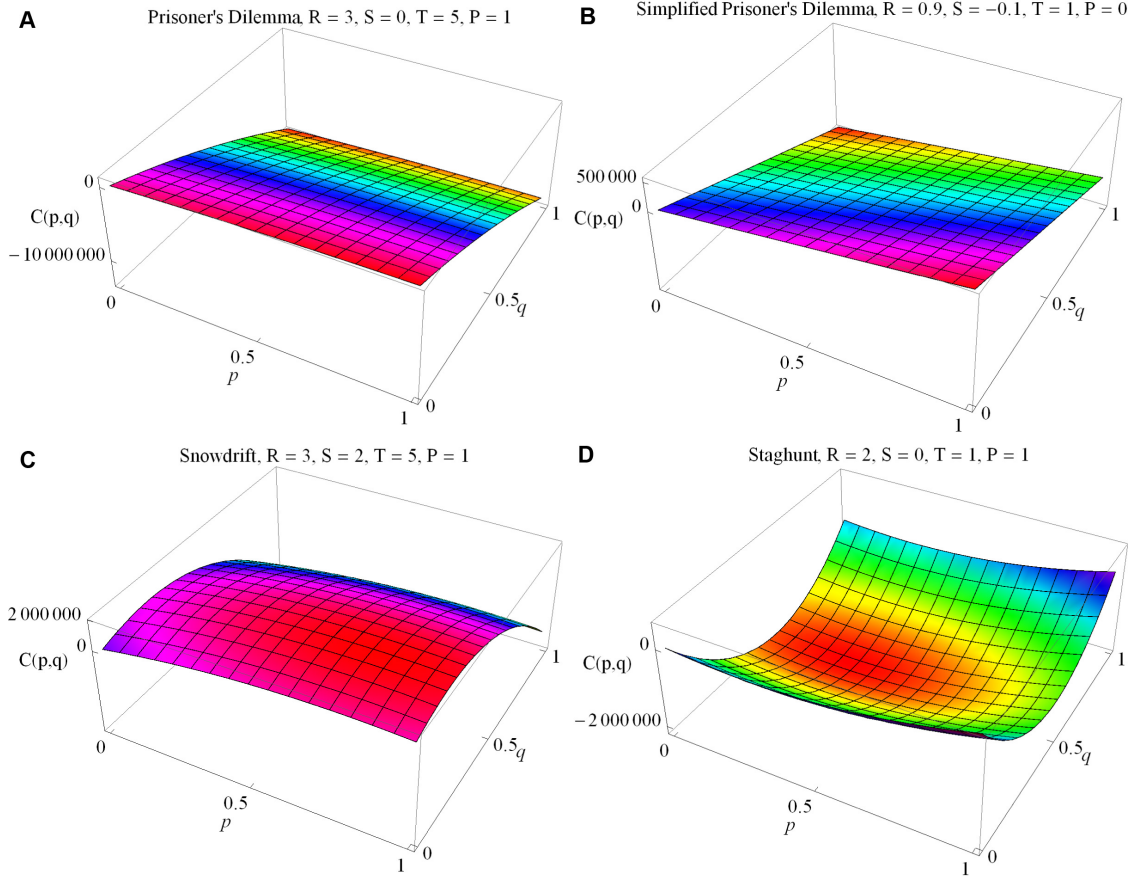


FIG. S1: 3-Dimensional plots of the condition $C(p, q)$ in inequality (69) for different games. Parameters: $M = 100, \mu = 0.01, \nu = 10$, (A) $R = 3, S = 0, T = 5, P = 1$, (B) $R = 0.9, S = -0.1, T = 1, P = 0$, (C) $R = 3, S = 2, T = 5, P = 1$, (D) $R = 2, S = 0, T = 1, P = 1$.

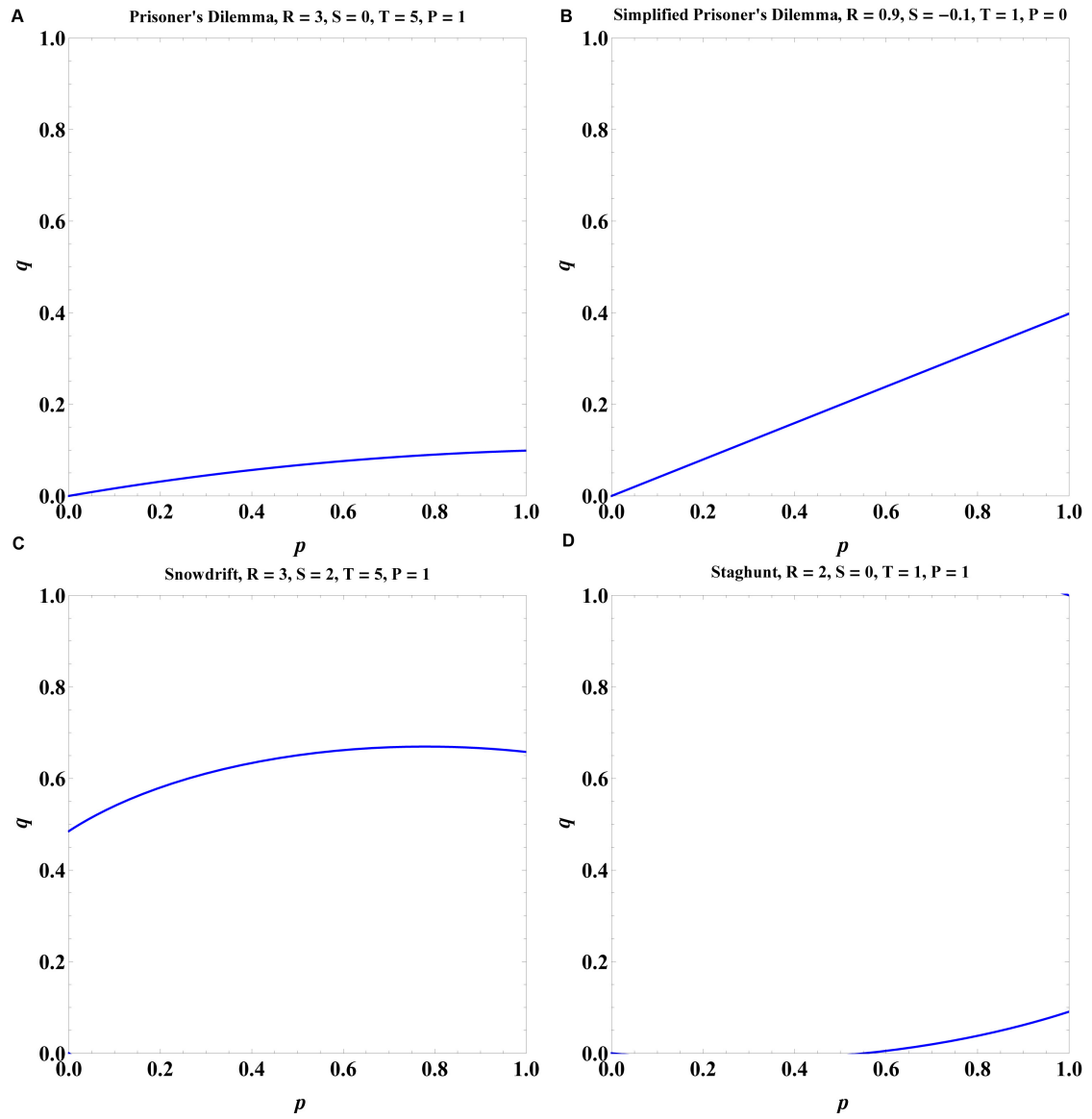


FIG. S2: The region (below the line plotted) in the unit square $[0, 1]^2$ where strategy (p, q) wins against $(0, 0)$. Parameters are as in Fig. S1.

It follows that strategy $\mathbf{S}_1 = (p, q)$ is favored over $\mathbf{S}_2 = (0, 0)$ if and only if:

$$\begin{aligned}
C(p, q) = & \lambda_1^i [p^2 R + p(1-p)S + (1-p)pT + p(p-2)P] \\
& + \lambda_2^i (pS - pT) \\
& + \lambda_3^i [p^2 R + p(2-p)S - p^2 T + p(p-2)P]/2 \\
& + \lambda_1^o [q^2 R + q(1-q)S + (1-q)qT + q(q-2)P] \\
& + \lambda_2^o (qS - qT) \\
& + \lambda_3^o [q^2 R + q(2-q)S - q^2 T + q(q-2)P]/2 > 0, \tag{69}
\end{aligned}$$

where these λ parameters are the same as derived before. The above condition can be seen as a quadric surface over the strategy space (p, q) (see Fig. S1), and only strategies $\mathbf{S}_1 = (p, q)$ that render positive $C(p, q)$ are selected against $\mathbf{S}_2 = (0, 0)$ (see Fig. S2).

