2 Simulations

2.1 Primary simulations with strategies defined in three dimensions

We developed, ran, and analysed a large number of agent-based simulations to further understand the evolutionary dynamics of our system. Specifically, two of us developed the initial simulations independently in two different languages (C.E. in Objective-C and U.F. in C++). We iteratively compared our output and refined our programs until our results converged in terms of both transitional dynamics and steady states. The specific results presented in the main paper and this supplement are based on the simulations of C.E.

Our overall objective was to examine the evolution of cooperative strategies under three basic scenarios. First, we simulated populations for which all social interactions are with ingroup members, and these interactions are either one-shot or repeated. This is the **repeated interactions scenario**. Second, we simulated populations involving one-shot interactions with ingroup members, one-shot interactions with outgroup members, and intergroup competition. We call this the **group competition** scenario. Finally, we simulated populations for which social interactions among ingroup members are repeated, social interactions with outgroup members are one-shot, and intergroup competition is present. We call this the **joint scenario**.

2.1.1 The social dilemma

The stage game is identical to that specified in (1) with $b = 2$, although we also consider $b = 4$ in Supplementary Figure 16. For the analytical work presented in the first part of this supplement, we implemented repeated interactions by assuming that, conditional on the present interaction between a pair of players, the relationship continued for at least one more interaction with probability $\delta \in [0, 1)$. In contrast, for simulations, the number of interactions per pair of players is a fixed

parameter, N, where $N \in \{1, 100\}$. These values of N are equivalent to the expected number of interactions under $\delta = 0$ and $\delta = 0.99$. We use a fixed number of interactions in the simulations, as explained below, because it allows us to conveniently standardise the intensity of group selection across the group competition and joint scenarios. In addition, because all strategies in our model are backward-looking, we have no concerns arising from forward-looking strategies, end-game effects, or backward induction. Note that we also consider $N = 1000$, which corresponds to $\delta = 0.999$, in Supplementary Figures 15 - 16.

2.1.2 Cancellation effects at the individual and group levels

A simulated population consists of 960 agents. Populations are subdivided into 40 groups of 24 agents each. Let $i \in I = \{1, \dots, 24\}$ and $j \in J = \{1, \dots, 40\}$ index agent and group respectively. Simulations ran for 150,000 generations.

In addition, we also examine cancellation effects at both the individual and group levels. Regarding cancellation effects at the individual level[4], we consider two different life cycles for all three scenarios. Under one life cycle, the population structure present at the game play stage is the same as the structure present when agents within a group compete to reproduce. In this case, game play and individual selection involve **coupled** population structures. Under the other life cycle, migration occurs between game play and competition within the group to reproduce. This means that the population structure present during game play is not the same as the structure present during competition and reproduction; game play and individual selection thus involve population structures that are **decoupled**. Because migration rates are less than one, simulated populations are never completely mixed. Thus, the claim that game play and individual selection are **decoupled** is a *relative* claim; structure at the two relevant stages of the life cycle are less coupled than they are when **coupled**.

Below we provide detailed information about the parameter space and initial conditions for each of the three scenarios. As explained in the main paper (Fig. 1), and as explained in detail below, we simulated evolution over strategies defined in two, three, or four dimensions. For each combination of initial condition, parameter values, life cycle, and scenario, we ran 50 independent simulations.

2.1.3 Strategies and payoffs for the social dilemma

We begin with ingroup interactions. Once two agents within a group are paired to play the social dilemma, they play the game N times, where $N \in \{1, 100\}$. Let n index a specific interaction, which simply means a single round of play for a pair of agents. For each interaction with a specific partner, each agent has an endowment. This endowment is normalised to 1. For a given pair, let $x_n \in [0, 1]$ be the transfer of the first mover for interaction n and let $y_n \in [0, 1]$ be the transfer of the second mover. Interactions are controlled by heritable strategies that are fixed for any given agent. Consider an arbitrary pair of agents in group j. Each agent's strategy for playing with an ingroup partner involves three quantities. These quantities are (i) $\tilde{x}_{ij}$, the initial transfer if first mover, (ii) a_{ij}, the left intercept of the response function, and (iii), d_{ij}, the right intercept of the response function. Putting all this together, let i be the first mover for an ingroup pairing and i' the second mover. Behaviours for the pair follow

$$
\begin{aligned}
n = 1, \quad & x_n = \tilde{x}_{ij} \\
& y_n = a_{i'j} + (d_{i'j} - a_{i'j})\tilde{x}_{ij} \\
n \in \{2, \ldots, N\}, \quad & x_n = a_{ij} + (d_{ij} - a_{ij})y_{n-1} \\
& y_n = a_{i'j} + (d_{i'j} - a_{i'j})x_n.
\end{aligned}
\tag{52}
$$

