Electronic supplementary material

Appendix A: Repeated *n*-player Prisoner's Dilemma for the smallest possible population size N(N = n) for general strategy

Each game involves all the *N* individuals in the population and consists of one or more rounds. We consider two strategies: ALLD and R. ALLD always defect no matter what other individuals do. R can be any strategy that cooperates at least once during each game when there are only one R and N - 1 ALLDs in the population. The payoffs, V(C|l) and V(D|l), have the same properties as above, given by (S1)-(S4).

First, let us consider whether strategy R is ESS_N or not. From (S1) and (S3), we have V(D|l) > V(C|l). This inequality means that a single mutant ALLD in a population of strategy R does not have a lower fitness and thus the first condition for R to be ESS_N is violated. Therefore, we conclude strategy R that is ESS_N does not exist.

Second, we examine whether ALLD is ESS_N or not. Since V(D|1) > V(C|1) and a mutant R cooperates at least once, selection opposes R invading ALLD, that is, the first condition for ALLD to be ESS_N is satisfied. The fixation probability of R is given by

$$\rho_{\rm R} = 1 / \left(1 + \sum_{k=1}^{N-1} \prod_{i=1}^{k} \frac{1 - w + wGi}{1 - w + wFi} \right),$$

where *i* denotes the number of R individuals and F_i and G_i are the expected payoffs of R and ALLD, respectively (see main text). Since $F_1 < G_1$ and $F_i \le G_i$ ($2 \le i \le N - 1$) from the definition of R, the second condition for ALLD to be ESS_N is satisfied. Therefore, we can conclude that ALLD is ESS_N.

To sum up, even in repeated *n*-player Prisoner's Dilemma, cooperation cannot evolve when population size and group size are the same. Note that the argument in this subsection applies for any payoff functions that satisfy (S1)-(S4): we do not have to assume specific payoff functions such V(C|k) = bk/n - c and V(D|k) = bk/n. Also, the argument does not presuppose weak selection.

Appendix B: One-shot *n*-player Prisoner's Dilemma for general population size Groups of *n* individuals are sampled from the population of size *N* and a game is played within each group. A game consists of only one round, in each of which individuals either cooperate or defect. When some individuals cooperate, all the individuals in the group gain a benefit from it while only the cooperating individuals have to pay a cost. Let V(C|l) and V(D|l) be the payoffs to individuals choosing cooperation and defection given that *l* of *n* individuals in the group choose cooperation. The *n*-player Prisoner's Dilemma demands that these payoffs have the following properties:

$$V(D|l) > V(C|l+1), \quad (S1)$$

$$V(D|l+1) > V(D|l), \quad (S2)$$

$$V(C|l+1) > V(C|l), \quad (S3)$$

$$(l+1)V(C|l+1) + (n-l-1)V(D|l+1) > lV(C|l) + (n-l)V(D|l), \quad (S4)$$

where $0 \le l \le n - 1$. Using (S1) and (S3), we can conclude that D is always traditional ESS while C never is. Now, let us examine for general *N* whether either or both C and D can be ESS_N. First, consider the case when a mutant D appears in a population of C. Using (S1) and (S3), we can obtain an inequality, that is,

$$(N-1)V(D|l) > (N-n)V(C|l+1) + (n-1)V(C|l).$$

This inequality implies that the first condition for C to be ESS_N is violated (let $a_k = V(D|k-1)$, $b_k = V(C|k)$ and l = n - 1 in (5) in the main text), that is, a single mutant D in a population of C has a higher fitness. Therefore, we conclude that C cannot be ESS_N .

Second, suppose that a mutant C has appeared in a population of D. From (S1) and (S2), we obtain

$$(N-1)V(C|l+1) < (N-n)V(D|l) + (n-1)V(D|l+1),$$

which suggests that the first condition for D to be ESS_N is satisfied (let $a_k = V(C|n - k + 1)$, $b_k = V(D|n - k)$ and l = 0 in (5) in the main text). The fixation probability of C is given by

$$\rho_{\rm C} = 1 / \left(1 + \sum_{k=1}^{N-1} \frac{1-w+wGi}{1-w+wFi} \right),$$

where *i* denotes the number of C individuals and F_i and G_i are the expected payoffs of C and D, respectively (see main text). From (S1) and (S2), we have

$$\sum_{k=1}^{n} \frac{\binom{i-1}{n-k}\binom{N-i}{k-1}}{\binom{N-1}{n-1}} V(C \mid n-k+1) < \sum_{k=1}^{n} \frac{\binom{i}{n-k}\binom{N-i-1}{k-1}}{\binom{N-1}{n-1}} V(D \mid n-k) ,$$

that is, $F_i < G_i$ ($1 \le i \le N - 1$). Hence, $\rho_C < 1/N$ and thus the second condition for D to be ESS_N is satisfied. Therefore, we can conclude that D is ESS_N.

To sum up, in nonrepeated *n*-player Prisoner's Dilemma, C is neither ESS_N nor traditional ESS, and D is not only ESS but also ESS_N . Hence, cooperation cannot emerge in populations consisting of defectors. Note that the argument in this subsection applies for any payoff functions that satisfy (S1)-(S4) and for any selection intensity.

Appendix C: For n=2, 3, no payoff matrix exists for which both A and B are traditional ESS but neither is ESS_N .

In two-player games,

 $2a_1 + a_2 < 2b_1 + b_2$

 $a_1 + 2a_2 > b_1 + 2b_2$

$$a_1 > b_1$$

 $a_2 < b_2$

All these inequalities cannot be satisfied simultaneously. Hence, for n=2, no payoff matrix exists for which both A and B are traditional ESS but neither is ESS_N . Similarly, in three player games,

$$3a_1+2a_2+a_3 < 3b_1+2b_2+b_3$$

 $a_1+2a_2+3a_3 > b_1+2b_2+3b_3$
 $a_1 > b_1$
 $a_3 < b_3$

All these inequalities cannot be met simultaneously. Hence, for n=3, no payoff matrix exists for which both A and B are traditional ESS but neither is ESS_N .

Appendix D: Figure illustrates the relationship between payoff parameter (*b/c*), group size (*n*) and the minimum number of rounds (*m*) required for $\rho_{ALLD} < 1/N$, $\rho_{TFTn-1} > \rho_{ALLD}$ or $\rho_{TFTn-1} > 1/N$ when *N* is large. The blue represents the number of rounds for which $\rho_{ALLD} = 1/N$, while the green represents that for which $\rho_{TFTn-1} = \rho_{ALLD}$ and the red represents that for which $\rho_{TFTn-1} = 1/N$. The parameter space is divided into the following four regions: (i) TFT_{n-1} is ESS_N and ALLD is not ESS_N ; (ii) both TFT_{n-1} and ALLD are ESS_N and $\rho_{TFTn-1} > \rho_{ALLD}$; (iii) both TFT_{n-1} and ALLD are ESS_N and $\rho_{TFTn-1} > \rho_{ALLD}$; (iii) both TFT_{n-1} and ALLD are ESS_N and $\rho_{TFTn-1} > \rho_{ALLD}$; (iii) both TFT_{n-1} and ALLD are the torus to figure 1 be when b/(nc) = 0.51.



Figure

the number of rounds(m)