For notational simplicity, we can rewrite the above condition as:

$$r_1 R + r_2 S > r_3 T + r_4 P, \tag{70}$$

where r_i 's are given by:

$$r_1 = (1 + \mu + \nu) \left((p - q)(p + q)\nu(2 + \mu + \nu) + M \left(q^2 \nu(2 + \mu + \nu) + p^2(3 + \mu + 2\nu) \right) \right), \tag{71}$$

$$\begin{aligned}
r_2 = & -(p - q)\nu(2 + \mu + \nu)(p(1 + \mu + \nu) + q(1 + \mu + \nu) - 2(2 + \mu + \nu)) \\
& - M \left(p^2(1 + \mu + \nu)(3 + \mu + 2\nu) - 2p(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu)) + \right. \\
& \left. + q\nu(2 + \mu + \nu)(q(1 + \mu + \nu) - 2(2 + \mu + \nu)) \right), \tag{72}
\end{aligned}$$

$$\begin{aligned}
r_3 = & (p - q)\nu(2 + \mu + \nu)(2 + p(1 + \mu + \nu) + q(1 + \mu + \nu)) \\
& - M \left(-2p\nu(2 + \mu + \nu) + p^2(1 + \mu + \nu)(3 + \mu + 2\nu) + q\nu(2 + \mu + \nu)(2 + q(1 + \mu + \nu)) \right), \tag{73}
\end{aligned}$$

$$\begin{aligned}
r_4 = & -(1 + \mu + \nu) \left((p - q)(-2 + p + q)\nu(2 + \mu + \nu) \right. \\
& \left. + M \left((-2 + q)q\nu(2 + \mu + \nu) - 2p(3 + \mu + 2\nu) + p^2(3 + \mu + 2\nu) \right) \right). \tag{74}
\end{aligned}$$

We make the following observations. For three special cases $p = 1$ and $q = 0$ (in-group cooperation), $p = 0$ and $q = 1$ (out-group cooperation), and $p = q = 1$ (unconditional cooperation), we have $r_1 = r_4$ and $r_2 = r_3$. In these cases, the condition in inequality (69) can thus be simplified to the single σ condition [10]:

$$\sigma R + S > T + \sigma P. \tag{75}$$

And the σ values for these three cases are respectively given by

$$\sigma(1, 0) = \frac{(1 + \mu + \nu)(\nu(2 + \mu + \nu) + M(3 + \mu + 2\nu))}{(3 + \mu + \nu)(M(1 + \mu) + \nu(2 + \mu + \nu))}, \quad (76)$$

$$\sigma(0, 1) = \frac{1 + \mu + \nu}{3 + \mu + \nu}, \quad (77)$$

$$\sigma(1, 1) = 1. \quad (78)$$

Note that for $p = 1$ and $q = 0$, the interaction structure of the population recovers to the sets model [7], and $\sigma(1, 0)$ is the same as in Ref. [7]. For $p = 1$ and $q = 1$, the population becomes well-mixed, leading to $\sigma(1, 1) = 1$ as in Refs. [3, 10]

Whereas for general p and q values, we find that $r_1 \neq r_4$ and $r_2 \neq r_3$ due to their nonlinear dependence on p and q . Thus we still need three independent structural coefficients to characterize the inequality condition as presented in (56).

Concerning the simplified ‘benefit-cost’ prisoner’s dilemma, we have $R = b - c$, $S = -c$, $T = b$, and $P = 0$. Thus we arrive at the following condition for in-group cooperators $\mathbf{S}_1 = (p, q)$ to be favored over pure defectors $\mathbf{S}_2 = (0, 0)$:

$$\frac{b}{c} > \frac{p(\lambda_1^i + \lambda_2^i + \lambda_3^i) + q(\lambda_1^o + \lambda_2^o + \lambda_3^o)}{p(\lambda_1^i - \lambda_2^i) + q(\lambda_1^o - \lambda_2^o)}. \quad (79)$$

Substituting the calculated λ expressions to above inequality, we arrive at the explicit, analytical condition for natural selection favoring (p, q) over $(0, 0)$:

$$\frac{b}{c} > \frac{\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 3\nu + \nu^2 + 2\mu(2 + \nu))}{(M - 1)\nu(2 + \mu + \nu)} + \frac{q}{p - q} \frac{M(1 + \nu)(1 + \mu + \nu)(3 + \mu + \nu)}{(M - 1)\nu(2 + \mu + \nu)}. \quad (80)$$

We should note that under no condition could out-group cooperators (*i.e.*, $1 \geq q > p \geq 0$) out-compete defectors.

When in-group cooperators abstain from helping out-group members (*i.e.*, $q = 0$), they have the greatest chance to prevail. The critical b/c ratio becomes

$$\frac{b}{c} > \frac{\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 3\nu + \nu^2 + 2\mu(2 + \nu))}{(M - 1)\nu(2 + \mu + \nu)}. \quad (81)$$

On the other hand, when cooperators do not discriminate against out-group members (*i.e.*, $p = q$), they never have a chance to dominate the population. The critical b/c reaches infinity since the situation is recovered to a standard well-mixed population where no in-group favoritism is at work.

B. Continuous strategies

In our coevolutionary model, we consider continuous strategies (p, q) over the unit square. Under some certain circumstances, in-group favoritism (that is, high in-group helping level, p , and low out-group helping level, q) can be most favored by natural selection in the long run mutation-selection equilibrium. To gain analytical insights, here we consider a global mutation model in which a mutated offspring adopts a strategy uniformly and randomly drawn from the unit square. In our computer simulations, we also consider a local mutation model, where a mutated offspring chooses a strategy from a Gaussian distribution with the parent's strategy as mean and with a small standard deviation. While we find no qualitatively different results, local mutation causes the stationary distribution of strategies more condensed than global mutation does.

Using the same approach conceived in Ref. [11] we can generalize the above results for n discrete strategies to the scenario of continuous (infinitely many) strategies. In this limiting case, the sums in the condition can be replaced by integrals. Thus a strategy $\mathbf{p} = (p_1, p_2, \dots, p_n) \in U_n$ is favored by natural selection if and only if:

$$\lambda_1 \int_{U_n} [\mathbf{A}(\mathbf{p}, \mathbf{p}) - \mathbf{A}(\mathbf{q}, \mathbf{q})] d\mathbf{q} + \lambda_2 \int_{U_n} [\mathbf{A}(\mathbf{p}, \mathbf{q}) - \mathbf{A}(\mathbf{q}, \mathbf{p})] d\mathbf{q} + \lambda_3 \int_{U_n} \int_{U_n} [\mathbf{A}(\mathbf{p}, \mathbf{q}) - \mathbf{A}(\mathbf{r}, \mathbf{q})] d\mathbf{q} d\mathbf{r} > 0. \quad (82)$$

Here the λ_i terms are the same as for the discrete strategies, and $\mathbf{A}(\mathbf{p}, \mathbf{q})$ is the payoff of strategy \mathbf{p} playing against strategy \mathbf{q} .

As for the present model of in-group favoritism, we need to separate in-group and out-group interactions as aforementioned. Denote strategy i by $\mathbf{s}_i = (p_i, q_i)$. For generality, here we can also interpret p_i (resp. q_i) as the probability of cooperating with in-group (resp. out-group) members. For the simplified prisoner's dilemma, p_i and q_i can be seen as the in-group/out-group helping level respectively. The payoff of strategy i playing against strategy k within the same group or from a different group is respectively given by

$$\begin{aligned} \mathbf{A}^i(\mathbf{s}_i, \mathbf{s}_j) &= R p_i p_j + S p_i (1 - p_j) + T (1 - p_i) p_j + P (1 - p_i) (1 - p_j), \\ \mathbf{A}^o(\mathbf{s}_i, \mathbf{s}_j) &= R q_i q_j + S q_i (1 - q_j) + T (1 - q_i) q_j + P (1 - q_i) (1 - q_j). \end{aligned} \quad (83)$$

Let us calculate the condition for strategy $\mathbf{s} = (p, q)$ to be favored by natural selection. To this

end, the three integrals in Eq. (82) for in-group interactions can be given by:

$$\begin{aligned}
\int_0^1 [\mathbf{A}^i(\mathbf{s}, \mathbf{s}) - \mathbf{A}^i(\mathbf{s}_j, \mathbf{s}_j)] dp_j &= \frac{2P}{3} - \frac{R}{3} - \frac{S}{6} - \frac{T}{6} + p(S + T - 2P) + p^2(P + R - S - T) \\
\int_0^1 [\mathbf{A}^i(\mathbf{s}, \mathbf{s}_j) - \mathbf{A}^i(\mathbf{s}_j, \mathbf{s})] dp_j &= \frac{S-T}{2}(2p-1) \\
\int_0^1 \int_0^1 [\mathbf{A}^i(\mathbf{s}, \mathbf{s}_j) - \mathbf{A}^i(\mathbf{s}_i, \mathbf{s}_j)] dp_i dp_j &= \frac{R+S-T-P}{4}(2p-1).
\end{aligned} \tag{84}$$

The three integrals in Eq. (82) for out-group interactions can be obtained by replacing p by q in the above equations. The λ expressions are the same as in the discrete n strategies. We arrive at the final condition for natural selection favoring strategy (p, q) :

$$\begin{aligned}
C(p, q) &= \lambda_1^i \left(\frac{2P}{3} - \frac{R}{3} - \frac{S}{6} - \frac{T}{6} + p(S + T - 2P) + p^2(P + R - S - T) \right) \\
&+ \lambda_2^i \left(\frac{S-T}{2}(2p-1) \right) + \lambda_3^i \left(\frac{R+S-T-P}{4}(2p-1) \right) \\
&+ \lambda_1^o \left(\frac{2P}{3} - \frac{R}{3} - \frac{S}{6} - \frac{T}{6} + q(S + T - 2P) + q^2(P + R - S - T) \right) \\
&+ \lambda_2^o \left(\frac{S-T}{2}(2q-1) \right) + \lambda_3^o \left(\frac{R+S-T-P}{4}(2q-1) \right) > 0.
\end{aligned} \tag{85}$$

It is easy to find that $C(p, q)$ always equals zero at the point $(1/2, 1/2)$ if the payoff matrix satisfies the condition of ‘equal gains from switching’ (i.e., $R + P = T + S$) [12]. In this case, the strategy $(1/2, 1/2)$ is neutral for any parameter choices.

