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**Author for correspondence:**

M. H. Duong

e-mail: [h.duong@bham.ac.uk](mailto:h.duong@bham.ac.uk)

# Cost efficiency of institutional incentives for promoting cooperation in finite populations

Manh Hong Duong<sup>1</sup>, The Anh Han<sup>2</sup>

<sup>1</sup>School of Mathematics, University of Birmingham, Birmingham B15 2TT, UK.

<sup>2</sup>School of Computing, Engineering and Digital Technologies, Teesside University, TS1 3BX, UK.

Institutions can provide incentives to enhance cooperation in a population where this behaviour is infrequent. This process is costly, and it is thus important to optimize the overall spending. This problem can be mathematically formulated as a multi-objective optimization problem where one wishes to minimize the cost of providing incentives while ensuring a minimum level of cooperation, sustained over time. Prior works that consider this question usually omit the stochastic effects that drive population dynamics. In this paper, we provide a rigorous analysis of this optimization problem, in a finite population and stochastic setting, studying both pairwise and multi-player cooperation dilemmas. We prove the regularity of the cost functions for providing incentives over time, characterize their asymptotic limits (infinite population size, weak selection and large selection) and show exactly when reward or punishment is more cost efficient. We show that these cost functions exhibit a phase transition phenomena when the intensity of selection varies. By determining the critical threshold of this phase transition, we provide exact calculations for the optimal cost of incentive, for any given intensity of selection. Numerical simulations are also provided to demonstrate analytical observations. Overall, our analysis provides for the first time a selection-dependent calculation of the optimal cost of institutional incentives (for both reward and punishment) that guarantees a minimum level of cooperation over time. It is of crucial importance for real-world applications of institutional incentives since intensity of selection is often found to be non-extreme and specific for a given population.

## 1. Introduction

The problem of promoting the evolution of cooperative behaviour within populations of self-regarding individuals has been intensively investigated across diverse fields of behavioural, social and computational sciences (Han, 2013; Nowak, 2006b; Perc et al., 2017; Sigmund, 2010; West et al., 2007). Various mechanisms responsible for promoting the emergence and stability of cooperative behaviours among such individuals have been proposed. They include kin and group selection (Hamilton, 1964; Traulsen and Nowak, 2006), direct and indirect reciprocities (Han et al., 2012; Krellner and Han, 2020; Nowak and Sigmund, 2005; Ohtsuki and Iwasa, 2006; Okada, 2020), spatial networks (Antonioni and Cardillo, 2017; Peña et al., 2016; Perc et al., 2013; Santos et al., 2006), reward and punishment (Boyd et al., 2003, 2010; Fehr and Gächter, 2000; Hauert et al., 2007a; Herrmann et al., 2008; Sigmund et al., 2001), and pre-commitments (Han et al., 2013, 2016; Martínez-Vaquero et al., 2017; Nesse, 2001; Sasaki et al., 2015). Institutional incentives, namely, rewards for cooperation and punishment of wrongdoing, are among the most important ones (Chen et al., 2015; García and Traulsen, 2019; Góis et al., 2019; Han and Tran-Thanh, 2018; Powers et al., 2018; Sigmund et al., 2001, 2010a; Vasconcelos et al., 2013; Wang et al., 2019; Wu et al., 2014). Differently from other mechanisms, in order to carry out institutional incentives, it is assumed that there exists an *external* decision maker (e.g. institutions such as the United Nations and the European Union) that has a budget to interfere in the population to achieve a desirable outcome. Institutional enforcement mechanisms are crucial for enabling large-scale cooperation. Most modern societies implemented certain forms of institutions for governing and promoting collective behaviors, including cooperation, coordination, and technology innovation (Bardhan, 2005; Bowles, 2009; Bowles and Gintis, 2002; Han et al., 2021; Ostrom, 1990; Scotchmer, 2004).

Providing incentives is costly and it is therefore important to minimize the cost while ensuring a sustained level of cooperation over time (Chen et al., 2015; Han and Tran-Thanh, 2018; Ostrom, 1990). Despite its paramount importance, so far there have been only few works exploring this question. In particular, Wang et al. (2019) use optimal control theory to provide an analytical solution for cost optimization of institutional incentives assuming deterministic evolution and infinite population sizes (modeled using replicator dynamics). This work therefore does not take into account various stochastic effects of evolutionary dynamics such as mutation and non-deterministic behavioral update (Hofbauer and Sigmund, 1998; Sigmund, 2010; Traulsen et al., 2006). In a deterministic system consisting of cooperators and defectors, once the latter disappear (for instance through strong institutional punishment), there is no further change to the system and thus no further interference in it is required. When mutation is present, this behaviour can however reoccur and become abundant over time, requiring institutions to spend more budget on providing further incentives. Moreover, a key factor of behavioral update, the intensity of selection (Sigmund, 2010)—which determines how strongly an individual bases her decision to copy another individual's strategy on their fitness difference—might strongly impact an institutional incentives strategy and its cost efficiency. Its value is usually found to be specific for a given population (Domingos et al., 2020; Rand et al., 2013; Traulsen et al., 2010; Zisis et al., 2015) and thus should be taken into account when designing suitable cost-efficient incentives. For instance, when selection is weak such that behavioral update is close to a random process (i.e. an imitation decision is independent of how large the fitness difference is), providing incentives would make little difference to cause behavioral change, however strong it is. When selection is strong, incentives that ensure a minimum fitness advantage to cooperators would already ensure a positive behavioral change.