For any given ingroup pairing and interaction n, endogenous fitness for the first and second movers are, respectively,

$$\Theta_1^n = 1 - x_n + by_n$$
$$\Theta_2^n = 1 - y_n + bx_n. \tag{53}$$

Theoretically, $\tilde{x}_{ij}$, a_{ij}, and d_{ij} are all continuous variables, and each can take any quantity in the interval $[0,1]$. For simulations, the quantities are on a finely grained lattice. Specifically, each of the three quantities for a specific agent has a value in the set $\{0, 0.025, \ldots, 1\}$.

Now we consider outgroup interactions. Outgroup interactions are possible in the group competition and joint scenarios, and in these scenarios each agent has an endowment of 1 for a single outgroup interaction. Additionally, each agent has a strategy that controls outgroup interactions. This strategy depends on three variables, which include (i) $\hat{x}_{ij}$, the initial transfer if first mover, (ii) u_{ij}, the left intercept of the response function, and (iii), v_{ij}, the right intercept of the response function. As with ingroup strategies, outgroup strategies are defined on the lattice $\{0, 0.025, \ldots, 0.975, 1\}^3$. For a given outgroup pairing, arbitrarily let i and j indicate the agent and group for the first mover and i' and j' the agent and group for the second mover. Outgroup interactions occur with probability 1, and the interaction in a matched pair is always one-shot. Transfers for this one-shot social dilemma take the form,

$$x_1 = \hat{x}_{ij}$$
$$y_1 = u_{i'j'} + (v_{i'j'} - u_{i'j'})\hat{x}_{ij}. \tag{54}$$

For a given outgroup pair, the endogenous fitness values for the first and second movers are, respectively,

$$\Omega_1 = 1 - x_1 + by_1$$
$$\Omega_2 = 1 - y_1 + bx_1. \tag{55}$$

Because $b = 2$ in our behavioural experiment in Papua New Guinea, we use $b = 2$ for most simulations. Under the repeated interactions scenario, the total fitness for i in j, denoted W_{ij}, is

a weighted sum of an exogenous fitness value, ω_0, and the total endogenous fitness value over all interactions with i's ingroup partner (53). Under the group competition and joint scenarios, the total fitness for i in j is a weighted sum of ω_0 and all endogenous fitness values, which consist of endogenous fitness values from all interactions with i's ingroup partner (53) and the endogenous fitness value from i's one-shot outgroup interaction (55). We explain this weighting in detail below. We also explain how we assigned values for ω_0 and how we translated W_{ij} values into reproduction and selection.

2.1.4   The repeated interactions scenario

Life cycles. The following specifies the sequence of events within a generation for simulations under the repeated interactions scenario. Each agent's strategy is specified by three variables, $\tilde{x}_{ij}$, a_{ij}, and d_{ij}.

- **Mutation.** When a strategy is reproduced, mutations potentially occur. In particular, for each of the three dimensions that control an agent's strategy, mutations occur independently according to mutation probability $\mu = 0.02$. If a mutation occurs, it simply means that the variable in question moves one step up or down, with equal probability, on the lattice for that variable. Mutations outside the lattice are not possible, and the probability of mutation is $\mu/2$ at the boundary of any given dimension of strategy space. For example, assume $\tilde{x}_{ij} \in \{0.025, 0.05, \ldots, 0.975\}$ in generation t. If the initial transfer value of i in j is replicated for a new agent in generation $t + 1$, the value moves up by 0.025 with probability $\mu/2$, it moves down by 0.025 with probability $\mu/2$, and it replicates faithfully with probability $1 - \mu$. If $\tilde{x}_{ij} = 0$, the value moves up with probability $\mu/2$, and it remains the same with probability $1 - \mu/2$. If $\tilde{x}_{ij} = 1$, the value moves down with probability $\mu/2$, and it remains the same with probability $1 - \mu/2$.