For the simplified b - c parameter prisoner’s dilemma, $C(p, q)$ is just a linear function of (p, q) over the unit square:

$$\begin{aligned}
C(p, q) &= -\frac{1}{2}(2 + \mu)(6 + 3\mu + 2\nu) [q[2(M-1)\nu(2 + \mu + \nu)(b + c(2 + \mu + \nu))] \\
&- p[2b(-1 + M)\nu(2 + \mu + \nu) - 2c\nu(2 + \mu + \nu)^2 - 2cM(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu))] \\
&- cM(1 + \nu)(1 + \mu + \nu)(3 + \mu + \nu)].
\end{aligned} \tag{86}$$

We can thus visualize the function $C(p, q)$ as a hyperplane in three-dimensional space (see Fig. S3). The (p, q) region rendering positive $C(p, q)$ values is selected by natural selection. If $C(p_i, q_i) > C(p_j, q_j)$ then strategy (p_i, q_i) is more abundant than strategy (p_j, q_j) in the mutation-selection equilibrium.

Let us consider these strategies located in the four corners: $(0, 0)$, defection, $(0, 1)$, out-group cooperation, $(1, 0)$, in-group cooperation, and $(1, 1)$, unconditional cooperation. We find that $C(0, 0) > C(0, 1)$ and $C(0, 0) > C(1, 1)$ always hold. This result suggests that defectors are always more abundant than both out-group cooperators and pure altruists. The abundance of in-group

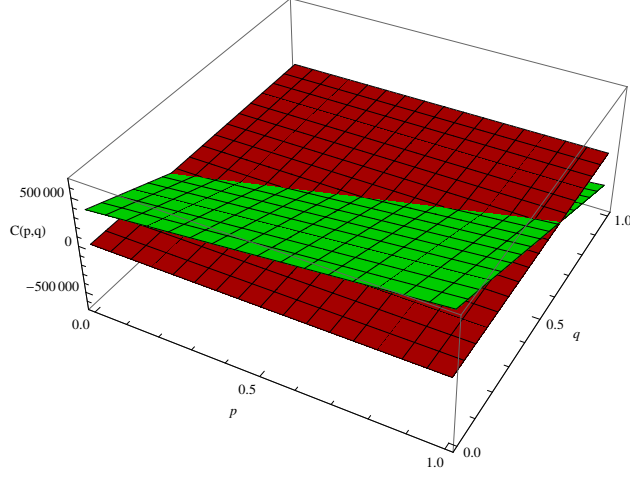


FIG. S3: Plot of the condition $C(p, q)$ for continuous strategies in the simplified prisoner's dilemma. These strategies having positive $C(p, q)$ values are favored by selection. The intersection of the surface and the zero-plane gives the critical line in the strategy space (p, q) . Strategies below this critical line (lower q values) are selected while being inhibited above this critical line (higher q values). Parameters: $M = 10$, $\mu = 4$, $\nu = 6$, $b = 1$, $c = 0.1$.

cooperators is larger than defectors, equivalently, $C(1, 0) > C(0, 0)$, if and only if:

$$\frac{b}{c} > \frac{\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu))}{(M - 1)\nu(2 + \mu + \nu)} \quad (87)$$

Interestingly, this condition is exactly the same as in the case where only these two discrete strategies are present and competing with each other. We can further prove that this is true only when the original 2×2 payoff matrix between two strategies satisfies the condition of 'equal gains from switching'. In this case, each payoff entry can be separated into two parts: what I do to the other and what the other does to me. Therefore, introducing more continuous strategies does not bring in changes in the ranking of the original two strategies with respect to each other. We also note that $(1/2, 1/2)$ is always a zero of the relative density function $C(p, q)$ for any model parameters. The sums of two diagonal corners are equal, that is $C(0, 0) + C(1, 1) = C(1, 0) + C(0, 1)$. The sum of the abundance of defectors and pure altruists equals that of in-group cooperators and out-group cooperators. Intuitively this is because $C(p, q)$ is a linear function of p and q and always has the root $(1/2, 1/2)$ for any parameter choices.

We can further divide the unit square into two regions by the critical line $C(p, q) = 0$, which can

be formally written as $q = K(p - 1/2) + 1/2$. The slope K is determined by the model parameters:

$$K = \frac{b(M-1)v(2+\mu+v) - c\left(v(2+\mu+v)^2 + M\left(3+\mu^2+2\mu(2+v)+v(3+v)\right)\right)}{(M-1)v(2+\mu+v)(b+c(2+\mu+v))}. \quad (88)$$

In the (p, q) plane, strategies below this critical line are favored by natural selection, while being suppressed above the critical line. A positive $K > 0$ requires the same condition as given in Eq. (87), suggesting that in-group cooperation $(1, 0)$ is most favored by natural selection and thus most abundant in the long-run mutation-selection equilibrium. Moreover, we find that the maximum slope K is $+1$ when the benefit-to-cost ratio, $b/c \rightarrow \infty$, and that the minimum K can reach $-\infty$ when the migration rate v tends to 0.

We further identify the condition for the population average p to be larger than the average q . Up to the same common factor, we can calculate the averages $\langle p \rangle$ and $\langle q \rangle$ as follows:

$$\begin{aligned} \langle p \rangle &\propto \int_0^1 \int_0^1 pC(p, q)dpdq \\ &\propto b(M-1)v(2+\mu+v) - c\left(v(2+\mu+v)^2 + M\left(3+\mu^2+3v+v^2+2\mu(2+v)\right)\right) \end{aligned} \quad (89)$$

$$\begin{aligned} \langle q \rangle &\propto \int_0^1 \int_0^1 qC(p, q)dpdq \\ &\propto (1-M)v(2+\mu+v)(b+c(2+\mu+v)). \end{aligned} \quad (90)$$

The condition for $\langle p \rangle > \langle q \rangle$ is equivalent to:

$$\frac{b}{c} > \frac{2v(2+\mu+v)^2 + M\left(3+\mu^2+3v+v^2+2\mu(2+v) - v(2+\mu+v)^2\right)}{2(M-1)v(2+\mu+v)}. \quad (91)$$

Interestingly, substituting the above condition into the expression of the slope K in Eq. (88), we find a very simple condition for $\langle p \rangle > \langle q \rangle$ in terms of the slope K :

$$\langle p \rangle > \langle q \rangle \Leftrightarrow K > -1. \quad (92)$$

In sum, we have two critical b/c ratios determined by the slopes $K = 0$ and $K = -1$. Increasing the strategy mutation rate μ always increases both critical b/c ratios, while increasing the number of groups, M , always reduces both critical b/c ratios. Increasing the migration rate v always reduces the critical b/c for $K = -1$, but there is an optimum v that minimizes the critical b/c ratio for $K = 0$.

In Fig. S4, we show the parameter space $(b/c, v)$ partitioned into three regions by the two slopes $K = 0$ and $K = -1$. In region 1 ($K > 0$), the average p is larger than average q and the

strategy (1, 0) is most common; in region 2 ($K < 0$ and $K > -1$), the average p is larger than average q and the strategy (0, 0) is most common; In region 3 ($K < -1$), the average p is smaller than average q (out-group favoritism) and the strategy (0, 0) is most common. For cooperative dilemmas ($b > c > 0$), some part of the parameter space (below $b/c \leq 1$) is inaccessible. For fixed $b/c > 1$, we can always choose a certain small migration rate such that $K < -1$, that is, some of out-group favoritism is evolved. This result is confirmed by our simulations in the main Fig. 3D.

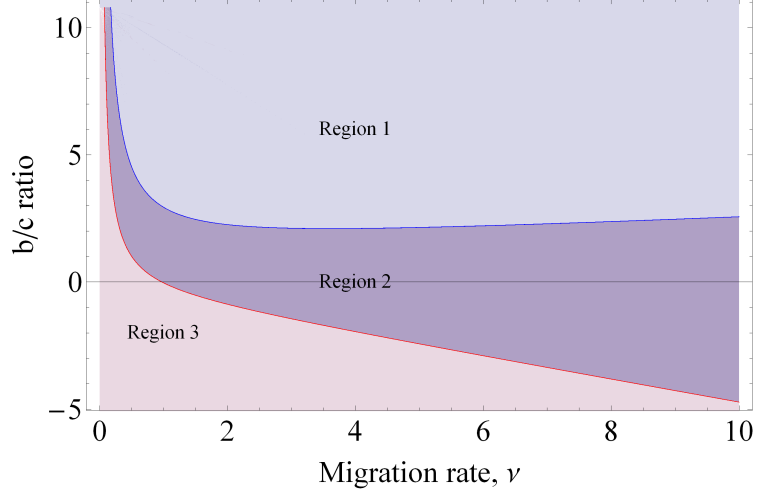


FIG. S4: Three regions in the $(b/c, \nu)$ -plane partitioned by the two conditions for the slope $K = 0$ and $K = -1$. In region 1 we have average $p > \text{average } q$ and the strategy (1, 0) is most common; in region 2 we have average $p > \text{average } q$ and (0, 0) is most common; in region 3 we have average $p < \text{average } q$ and (0, 0) is most common. Because of the cooperative dilemma ($b > c > 0$), some region of the parameter space (i.e., $b/c \leq 1$) is inaccessible. Parameters: $M = 10, \mu = 0.01$.