In a stochastic, finite population context, so far this problem has been investigated primarily based on agent-based and numerical simulations (Chen et al., 2015; Cimpéanu et al., 2019, 2021; Han and Tran-Thanh, 2018; Han et al., 2018; Sasaki et al., 2012). Results demonstrate several interesting phenomena, such as the significant influence of the intensity of selection on incentive strategies and optimal costs. However, there is no satisfactory rigorous analysis available at present that allows one to determine the optimal way of providing incentives. This

is a challenging problem because of the large but finite population size and the complexity of stochastic processes governing the population dynamics.

In this paper, we provide exactly such a rigorous analysis. We study cooperation dilemmas in both pairwise (the Donation game) and multi-player (the Public Goods game) settings (Sigmund, 2010). They are among the most well studied models for studying the evolution of cooperative behaviour where individually defection is always preferred over cooperation while mutual cooperation is the preferred collective outcome for the population as a whole. Adopting a popular stochastic evolutionary game approach for analysing well-mixed finite populations (Imhof et al., 2005; Nowak, 2006a; Nowak et al., 2004), we derive the total expected costs of providing institutional reward or punishment, characterize their asymptotic limits (namely, for infinite population, weak selection and strong selection) and show the existence of a phase transition phenomena in the optimization problem when the intensity of selection varies. We calculate the critical threshold of phase transitions and study the minimization problem when the selection is under and above the critical value. We furthermore provide numerical simulations to demonstrate the analytical results.

The rest of the paper is organized as follows. In Section 2 we introduce the models and methods, deriving mathematical optimization problems that will be studied. The main results of the paper are presented in Section 3. In Section 4 we discuss possible extensions for future work. Finally, detailed computations, technical lemmas and proofs the main results are provided in the attached Supporting Information (SI).

## 2. Models and methods

### (a) Cooperation dilemmas

We consider a well-mixed, finite population of  $N$  self-regarding individuals or players, who interact with each other using one of the following one-shot (i.e. non-repeated) cooperation dilemmas, the Donation Game (DG) or its multi-player version, the Public Goods Game (PGG). In these games, a player can either choose to cooperate (i.e. a cooperator, or C player) or to defect (i.e. a defector, or D player).

Let  $\Pi_C(i)$  and  $\Pi_D(i)$  be the average payoffs of a C player and a D player in a population with  $i$  C players and  $N - i$  D players, respectively (see also Section 2.3 for more details). We show below that the difference  $\delta = \Pi_C(i) - \Pi_D(i)$  does not depend on  $i$ . For cooperation dilemmas, it is always the case that  $\delta < 0$ .

#### Donation Game (DG)

The payoff matrix of the DG (for row player) is given as follows

$$\begin{array}{cc} & \begin{array}{cc} C & D \end{array} \\ \begin{array}{c} C \\ D \end{array} & \begin{pmatrix} b - c & -c \\ b & 0 \end{pmatrix}, \end{array}$$

where  $c$  and  $b$  represent the cost and benefit of cooperation, where  $b > c$ . DG is a special version of the Prisoner's Dilemma game (PD).

Denoting  $\pi_{X,Y}$  the payoff of a strategist  $X$  when playing with strategist  $Y$  from the payoff matrix above, we obtain

$$\begin{aligned} \Pi_C(i) &= \frac{(i-1)\pi_{C,C} + (N-i)\pi_{C,D}}{N-1} = \frac{(i-1)(b-c) + (N-i)(-c)}{N-1}, \\ \Pi_D(i) &= \frac{i\pi_{D,C} + (N-i-1)\pi_{D,D}}{N-1} = \frac{ib}{N-1}. \end{aligned}$$

Thus,

$$\delta = \Pi_C(i) - \Pi_D(i) = -\left(c + \frac{b}{N-1}\right).$$

## Public Goods Game (PGG)

In a PGG, players interact in a group of size  $n$ , where they decide to cooperate, contributing an amount  $c > 0$  to a common pool, or to defect and contributes nothing to the pool. The total contribution in a group will be multiplied by a factor  $r$ , where  $1 < r < n$  (for the PGG to be a social dilemma), which is then shared equally among all members of the group, regardless of their strategy.

We obtain (Hauert et al., 2007b)

$$\begin{aligned} \Pi_C(i) &= \sum_{j=0}^{n-1} \frac{\binom{i-1}{j} \binom{N-i}{n-1-j}}{\binom{N-1}{n-1}} \left( \frac{(j+1)rc}{n} - c \right) = \frac{rc}{n} \left( 1 + (i-1) \frac{n-1}{N-1} \right) - c, \\ \Pi_D(i) &= \sum_{j=0}^{n-1} \frac{\binom{i}{j} \binom{N-1-i}{n-1-j}}{\binom{N-1}{n-1}} \frac{jrc}{n} = \frac{rc(n-1)}{n(N-1)} i. \end{aligned}$$

Thus,

$$\delta = \Pi_C(i) - \Pi_D(i) = -c \left( 1 - \frac{r(N-n)}{n(N-1)} \right).$$

## (b) Cost of institutional reward and punishment

To reward a cooperator (respectively, punish a defector), the institution has to pay an amount  $\theta/a$  (resp.,  $\theta/b$ ) so that the cooperator's (defector's) payoff increases (decreases) by  $\theta$ , where  $a, b > 0$  are constants representing the efficiency ratios of providing the corresponding incentive. As we study reward and punishment separately, without losing generality, we set  $a = b = 1$  (Chen et al., 2015; Sigmund et al., 2001). Thus, the key question here is: *what is the optimal value of the individual incentive cost  $\theta$  that ensures a sufficient desired level of cooperation in the population (in the long run) while minimizing the total cost spent by the institution?*