- **Movement of groups in the metapopulation.** Each generation, groups are randomly paired with each other for outgroup game play and potential intergroup competitions. Because outgroup game play and intergroup competition do not occur in the repeated interactions scenario, the pairing of groups is not directly relevant. Nonetheless, we maintain the random pairing of groups. We also maintain the movement of groups in the metapopulation, which is relevant for examining cancellation effects at the group level[5] in the group competition and joint scenarios. Specifically, at the beginning of each generation after the first, $\Xi \in \{0, 20, 40\}$ groups are randomly sampled to enter a pool of groups who will move around in the metapopulation. In effect, this process vacates Ξ territories. The sampled groups in the pool are then randomly redistributed back to these vacant territories. As a result, large values of Ξ reduce the probability, all else equal, that a group winning an intergroup competition (i.e. group competition and joint scenarios) in the previous generation will compete against its descendent group in the current generation. Small values of Ξ increase this probability. Accordingly, cancellation effects at the group level increase as Ξ declines.

- **Migration (Coupled).** When the life cycle couples population structure during game play with structure at the individual selection stage, migration occurs just before game play. Specifically, for each j, $m_j \in \{8, 16\}$ randomly selected agents leave the group and join a common pool of migrants. The agents in this pool of migrants are then randomly redistributed back to the 40 groups in the population subject to the constraint that each group ends up with 24 agents.

- **Social dilemma.** For each j, agents are randomly assigned to form ingroup pairs. Each pair plays the social dilemma game for $N \in \{1, 100\}$ interactions. The first mover is randomly selected with uniform probability. The unweighted exogenous fitness parameter is simply equal to the number of endowments, and so $\omega_0 = N$. Fitness is a convex combination of ω_0 and payoffs derived from social interactions endogenous to the model. The weighting

55

parameter for this convex combination is $\zeta \in (0, 1)$ Thus, for the first mover in a pair, $W_{ij} = (1 - \zeta)N + \zeta \sum_{n=1}^{N} \Theta_1^n$, and for the second mover $W_{ij} = (1 - \zeta)N + \zeta \sum_{n=1}^{N} \Theta_2^n$.

- **Migration (Decoupled).** When the life cycle decouples population structure during game play with structure at the individual selection stage, migration occurs just after game play. Specifically, for each j, $m_j \in \{8, 16\}$ randomly selected agents leave the group and join a common pool of migrants. The agents in this pool of migrants are then randomly redistributed back to the 40 groups in the population subject to the constraint that each group ends up with 24 agents.

- **Reproduction.** For each j, reproduction means replacing the group of 24 agents in t with a new group of 24 agents in $t + 1$. The reproduction of strategies is proportional to an agent's fitness relative to the sum of all fitness values in the agent's deme. Moreover, the reproduction of strategies is independent across the three dimensions used to define strategies. Specifically, for each of the 24 agents in group j, the value of $\tilde{x}_{ij}$ is replicated in the next generation with probability $W_{ij} / \sum_i W_{ij}$. Similarly, the values of a_{ij} and d_{ij} are each independently replicated with probability $W_{ij} / \sum_i W_{ij}$.

Basic effects of population structure on the evolution of cooperation. Quite apart from the effects of intergroup competition, population structure per se can affect the evolution of cooperation by creating assortment. Demographic and ecological details, however, are crucial[4, 6, 7]. Supplementary Figures 15 - 16 show that in our simulations decreasing migration rates (increasing population structure) generally support the evolution of *relatively* high levels of cooperation when interactions are one-shot ($N = 1$) or repeated ($N \in \{100, 1000\}$), and strategies are three-dimensional. Interestingly, however, the levels of cooperation that evolve are well below the maximum levels of cooperation that could evolve. This is even true under exceptional conditions, namely when the migration rate is zero, and ingroup relationships are extraordinarily long-lived ($N = 1000$). This

is consistent with our finding that the dimensionality of strategy space plays an utterly decisive, if arbitrary role in the evolution of cooperation under repeated interactions.