Let us now look at the low mutation limit $\mu \rightarrow 0$. At this limit, the slope K becomes:

$$K = \frac{b(M-1)\nu(2+\nu) - c\left(\nu(2+\nu)^2 + M(3+3\nu+\nu^2)\right)}{(M-1)\nu(2+\nu)(b+c(2+\nu))}. \quad (93)$$

And the difference between population averages p and q is given by:

$$\langle p \rangle - \langle q \rangle \propto 2b(M-1)\nu(2+\nu) + c\left(-2\nu(2+\nu)^2 + M(-3+\nu+3\nu^2+\nu^3)\right). \quad (94)$$

Hence $\langle p \rangle - \langle q \rangle > 0$ requires

$$2b(M-1)\nu(2+\nu) + c\left(-2\nu(2+\nu)^2 + M(-3+\nu+3\nu^2+\nu^3)\right) > 0. \quad (95)$$

Since $(M - 1)\nu(2 + \nu)$ is positive and b, c are also positive, we can formally write the above condition as:

$$\frac{b}{c} > \frac{2\nu(2 + \nu)^2 - M(-3 + \nu + 3\nu^2 + \nu^3)}{2(M - 1)\nu(2 + \nu)}, \quad (96)$$

It is easy to find that this condition is exactly equivalent to $K > -1$.

Note that the numerator in the above inequality (96) could be negative if

$$2\nu(2 + \nu)^2 < M(-3 + \nu + 3\nu^2 + \nu^3). \quad (97)$$

For instance, for large number of groups M and the migration rate $\nu \sim \sqrt{M}$, $2\nu(2 + \nu)^2 < M(-3 + \nu + 3\nu^2 + \nu^3)$ is fulfilled. In this case the selection of some in-group favoritism, i.e., $\langle p \rangle > \langle q \rangle$, is always guaranteed for any b/c ratio.

C. Heterogeneous interaction rates

In the analysis above, we consider uniform interaction rates within and between groups (*i.e.*, everyone is equally likely paired up with one another to play games). We can further modify this assumption and take into account heterogeneous rates for individuals' in-group and out-group interactions. To do this, we introduce an additional model parameter, $\theta \in (0, 1)$, which is the proportion of time per updating step that a focal individual interacts with in-group members. For $\theta > 1/2$, individuals interact more often with members of their own group than with those of other groups; for $\theta = 1/2$, the original model is recovered; for $\theta < 1/2$, individuals are biased toward out-group interactions rather than in-group interactions. Varying the parameter θ changes the relative payoff contribution from in-group games versus out-group games.

It is straightforward to see that the strategy selection condition (85) now is a weighted sum of in-group and out-group contributions and thus is modified as

$$\begin{aligned} C(p, q) = & \theta \left[\lambda_1^i \left(\frac{2P}{3} - \frac{R}{3} - \frac{S}{6} - \frac{T}{6} + p(S + T - 2P) + p^2(P + R - S - T) \right) \right. \\ & + \lambda_2^i \left(\frac{S - T}{2} (2p - 1) \right) + \lambda_3^i \left(\frac{R + S - T - P}{4} (2p - 1) \right) \left. \right] \\ & + (1 - \theta) \left[\lambda_1^o \left(\frac{2P}{3} - \frac{R}{3} - \frac{S}{6} - \frac{T}{6} + q(S + T - 2P) + q^2(P + R - S - T) \right) \right. \\ & + \lambda_2^o \left(\frac{S - T}{2} (2q - 1) \right) + \lambda_3^o \left(\frac{R + S - T - P}{4} (2q - 1) \right) \left. \right] > 0, \quad (98) \end{aligned}$$

where the structural coefficients λ 's are the same as before. For the simplified b - c prisoner's

dilemma, we obtain the condition for natural selection to favor strategy (p, q) :

$$\begin{aligned}
C(p, q) = & \frac{1}{2}\mu(2 + \mu)(6 + 3\mu + 2\nu) [(M - 1)(2q - 1)(\theta - 1)\nu(\mu + \nu + 2)(b + c(\mu + \nu + 2)) \\
& - (2p - 1)\theta(-b(M - 1)\nu(\mu + \nu + 2)) \\
& + c(\nu(\mu + \nu + 2)^2 + M(3 + \mu^2 + 2\mu(\nu + 2) + \nu(\nu + 3)))] > 0.
\end{aligned} \tag{99}$$

Again we find that the (p, q) strategy space is intersected by the critical line, $q = K'(p - 1/2) + 1/2$, where $K' = \frac{\theta}{1-\theta}K$ and K is the original slope as given in Eq. (93). Strategies below this line are favored while those above this line are suppressed. Since $\frac{\theta}{1-\theta} > 0$, the condition for evolution of maximum in-group favoritism is the same as in the original model: $K' > 0 \Leftrightarrow K > 0$. The condition for evolution of some in-group favoritism becomes

$$\langle p \rangle > \langle q \rangle \Leftrightarrow K' > -1 \Leftrightarrow K > \frac{\theta - 1}{\theta}. \tag{100}$$

After some algebra, we can further show that: if $K > 0$, we have $\langle q \rangle < 1/2 < \langle p \rangle$; if $\frac{\theta-1}{\theta} < K < 0$, $\langle q \rangle < \langle p \rangle < 1/2$; if $K < \frac{\theta-1}{\theta}$, $\langle p \rangle < \langle q \rangle < 1/2$. Moreover, $\langle q \rangle$ always increases with θ ; whereas $\langle p \rangle$ is an increasing function of θ if $K > 0$, but decreases with θ if $K < 0$.

D. Local mutation model

Based on above calculations, we can also analyze the local mutation model using an approach analogous to the adaptive dynamics [13]. Suppose the resident population uses strategy $\mathbf{s} = (p, q)$. Now a mutant strategy $\mathbf{s}' = (p', q')$ arises. Without loss of generality, we assume one mutation at a time. The long-run competition between \mathbf{s} and \mathbf{s}' is determined by the condition $C(\mathbf{s}', \mathbf{s})$ in the left hand side of Inequality (7). To calculate this, the payoff matrix for the mutant strategy \mathbf{s}' regarding in-group interactions is

$$\begin{array}{cc}
& \mathbf{s}' & \mathbf{s} \\
\mathbf{s}' & \left(\begin{array}{cc} p'(b - c) & pb - p'c \end{array} \right) \\
\mathbf{s} & \left(\begin{array}{cc} p'b - pc & p(b - c) \end{array} \right)
\end{array} \tag{101}$$

The payoff matrix for the mutant strategy \mathbf{s}' regarding out-group interactions is

$$\begin{array}{cc}
& \mathbf{s}' & \mathbf{s} \\
\mathbf{s}' & \left(\begin{array}{cc} q'(b - c) & qb - q'c \end{array} \right) \\
\mathbf{s} & \left(\begin{array}{cc} q'b - qc & q(b - c) \end{array} \right)
\end{array} \tag{102}$$

Now consider a mutant strategy s' arises in the infinitesimal neighborhood of the resident strategy s . In this limit, the gradient of the function $C(s', s)$ with respect to s' , evaluated at the resident strategy s , gives the most likely evolutionary adaptation in which a mutant s' sufficiently close to s has the largest chance of invasion success. This yields the following deterministic differential equations for the most likely path of mutant invasion:

$$\dot{p} = \left. \frac{\partial}{\partial p'} C(s', s) \right|_{s'=s}, \quad (103)$$

$$\dot{q} = \left. \frac{\partial}{\partial q'} C(s', s) \right|_{s'=s}. \quad (104)$$

Omitting intermediate calculation steps, we obtain the explicit differential equations as below:

$$\begin{aligned} \dot{p} = & \frac{1}{2} \mu (2 + \mu) (6 + 3\mu + 2\nu) (b(-1 + M)\nu(2 + \mu + \nu) \\ & - c(\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu))))), \end{aligned} \quad (105)$$

$$\dot{q} = -\frac{1}{2} (M - 1) \mu (2 + \mu) \nu (2 + \mu + \nu) (6 + 3\mu + 2\nu) (b + c(2 + \mu + \nu)). \quad (106)$$

We can see that $\dot{q} < 0$ always holds, while the sign of \dot{p} is positive if and only if:

$$\frac{b}{c} > \frac{\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu))}{(M - 1)\nu(2 + \mu + \nu)} \quad (107)$$

which is exactly the same as inequality (87). Natural selection always disfavors the tendency to help out-group members (Fig. S5). Only when the above inequality holds, does selection promote the predisposition of helping in-group members; otherwise, the pure defection corner $(0, 0)$ is most selected (Fig. S5). It should be noted that we get the same results if using the gradient of the condition $C(p, q)$ in inequality (85) for strategy (p, q) against all mutants over the entire strategy space.