### Deriving the expected cost of providing institutional incentives

We adopt here the finite population dynamics with the Fermi strategy update rule (Traulsen et al., 2006), stating that a player  $A$  with fitness  $f_A$  adopts the strategy of another player  $B$  with fitness  $f_B$  with a probability given by,  $P_{A,B} = \left( 1 + e^{-\beta(f_B - f_A)} \right)^{-1}$ , where  $\beta$  represents the intensity of selection (see details in Section (c)). We compute the expected number of times the population contains  $i$  C players,  $1 \leq i \leq N-1$ . For that, we consider an absorbing Markov chain of  $(N+1)$  states,  $\{S_0, \dots, S_N\}$ , where  $S_i$  represents a population with  $i$  C players.  $S_0$  and  $S_N$  are absorbing states. Let  $U = \{u_{ij}\}_{i,j=1}^{N-1}$  denote the transition matrix between the  $N-1$  transient states,  $\{S_1, \dots, S_{N-1}\}$ . The transition probabilities can be defined as follows, for  $1 \leq i \leq N-1$ :

$$\begin{aligned} u_{i,i\pm j} &= 0 \quad \text{for all } j \geq 2, \\ u_{i,i\pm 1} &= \frac{N-i}{N} \frac{i}{N} \left( 1 + e^{\mp \beta[\Pi_C(i) - \Pi_D(i) + \theta]} \right)^{-1}, \\ u_{i,i} &= 1 - u_{i,i+1} - u_{i,i-1}. \end{aligned} \tag{2.1}$$

The entries  $n_{ij}$  of the so-called fundamental matrix  $\mathcal{N} = (n_{ij})_{i,j=1}^{N-1} = (I - U)^{-1}$  of the absorbing Markov chain gives the expected number of times the population is in the state  $S_j$  if it is started in the transient state  $S_i$  (Kemeny and Snell, 1976). As a mutant can randomly occur either at  $S_0$  or  $S_N$ , the expected number of visits at state  $S_i$  is thus,  $\frac{1}{2}(n_{1i} + n_{N-1,i})$ .

The total cost per generation is

$$\theta_i = \begin{cases} i \times \theta & \text{in the case of institutional reward,} \\ (N - i) \times \theta & \text{in the case of institutional punishment.} \end{cases}$$

Hence, the expected total cost of interference for institutional reward and institutional punishment are respectively

$$E_r(\theta) = \frac{\theta}{2} \sum_{i=1}^{N-1} (n_{1i} + n_{N-1,i})i \quad \text{and} \quad E_p(\theta) = \frac{\theta}{2} \sum_{i=1}^{N-1} (n_{1i} + n_{N-1,i})(N - i). \quad (2.2)$$

### Cooperation frequency

Since the population consists of only two strategies, the fixation probabilities of a C (D) player in a homogeneous population of D (C) players when the interference scheme is carried out are, respectively,

$$\rho_{D,C} = \left( 1 + \sum_{i=1}^{N-1} \prod_{k=1}^i \frac{1 + e^{\beta(\Pi_C(k) - \Pi_D(k) + \theta)}}{1 + e^{-\beta(\Pi_C(k) - \Pi_D(k) + \theta)}} \right)^{-1},$$

$$\rho_{C,D} = \left( 1 + \sum_{i=1}^{N-1} \prod_{k=1}^i \frac{1 + e^{\beta(\Pi_D(k) - \Pi_C(k) - \theta)}}{1 + e^{-\beta(\Pi_D(k) - \Pi_C(k) - \theta)}} \right)^{-1}.$$

Computing the stationary distribution using these fixation probabilities, we obtain the frequency of cooperation (See Section 2.3)

$$\frac{\rho_{D,C}}{\rho_{D,C} + \rho_{C,D}}.$$

Hence, this frequency of cooperation can be maximized by maximizing

$$\max_{\theta} (\rho_{D,C} / \rho_{C,D}). \quad (2.3)$$

The fraction in Equation (2.3) can be simplified as follows (Nowak, 2006a)

$$\begin{aligned} \frac{\rho_{D,C}}{\rho_{C,D}} &= \prod_{k=1}^{N-1} \frac{T^-(k)}{T^+(k)} = \prod_{k=1}^{N-1} \frac{1 + e^{\beta[\Pi_C(k) - \Pi_D(k) + \theta]}}{1 + e^{-\beta[\Pi_C(k) - \Pi_D(k) + \theta]}} \\ &= e^{\beta \sum_{k=1}^{N-1} (\Pi_C(k) - \Pi_D(k) + \theta)} \\ &= e^{\beta(N-1)(\delta + \theta)}. \end{aligned} \quad (2.4)$$

In the above transformation,  $T^-(k)$  and  $T^+(k)$  are the probabilities to increase or decrease the number of C players (i.e.  $k$ ) by one in each time step, respectively.

We consider non-neutral selection, i.e.  $\beta > 0$  (under neutral selection, there is no need to use incentives). Assuming that we desire to obtain at least an  $\omega \in [0, 1]$  fraction of cooperation, i.e.  $\frac{\rho_{D,C}}{\rho_{D,C} + \rho_{C,D}} \geq \omega$ , it follows from Equation (2.4) that

$$\theta \geq \theta_0(\omega) = \frac{1}{(N-1)\beta} \log \left( \frac{\omega}{1-\omega} \right) - \delta. \quad (2.5)$$

Therefore it is guaranteed that if  $\theta \geq \theta_0(\omega)$ , at least an  $\omega$  fraction of cooperation can be expected. From this condition it implies that the lower bound of  $\theta$  monotonically depends on  $\beta$ . Namely, when  $\omega \geq 0.5$ , it increases with  $\beta$  while decreases for  $\omega < 0.5$ .

## Optimization problems

Bringing all ingredients together, we obtain the following cost-optimization problems of institutional incentives in stochastic finite populations

$$\min_{\theta \geq \theta_0(\omega)} E(\theta), \quad (2.6)$$

where  $E$  is either  $E_r$  or  $E_p$ , defined in (2.2), which respectively corresponds to institutional reward and punishment. We show in Supporting Information (SI) that  $\theta \mapsto E(\theta)$  is a smooth function on  $\mathbb{R}$ .

## (c) Methods: Evolutionary Dynamics in Finite Populations

We adopt in our analysis the Evolutionary Game Theory (EGT) methods for finite populations (Imhof et al., 2005; Nowak, 2006a; Nowak et al., 2004). Herein, individuals' payoff represents their *fitness* or social *success*, and evolutionary dynamics is shaped by social learning (Hofbauer and Sigmund, 1998; Sigmund, 2010), whereby the most successful players will tend to be imitated more often by the other players. Here, social learning is modeled using the pairwise comparison rule (Traulsen et al., 2006), that is, a player  $A$  with fitness  $f_A$  adopts the strategy of another player  $B$  with fitness  $f_B$  with probability given by the Fermi function,

$$P_{A,B} = \left(1 + e^{-\beta(f_B - f_A)}\right)^{-1},$$

where  $\beta$  conveniently describes the selection intensity ( $\beta = 0$  represents neutral drift while  $\beta \rightarrow \infty$  represents increasingly deterministic selection).

In the absence of mutations or exploration, the end states of evolution are inevitably monomorphic: once such a state is reached, it cannot be escaped through social learning. We assume that, with a certain mutation probability, an individual switches randomly to a different strategy without imitating another individual. In addition, we assume here the small mutation limit (Fudenberg and Imhof, 2005; Imhof et al., 2005; Nowak et al., 2004). Thus, at most two strategies are present in the population at a time. The evolutionary dynamics can be described by a Markov Chain, where each state represents a homogeneous population and the transition probabilities between any two states are given by the fixation probability of a single mutant (Fudenberg and Imhof, 2005; Imhof et al., 2005; Nowak et al., 2004). The resulting Markov Chain has a stationary distribution, which describes the average time the population spends in an end state. The small mutation limit allows us to obtain an analytical form of the frequency of cooperation (see below). It is noteworthy that although we focus here on the small mutation limit, this approach has been shown to be widely applicable to scenarios which go well beyond the strict limit of very small mutation rates (Domingos et al., 2020; Rand et al., 2013; Sigmund et al., 2010b; Zisis et al., 2015).

The fixation probability that a single mutant  $A$  taking over a whole population with  $(N - 1)$   $B$  players is as follows (see e.g. references for details (Karlin and Taylor, 1975; Nowak et al., 2004; Traulsen et al., 2006))

$$\rho_{B,A} = \left(1 + \sum_{i=1}^{N-1} \prod_{j=1}^i \frac{T^-(j)}{T^+(j)}\right)^{-1},$$

where  $T^\pm(k) = \frac{N-k}{N} \frac{k}{N} \left[1 + e^{\mp\beta[\Pi_A(k) - \Pi_B(k)]}\right]^{-1}$  describes the probability to change the number of  $A$  players by  $\pm$  one in a time step. Specifically, when  $\beta = 0$ ,  $\rho_{B,A} = 1/N$ , representing the transition probability at neural limit.

Considering the set of two strategies  $C$  and  $D$  (see (Fudenberg and Imhof, 2005; Imhof et al., 2005) for the calculation for any number of strategies). Their stationary distribution is given by the normalised eigenvector associated with the eigenvalue 1 of the transposed of a matrix (Fudenberg

$$M = \begin{pmatrix} 1 - \rho_{C,D} & \rho_{C,D} \\ \rho_{D,C} & 1 - \rho_{D,C} \end{pmatrix},$$

which is  $\left\{ \frac{\rho_{D,C}}{\rho_{D,C} + \rho_{C,D}}, \frac{\rho_{C,D}}{\rho_{D,C} + \rho_{C,D}} \right\}$ . The first term is the frequency of cooperation and the second one is that of defection.

### 3. Main results

The present paper provides a rigorous analysis for the expected total cost of providing institutional incentive (2.2) and the associated optimization problem (2.6). In this section, we state our main analytical results, Theorems 3.1, 3.2 and 3.3, and provide numerical simulations to illustrate the analytical results. The proofs of these results, which require a delicate analysis of the cost functions, are presented in SI.

In the following theorems,  $E$  denotes the cost function either for institutional reward,  $E_r$ , or institutional punishment,  $E_p$ , as obtained in (2.2). Also,  $H_N$  denotes the well-known harmonic number

$$H_N := \sum_{j=1}^{N-1} \frac{1}{j}. \tag{3.1}$$

Our first main result provides qualitative properties and asymptotic limits of  $E$ .

**Theorem 3.1** (Qualitative properties and asymptotic limits of total cost functions).

(I) (finite population estimates) The expected total cost of providing incentive satisfies the following estimates for all finite populations of size  $N$

$$\frac{N^2\theta}{2} \left( H_N + \frac{1}{N-1} \right) \leq E(\theta) \leq N(N-1)\theta(H_N + 1). \tag{3.2}$$

(II) (infinite population limit) The expected total cost of providing incentive satisfies the following asymptotic behaviour when the population size  $N$  tends to  $+\infty$

$$\lim_{N \rightarrow +\infty} \frac{E(\theta)}{\frac{N^2\theta}{2}(\ln N + \gamma)} = \begin{cases} 1 + e^{-\beta|\theta-c|} & \text{for DG,} \\ 1 + e^{-\beta|\theta-c|} e^{\beta c \frac{c}{n}} & \text{for PGG,} \end{cases} \tag{3.3}$$

where  $\gamma = 0.5772\dots$  is the Euler-Mascheroni constant.