E. Co-evolution of cooperation and aggression

In this paper, the theoretical framework for “in-group/out-group” evolutionary games can be easily extended to study a variety of social behaviors that are triggered by minimal group construction. Here we demonstrate the omnipotence of our analytical theory by studying the co-evolution of cooperation and aggression. Previously, we have focused on the positive side of social behavior — individual helping behavior biased towards in-group or out-group. Let us now consider both ‘in-group love’ and ‘out-group hatred’ as what follows.

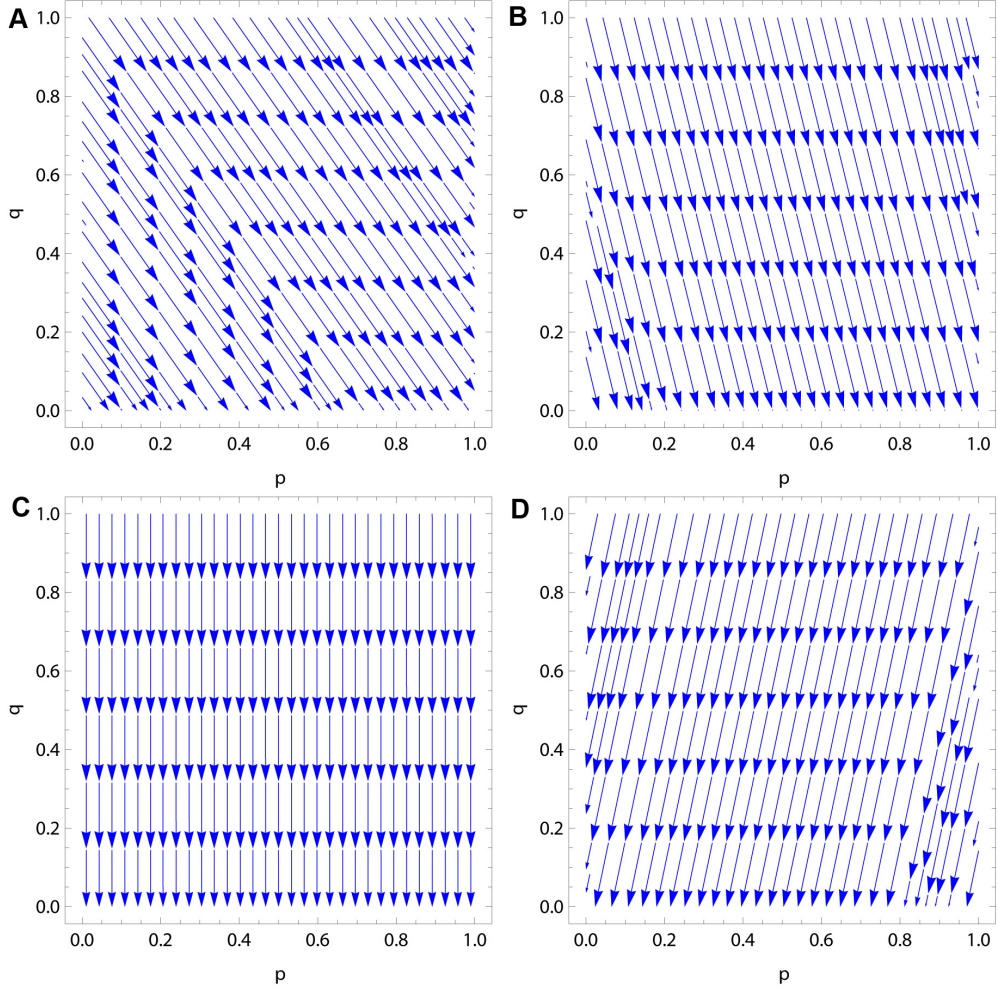


FIG. S5: “Adaptive dynamics” analysis of the local mutation model. Shown are the stream plots in the strategy space for different b/c ratios. As in the global mutation model, the same critical b/c ratio is needed for maximum in-group favoritism $(1, 0)$ to be most favored. There is no branching point in the strategy space. Parameters: $M = 4$, $\mu = 4$, $\nu = 6$, $b = 1$, (A) $c = 0.02$, (B) $c = 0.08$, (C) $c = 0.1529$, (D) $c = 0.3$.

Regarding in-group pairwise interactions, individuals cooperate with an in-group member with probability p . Cooperation implies a cost c for the donor and a benefit b for the recipient. Whereas for out-group interactions, individuals punish an out-group member with probability q . Punishment incurs a cost α for the punisher and makes another out-group member lose γ . We have the payoff matrix for in-group cooperation $\mathbf{A}^i = [b - c, -c; b, 0]$ and that for out-group aggression $\mathbf{A}^o = [-\alpha - \gamma, -\alpha; -\gamma, 0]$. We are interested in under what condition the strategy $(1, 1)$, which is termed as ‘parochial altruism’ in Refs. [14, 15], is most selected.

As discussed previously, the condition $C(p, q)$ is also a linear function of p and q because both

payoff matrices \mathbf{A}^i and \mathbf{A}^o satisfy the condition of ‘equal gains from switching’. Moreover, because of the global uniform mutation and the particular payoff matrices used, $(1/2, 1/2)$ is always a zero of the condition $C(p, q)$, and thus it is neutral for any parameter choices. Let us focus on the four corners. We note that $C(1, 1) > C(1, 0)$ and $C(0, 1) > C(0, 0)$ require the same condition:

$$\frac{\gamma}{\alpha} > 2 + \mu + \nu. \quad (108)$$

And $C(1, 1) > C(0, 1)$ and $C(1, 0) > C(0, 0)$ also imply the same condition:

$$\frac{b}{c} > \frac{\nu(2 + \mu + \nu)^2 + M(3 + \mu^2 + 2\mu(2 + \nu) + \nu(3 + \nu))}{(M - 1)\nu(2 + \mu + \nu)}. \quad (109)$$

Hence the strategy $(1, 1)$, i.e., parochial altruism, is most favored by selection if and only if above two inequalities are both fulfilled. Figure S6A shows an example, where both conditions are fulfilled and thus the most common strategy is parochial altruism. Fig. S6B shows that if neither of the conditions is fulfilled, defection $(0, 0)$ is most common.

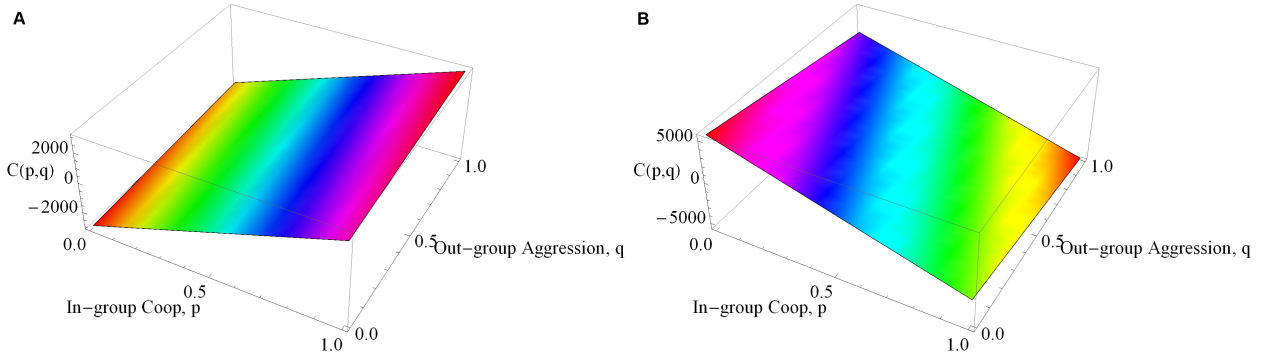


FIG. S6: Co-evolution of cooperation and aggression. In panel (A) parochial altruism $(1, 1)$ is most selected. Panel (B) shows the case where defection $(0, 0)$ is most favored. Parameters: $M = 10$, $\mu = 1$, $\nu = 3$, $b = 1$, $\alpha = 0.1$, (A) $c = 0.1$, $\gamma = 0.7$, (B) $c = 0.8$, $\gamma = 0.2$.

It should be noted that in Ref. [14] the authors questioned the validity of evolutionary multi-level selection theories based on group conflicts and some individual selection models for explaining their experimental observations of parochial altruism in humans. They also called for further theoretical efforts for explicitly examining the interactions between individuals stemming from different groups in evolutionary models. Since selection in our model operates only on the individual level and we consider both in-group and out-group interactions, our analytical results here make good progress towards understanding the evolution of parochial altruism [14, 15].

IV. SIMULATIONS

In addition to the theoretical analysis, we have performed extensive agent-based simulations to validate our analytical predictions as well as to study the evolutionary dynamics under non-vanishing selection strength.