(III) (weak selection limit) The expected total cost of providing incentive satisfies the following asymptotic limit when the selection strength  $\beta$  tends to 0

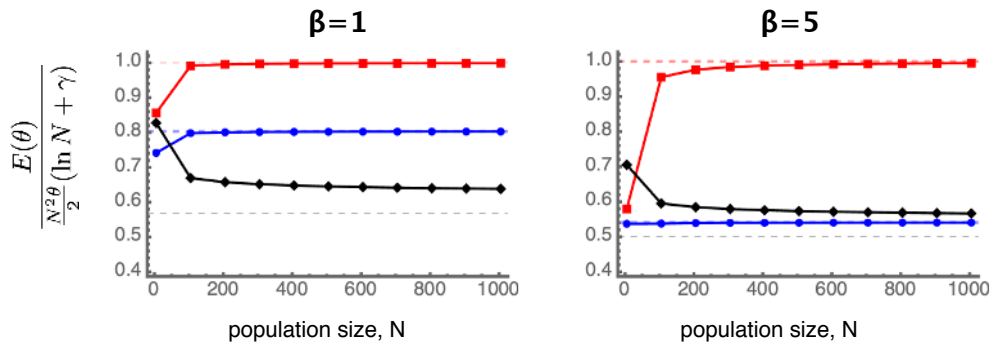
$$\lim_{\beta \rightarrow 0} E(\theta) = N^2\theta H_N. \tag{3.4}$$

(IV) (strong selection limit) The expected total cost of providing incentive satisfies the following asymptotic limit when the selection strength  $\beta$  tends to  $+\infty$

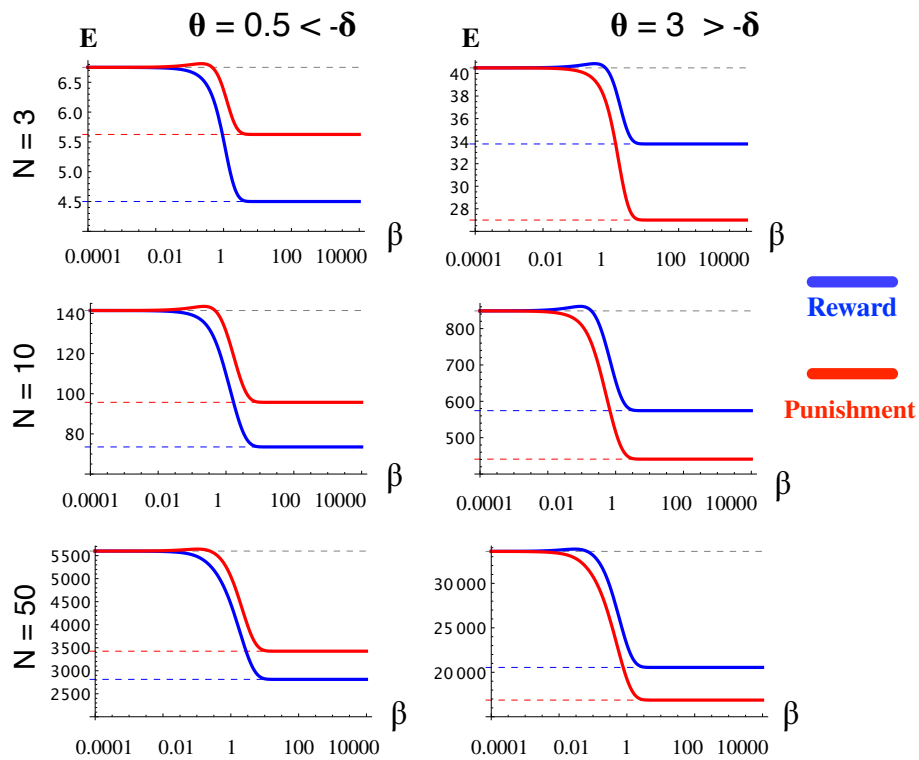
$$\lim_{\beta \rightarrow +\infty} E_r(\theta) = \begin{cases} \frac{N^2\theta}{2} \left( \frac{1}{N-1} + H_N \right) & \text{for } \theta < -\delta, \\ N^2\theta H_N & \text{for } \theta = -\delta, \\ \frac{N^2\theta}{2} (1 + H_N) & \text{for } \theta > -\delta. \end{cases} \tag{3.5}$$

$$\lim_{\beta \rightarrow +\infty} E_p(\theta) = \begin{cases} \frac{N^2\theta}{2} (1 + H_N) & \text{for } \theta < -\delta, \\ N^2\theta H_N & \text{for } \theta = -\delta, \\ \frac{N^2\theta}{2} \left( H_N + \frac{1}{N-1} \right) & \text{for } \theta > -\delta. \end{cases} \tag{3.6}$$

The lower and upper bounds obtained in part (I) of the theorem suggest the total expected cost function  $E$  for both reward and punishment behaves asymptotically in order of  $(N^2 H_N) \times \theta$



**Figure 1. Large population size limit.** We calculate numerically the expected total cost of incentive  $E$  for reward and punishment, varying population size  $N$ , for different values of  $\theta$  and  $\beta$ . The dashed lines represent the corresponding theoretical limiting values obtained in Theorem 3.1 for the large population size limit,  $N \rightarrow +\infty$ . We observe that numerical results are in close accordance with those obtained theoretically. Results are obtained for DG with  $b = 2$ ,  $c = 1$ .



**Figure 2. Weak and strong selection limits.** We calculate numerically the total expected cost of incentive  $E$  for reward and punishment, for varying the intensity of selection, for different values of  $N$  and  $\beta$ . The dashed lines represent the corresponding theoretical limiting values obtained in Theorem 3.1 for weak and strong selection limits. We observe that numerical results are in close accordance with those obtained theoretically. Results are obtained for DG with  $b = 2$ ,  $c = 1$ .

for sufficiently large  $N$ . It is confirmed in part (II), noting that  $H_N \sim \ln N$ . We also show that the



leading asymptotic coefficient of  $E$  depends on the game (i.e., DG or PGG) and its parameters. Hence, it is important to adopt a precise optimal value of  $\theta$  (e.g., obtained by solving the optimization problem (2.6)), as a small increase of this individual incentive cost can lead to significant increase in  $E$ , especially when the population size is large. Figure 1 numerically demonstrates this asymptotic limit.

Parts (III) and (IV) of the theorem provide theoretical estimations of  $E$  under the weak ( $\beta \rightarrow 0$ ) and strong ( $\beta \rightarrow +\infty$ ) selection limits. For the weak selection limit, the expected total costs are the same for reward and punishment, i.e.  $E_r(\theta) = E_p(\theta)$ . For the strong selection limit,  $E_r$  is smaller, equal or greater than  $E_p$  depending on whether  $\theta$  is smaller, equal, or greater than  $-\delta$ . Figure 2 provides numerical validation of the theoretical weak and strong selection asymptotic behaviors of  $E$ , for different population sizes  $N$ . We can observe that, for a given individual incentive cost  $\theta$ , the range of  $E$  increases significantly for larger  $N$ .

Our second main result concerns the optimization problem (2.6). We show that the cost function  $E$  exhibits a phase transition when the selection intensity  $\beta$  varies.

**Theorem 3.2** (Optimization problems and phase transition phenomenon).

(I) (phase transition phenomena and behaviour under the threshold) Define

$$F^* = \begin{cases} \min\{F(u) : P(u) > 0\} & \text{in the reward case,} \\ \min\{\hat{F}(u) : \hat{P}(u) > 0\} & \text{in the punishment case,} \end{cases}$$

where  $P(u)$  and  $F(u)$  as well as  $\hat{P}$  and  $\hat{F}$  are defined in the Supporting Information (See Section 1 and Section 2 there, respectively). There exists a threshold value  $\beta^*$  given by

$$\beta^* = -\frac{F^*}{\delta} > 0,$$

such that  $\theta \mapsto E(\theta)$  is non-decreasing for all  $\beta \leq \beta^*$  and is non-monotonic when  $\beta > \beta^*$ . As a consequence, for  $\beta \leq \beta^*$

$$\min_{\theta \geq \theta_0} E(\theta) = E(\theta_0). \quad (3.7)$$

(II) (behaviour above the threshold value) For  $\beta > \beta^*$ , the number of changes of the sign of  $E'(\theta)$  is at least two for all  $N$  and there exists an  $N_0$  such that the number of changes is exactly two for  $N \leq N_0$ . As a consequence, for  $N \leq N_0$ , there exist  $\theta_1 < \theta_2$  such that for  $\beta > \beta^*$ ,  $E(\theta)$  is increasing when  $\theta < \theta_1$ , decreasing when  $\theta_1 < \theta < \theta_2$  and increasing when  $\theta > \theta_2$ . Thus, for  $N \leq N_0$ ,

$$\min_{\theta \geq \theta_0} E(\theta) = \min\{E(\theta_0), E(\theta_2)\}.$$

The proof of Theorems 3.1 and 3.2 for the case of reward and punishment are given in Section 1 and Section 2 in the SI, respectively. We also provide explicit computations for  $N = 3$  and  $N = 4$  to illustrate these theorems in Section 3 in the SI. Based on numerical simulations, we conjecture that the requirement that  $N \leq N_0$  could be removed and Theorem 3.2 is true for all finite  $N$ . In SI (Figure S2), using numerical calculation we have shown that  $N_0 = 100$  satisfies the conjecture, ensuring the validity of the numerical examples below. Theorem 3.2 gives rise to the following algorithm to determine the optimal value  $\theta^*$  for  $N \leq N_0$ .

**Algorithm 3.1** (Finding optimal cost of incentive  $\theta^*$ ).

**Inputs:** i)  $N \leq N_0$ : population size, ii)  $\beta$ : intensity of selection, iii) game and parameters: PD ( $c$  and  $b$ ) or PGG ( $c$ ,  $r$  and  $n$ ), iv)  $\omega$ : minimum desired cooperation level.

- (1) Compute  $\delta \left\{ \begin{array}{l} \text{in PD: } \delta = -(c + \frac{b}{N-1}); \\ \text{in PGG: } \delta = -c \left(1 - \frac{r(N-n)}{n(N-1)}\right) \end{array} \right\}$ .
- (2) Compute  $\theta_0 = \frac{1}{(N-1)\beta} \log\left(\frac{\omega}{1-\omega}\right) - \delta$ ;

(3) Compute

$$F^* = \begin{cases} \min\{F(u) : P(u) > 0\} & \text{in the reward case,} \\ \min\{\hat{F}(u) : \hat{P}(u) > 0\} & \text{in the punishment case,} \end{cases}$$

where  $P(u)$  and  $F(u)$ , as well as  $\hat{P}$  and  $\hat{F}$  are defined in the Supporting Information.

(4) Compute  $\beta^* = -\frac{F^*}{\delta}$ .

(5) If  $\beta \leq \beta^*$ :

$$\theta^* = \theta_0, \quad \min E(\theta) = E(\theta_0).$$

(6) Otherwise (i.e. if  $\beta > \beta^*$ )

(a) Compute  $u_2$  that is the largest root of the equation  $F(u) + \beta\delta = 0$  for the reward case or that of  $\hat{F}(u) + \beta\delta = 0$  for the punishment case.