A. Two discrete strategies: (p, q) versus $(0, 0)$

We present a systematic study of the evolutionary dynamics between two discrete strategies, (p, q) versus $(0, 0)$. Figure S7A shows how the ratio of out-group helping to in-group, q/p , impacts the evolution of cooperation. The simulation results agree very well with the analytical predictions [Eq. (80)]. We can see that when cooperators abstain from helping out-group members ($q/p = 0$), cooperation has the greatest chance to predominate in the population. Whereas, cooperation has no chance to prevail if individuals treat in-group and out-group members equally ($q/p = 1$). Therefore, some degree of in-group favoritism, *i.e.* ($p > q$), is necessary for the evolution of cooperation.

Now we focus on studying the case of maximum in-group favoritism $(1, 0)$ versus defection $(0, 0)$. Figure S7B shows the critical c/b ratio, given by Eq. (81), as a function of the strategy mutation rate u and the migration rate v in the limit of weak selection. We can see that strategy mutation (exploration) always harms cooperation while an intermediate migration rate most promotes cooperation. In what follows, we also perform extensive agent-based simulations to have an in-depth investigation of how varying each model parameter affects cooperation.

Figure S8 shows, for different combinations of cost of cooperation c and selection strength β , the equilibrium frequency of cooperators as a function of the mutation rate u and the migration rate v . Increasing c and β values both inhibit the evolution of cooperation. Individual strategy mutation or exploration always harms cooperation, leading to increased critical b/c threshold. Intermediate migration rate between different group most enhances cooperation, although the positive effect of migration on cooperation is greatly diminished by increased selection pressure. Figure S8 demonstrates that our theoretical results in the limit of weak selection can carry over to intermediate selection strength and remain qualitatively the same. For even larger β values, the population is predominated by defection (Fig. S8) as in-group cooperators become more prone to free-riders from their own groups.

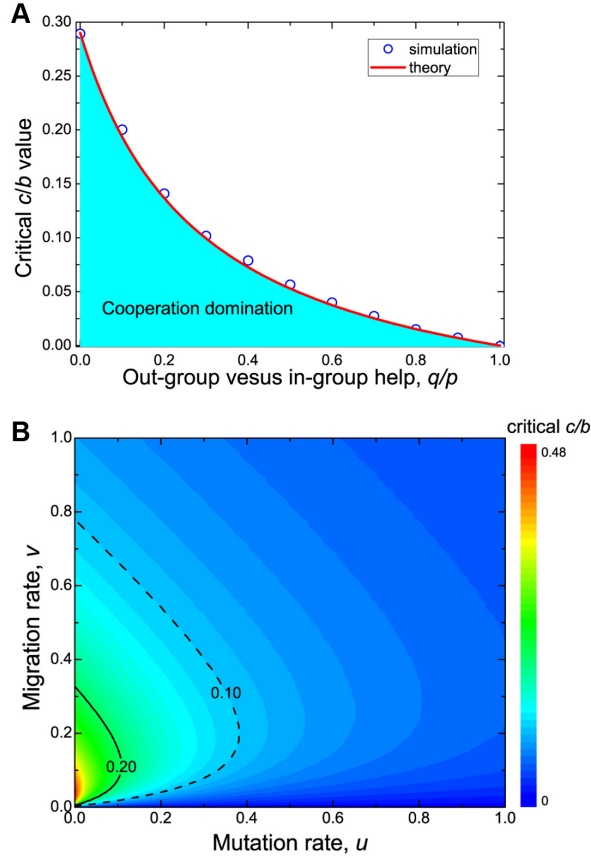


FIG. S7: Evolutionary dynamics of in-group cooperators versus defectors. (A) shows the critical cost-to-benefit ratio, c/b , below which cooperators are more abundant than defectors, as a function of the ratio of out-group helping to in-group helping, q/p . (B) shows the critical c/b value as a function of the mutation rate, u , and the migration rate, v . When cooperators deal their help only towards in-group members ($q/p = 0$), cooperators have their greatest chance to prevail. Increasing mutation rate u harms the evolution of cooperation, while an intermediate migrate rate v most enhances the evolution of cooperation. Our analytical theory agrees well with computer simulations. Parameters: $N = 100$, $M = 10$, $b = 1$, $p = 1$, $\beta = 0.001$, $u = 0.04$, $v = 0.06$. Equilibrium frequencies of strategies are averaged over $T = 10^8$ time steps.

Figure S9 plots the equilibrium frequency of cooperators as a function of intensity of selection β for different costs of cooperation c . We note that in this case the analytical prediction for the critical c/b ratio, below which cooperators are more abundant than defectors, is ≈ 0.34 . Under weak selection, the frequency of cooperators linearly increases with β if $c < 0.34$. For the other limit, strong selection always disfavors cooperation. Therefore there exists an optimum β in between 0 and ∞ that renders the maximal level of cooperation for $c < 0.34$ (Fig. S9). For $c > 0.34$, the

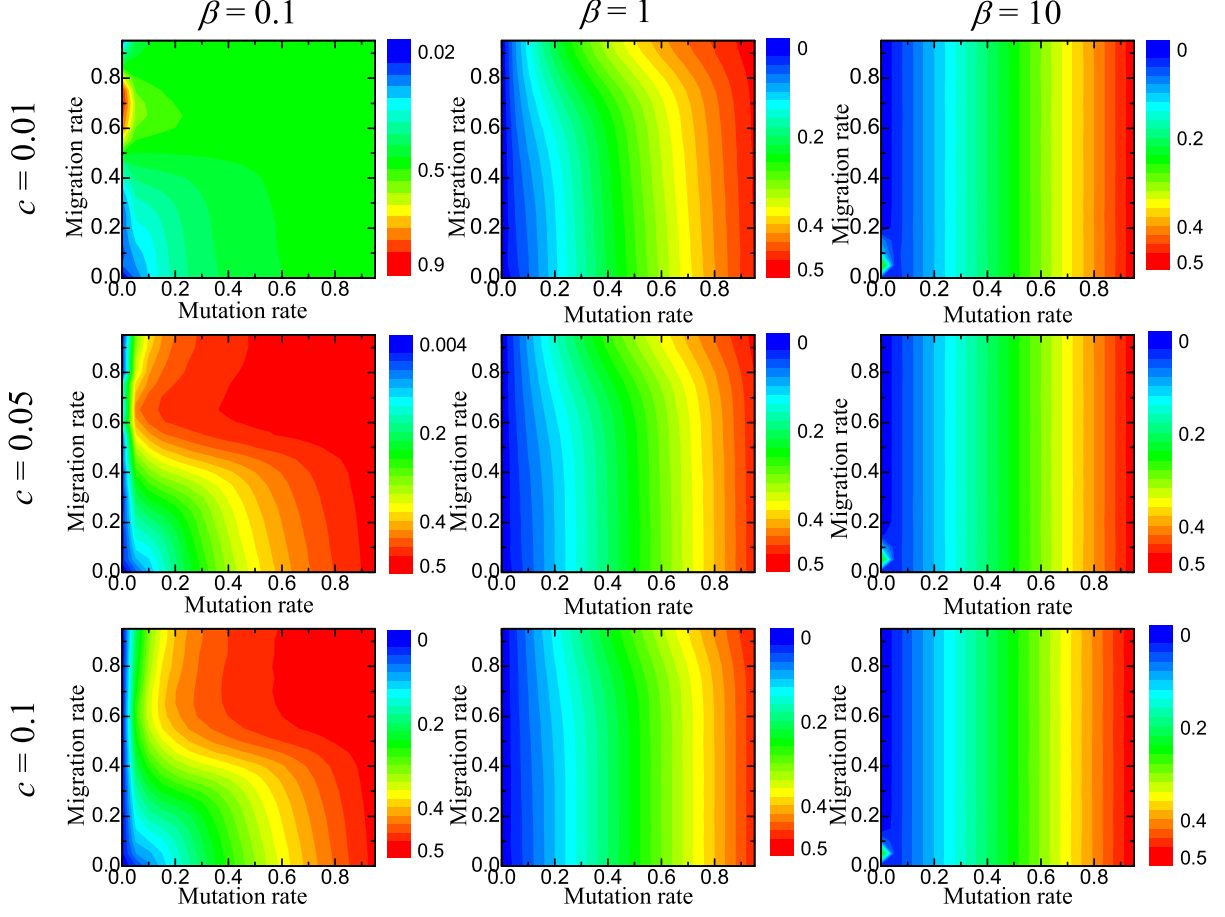


FIG. S8: Frequency of cooperators as a function of the mutation rate u and the migration rate v , for different sets of cost of cooperation and intensity of selection. Although the evolution of cooperation turns to be dismal with increasing c and β , we observe that the results for intermediate selection ($\beta \approx 0.1$) strength remain qualitatively the same as for weak selection ($\beta \ll 1$). For even larger β values, the population is predominated by defection. Parameters: $N = 100$, $M = 10$, $b = 1$, $c = 0.01, 0.05$, and 0.1 , $\beta = 0.1, 1$, and 10 . Results are averaged over $T = 10^7$ time steps.

frequency of cooperation monotonically decreases with increasing β .