(b) Compute  $\theta_2 = \frac{\log u_2}{\beta} - \delta$ .

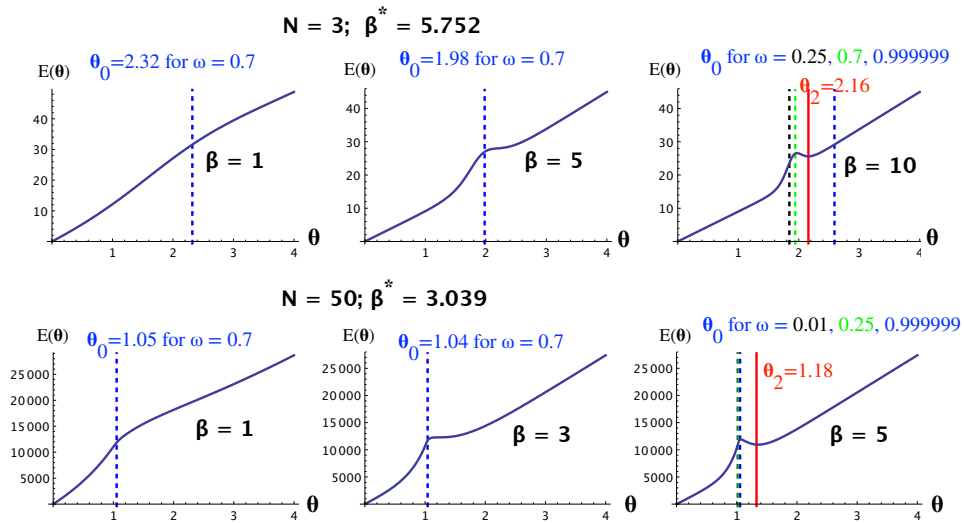
• If  $\theta_2 \leq \theta_0$ :  $\theta^* = \theta_0$ ,  $\min E(\theta) = E(\theta_0)$ ;

• Otherwise (if  $\theta_2 > \theta_0$ ):

– If  $E(\theta_0) \leq E(\theta_2)$ :  $\theta^* = \theta_0$ ,  $\min E(\theta) = E(\theta_0)$ ;

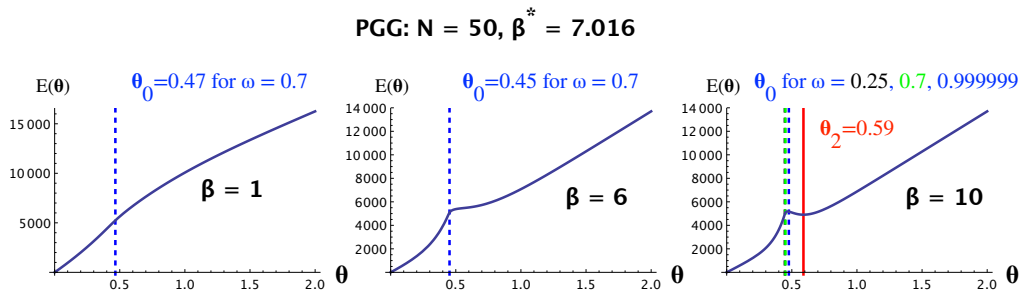
– if  $E(\theta_2) < E(\theta_0)$ :  $\theta^* = \theta_2$ ,  $\min E(\theta) = E(\theta_2)$ .

**Output:**  $\theta^*$  and  $E(\theta^*)$ .



**Figure 3.** Using Algorithm 3.1 to find optimal  $\theta$  that minimizes  $E(\theta)$  (for institutional reward) while ensuring a minimum level of cooperation  $\omega$ . We use as examples a small population size ( $N = 3$ , top row) and a larger one ( $N = 50$ , bottom row), for DG ( $b = 1.8$ ,  $c = 1$ ).

To illustrate Theorem 3.2 and Algorithm 3.1, we focus on the case of reward. Figure 3 shows the cost function  $E_r$  as a function of  $\theta$ , for different values of  $N$ ,  $\beta$  and  $\omega$  for illustrating the phase transition when varying  $\beta$ , in a DG. We can see that in all cases, these numerical observations are in close accordance with theoretical results. For example, with  $N = 3$  (see top row), we found  $\beta^* = f^*/\delta = 10.9291/1.9 = 5.752$ . For  $\beta < \beta^*$ ,  $E(\theta)$  are increasing functions of  $\theta$ . Thus, the optimal cost of incentive  $\theta^* = \theta_0$ , for a given required minimum level of cooperation  $\omega$ . For example, with  $N = 3$ , for  $\beta = 1$  to ensure at least 70% of cooperation ( $\omega = 0.7$ ), then  $\theta^* = \theta_0 = 2.32$ . When  $\beta \geq \beta^*$  one needs to compare  $E(\theta_0)$  and  $E(\theta_2)$ . For example, with  $N = 3$ ,  $\beta = 10$ : for  $\omega = 0.25$  (black dashed



**Figure 4.** Using Algorithm 3.1 to find optimal  $\theta$  that minimizes  $E(\theta)$  while ensuring a minimum level of cooperation  $\omega$ , for PGG ( $r = 3$ ,  $n = 5$ ,  $c = 1$ ) with  $N = 50$ . Similar observations to those in DG, are obtained.

line), then  $E(\theta_0) = 23.602 < 25.6124 = EC(\theta_2)$ , so  $\theta^* = \theta_0 = 1.845$ ; for  $\omega = 0.7$  (green dashed line), then  $E(\theta_0) = 26.446 > 25.6124 = EC(\theta_2)$ , so  $\theta^* = \theta_2 = 2.16$  (red solid line); for  $\omega = 0.999999$  (blue dashed line), since  $\theta_2 < \theta_0$ ,  $\theta^* = \theta_0 = 2.59078$ .