Figure S10 shows that the frequency of cooperation is always a monotonic decreasing function of cost of cooperation c for different mutation rates u . This result also evidences the emergence of cooperation as a result of a tradeoff between two opposing forces – selection and mutation. In other words, we observe a “crossover” of cooperator abundance with increasing u . For small c values that favor the evolution of cooperation, increasing mutation rate u brings down the cooperation level. Whereas for large c values that are disadvantageous for cooperators, increasing mutation

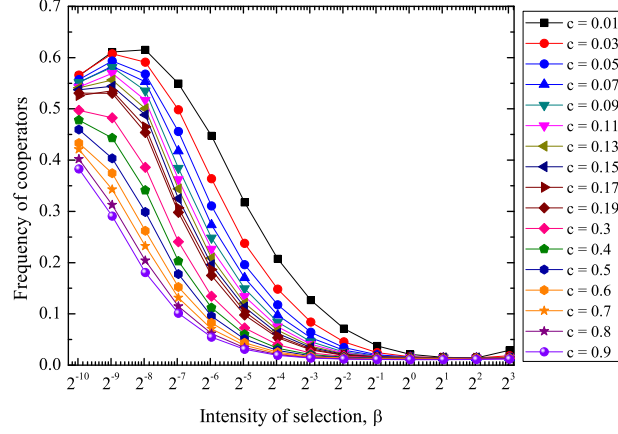


FIG. S9: Frequency of cooperators as a function of intensity of selection β for different costs of cooperation. For $\beta \ll 1$, we have the critical $(c/b)^* = 0.340$ given by our analytic calculations. Parameters: $N = 100$, $M = 10$, $u = 0.02$, $v = 0.04$. Results are averaged over $T = 10^8$ time steps.

rate u helps elevate the frequency of cooperators toward $1/2$.

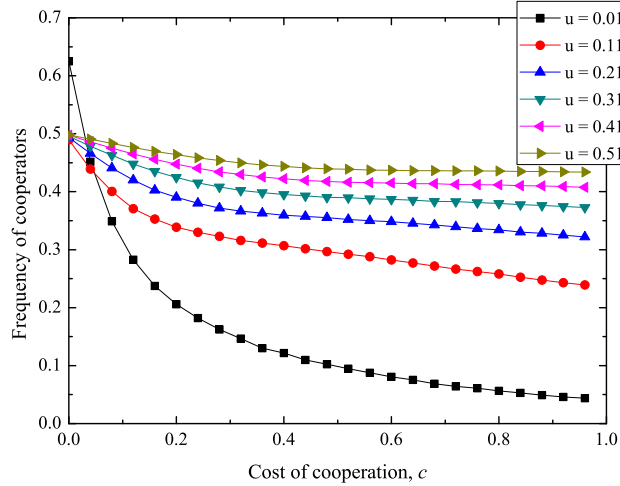


FIG. S10: Frequency of cooperation as a function of cost of cooperation for different mutation rates. Parameters: $N = 100$, $M = 10$, $v = 0.04$, $b = 1$, $\beta = 0.01$. Results are averaged over $T = 10^8$ time steps.

In Fig. S11 we study the role of migration in the evolution of cooperation. It is noted that intermediate migration tendency v most promotes cooperation. The frequency of cooperators is quite low at small migration rates v ($v = 0.01$ in Fig. S11). With increasing v cooperators become more abundant in the population for small c ($v = 0.11$ in Fig. S11). At some certain intermediate v , the frequency of cooperators reaches the maximal level ($v = 0.21$ in Fig. S11), and drops down

with further increasing v .

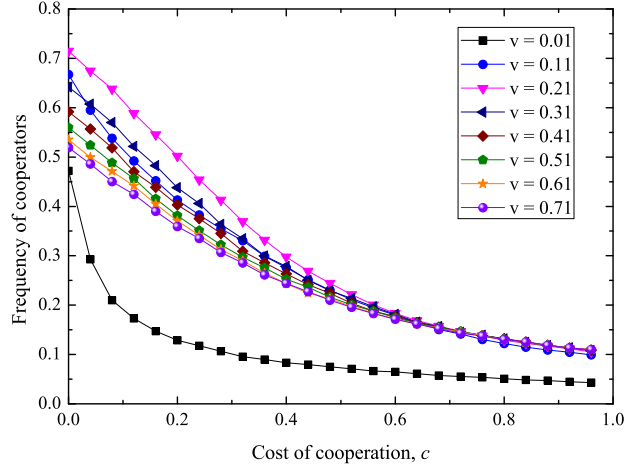


FIG. S11: Frequency of cooperation as a function of cost of cooperation for different migration rates. Parameters: $N = 100$, $M = 10$, $u = 0.02$, $b = 1$, $\beta = 0.01$. Results are averaged over $T = 10^8$ time steps.

The number of groups M plays a decisive role in determining the evolutionary fate of cooperators. As shown in Fig. S12, the larger the number of groups, the greater the chance for cooperators to prevail. In excellent agreement with simulations, the critical c/b ratio, below which cooperators win over defectors, increases monotonically with the number of groups M until a plateau is reached (Fig. S12A). For other parameters fixed, increasing number of groups M also boosts the abundance of cooperators (Fig. S12B). This result suggests the importance of the diversity of group identity in the maintenance and promotion of cooperation.

B. Coevolutionary dynamics in heterogeneous populations

We have run extensive agent-based simulations for both global and local mutation models. As shown in Fig. S13, the simulation results and our analytical theory are in perfect agreement. To have a clear picture, here we show the stationary distributions of these strategies that are selected (namely, their abundance is larger than the average 4×10^{-4}). We can see that the critical lines in the strategy space determined by simulations agree very well with the theoretical predictions (Fig. S13).

Figure S14 plots the effect of increasing selection pressure on the resulting distribution of s-strategies. In this case, maximum in-group favoritism $(1, 0)$ is most favored by weak selection (small β values in Fig. S14). Slightly increased intensity of selection β pushes the distribution

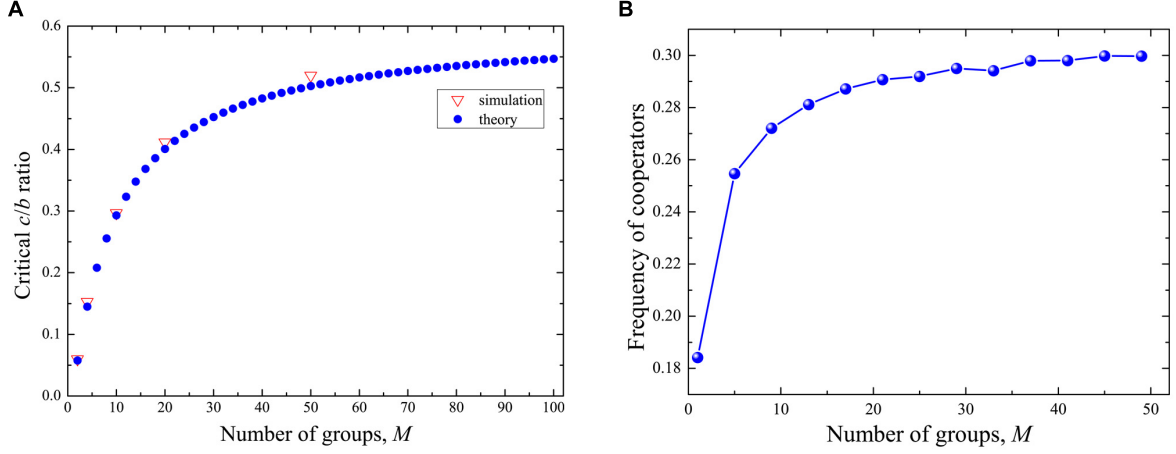


FIG. S12: The role of number of groups, M , in evolution of cooperation. Panel (A) shows the critical c/b ratio as a function of M . Panel (B) shows that the equilibrium frequency of cooperation increases monotonically with M . Parameters: $N = 100$, $u = 0.04$, $v = 0.08$, $b = 1$, (A) $\beta = 0.001$, (B) $\beta = 0.1$, $c = 0.01$. Results are averaged over $T = 2 \times 10^8$ time steps.

further towards $(1, 0)$, leading to enhanced level of in-group favoritism. Once the β value exceeds a certain threshold, the most selected region of the strategy space (the peak of the distribution of strategies) starts to gradually move along the p -axis from $(1, 0)$ to $(0, 0)$. This is because that under strong selection in-group cooperators having high p values face the exploitation of some in-group members with low p values. These individuals with low p values are free riding on the efforts of those with high p values. For $\beta \rightarrow \infty$, it even does not pay to help members of their own group.

In comparison with the global mutation model, local mutation results in more condensed distributions of strategies (Fig. S15). Additionally, localized mutation reduces the fluctuations in the stationary distributions and thus renders the distribution of strategies smooth. We can clearly observe a peak in these distributions. In the theoretical analysis, we have demonstrated that both global mutation and local mutation models require the same condition for maximum in-group favoritism $(1, 0)$ to be most selected. Our simulations confirm this prediction (Fig. S15). We also study the effect of increasing β on the resulting distribution of strategies. We observe the qualitatively same pattern as in the global mutation (cf. Figs. S13A, S14 and Fig. S15). Taken together, the present work shows that our results in the main text are robust with respect to various model variations.

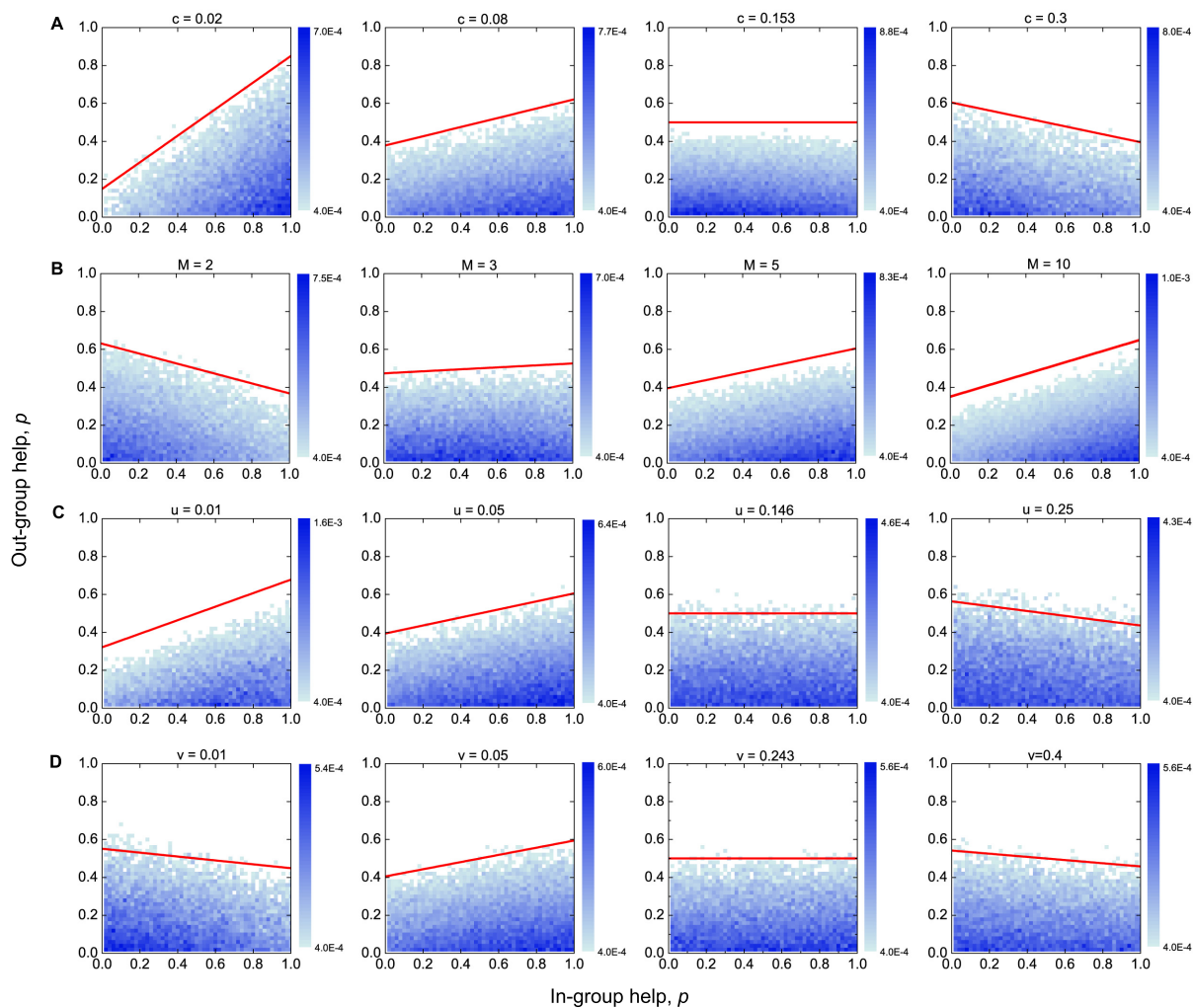


FIG. S13: Perfect agreement between analytical predictions and numeric simulations. Shown are the distributions of the strategies that are favored by selection (frequency larger than the average 4×10^{-4}) in agent-based simulations. Theoretical predictions are given by the straight lines. These strategies below the critical line (lower q values) are selected. Parameters are as in Fig. 2 in the main text.

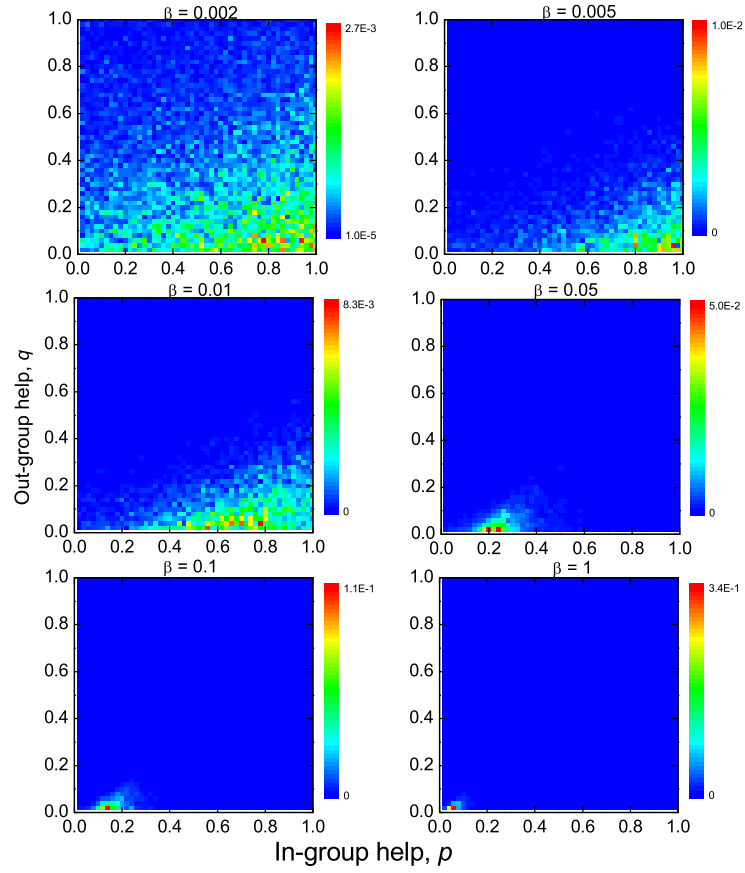


FIG. S14: The impact of intensity of selection β on the resulting distribution of strategies. Increasing β first enhances the evolution of in-group favoritism, but opposes it after β exceeds a certain threshold. Parameters: $N = 100$, $M = 100$, $u = 0.002$, $v = 0.1$, $b = 1$, $c = 0.1$. Results are averaged over $T = 10^9$ time steps.

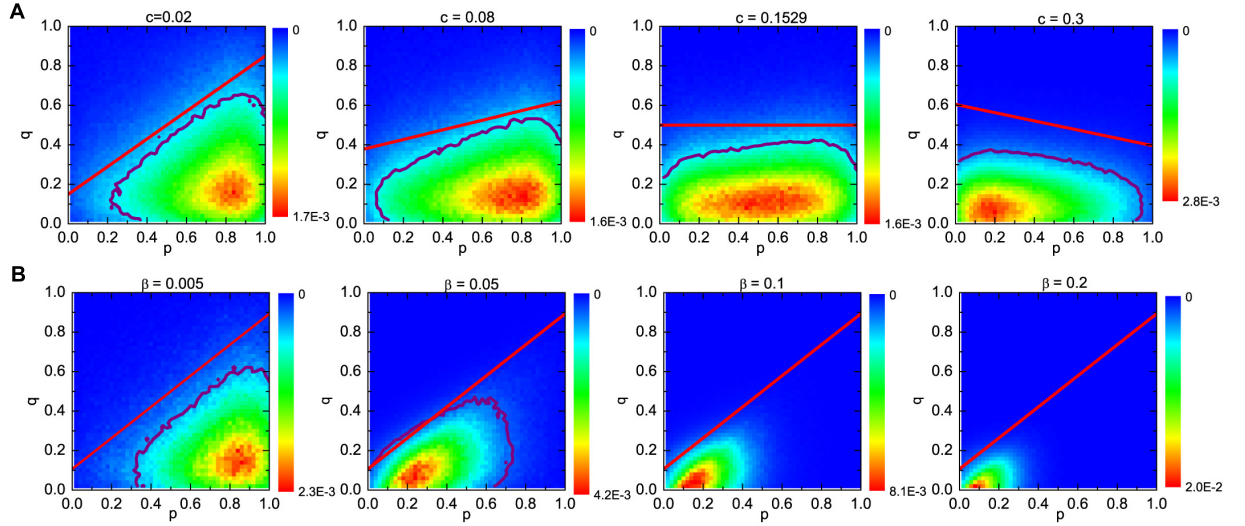


FIG. S15: Local mutation model. Shown are the stationary distributions of strategies over the unit square with varying (A) cost of cooperation, c , and (B) intensity of selection, β , as indicated. The numeric simulations agree very well with the adaptive dynamics analysis. Compared with the global mutation model, localized mutations lead to more concentrated distributions with a legible peak because the strategy of a mutated offspring is constrained within the small neighborhood of the parental strategy. Parameters: $N = 100$, $b = 1$, (A) $M = 4$, $u = 0.04$, $v = 0.06$, the standard deviation of the Gaussian mutation kernel is 0.01, $\beta = 0.005$, (B) $M = 10$, $c = 0.02$, $u = 0.02$, $v = 0.06$. Results are averaged over $T = 10^9$ time steps.

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