Similarly, with a larger population size ( $N = 50$ , see Figure 1 in the SI, bottom row), we obtained  $\beta^* = 3.15/1.03673 = 3.039$ . In general, similar observations are obtained as in case of a small population size  $N = 3$ . Except that when  $N$  is large, the values of  $\theta_0$  for different non-extreme values of minimum required cooperation  $\omega$  (say,  $\omega \in (0.01, 0.99)$ ) is very small (given the log scale of  $\omega/(1 - \omega)$  in the formula of  $\omega_0$ ). This value is also smaller than  $\theta_0$ , with a cost  $E(\theta_0) > E(\theta_2)$ , making  $\theta_2$  the optimal cost of incentive. Similar results are obtained for PGG (see Figure 4). When  $\omega$  is extremely high (i.e. greater than  $1 - 10^{-k}$ , for a large  $k$ ) (we don't look at extremely low value since we would like to ensure at least a sufficient level of cooperation), then we can also see other scenarios where the optimal cost is  $\theta_0$  (see Figure 1 in the SI, bottom row). We thus can observe that for  $\omega \in (0.01, 0.99)$ , for sufficiently large population size  $N$  and large enough  $\beta$  ( $\beta > \beta^* + \text{a bit more}$ ), then the optimal value of  $\omega$  is always  $\theta_2$ . Otherwise,  $\theta_0$  is the optimal cost.

Our last result provides a comparison of the expected total costs for providing institutional reward and punishment, for different individual incentive cost  $\theta$ .

**Theorem 3.3** (reward vs punishment costs). *The difference between the expected total costs of reward and punishment is given by*

$$(E_r - E_p)(\theta) = \begin{cases} < 0, & \text{for } \theta < -\delta, \\ = 0, & \text{for } \theta = -\delta, \\ > 0, & \text{for } \theta > -\delta. \end{cases} \quad (3.8)$$

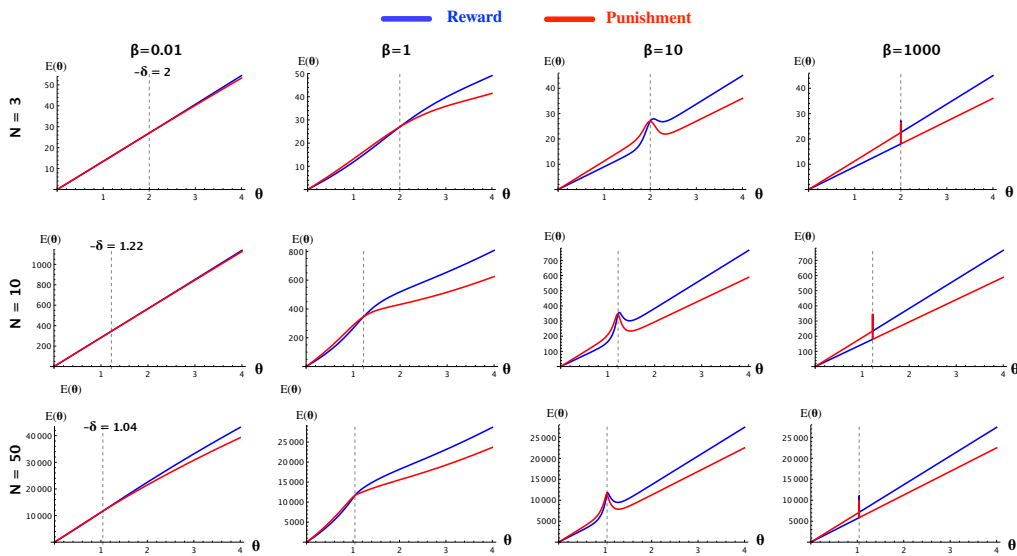
As a consequence, when  $\beta \leq \min\{\beta_r^*, \beta_p^*\}$  we have

$$E_r^* = E_r(\theta_0), \quad E_p^* = E_p(\theta_0).$$

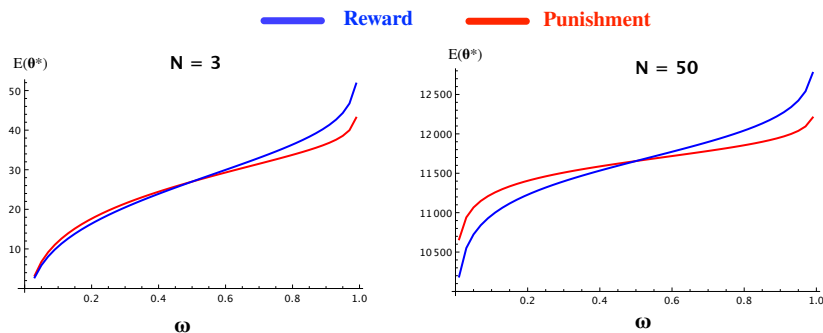
In this case,

$$(E_r^* - E_p^*) = E_r(\theta_0) - E_p(\theta_0) = \begin{cases} < 0 & \text{for } \omega < 0.5, \\ = 0 & \text{for } \omega = 0.5, \\ > 0 & \text{for } \omega > 0.5. \end{cases} \quad (3.9)$$

The proof of Theorem 3.4 is given in Section 3 in the SI. Numerical calculation in Figure 5 shows the expected total costs for reward and punishment (DG), for varying  $\theta$ . We observe that reward is less costly than punishment ( $E_r < E_p$ ) for  $\theta < -\delta$  and vice versa when  $\theta > -\delta$ . It is exactly as shown analytically in Theorem 3.3. This analytical result is confirmed here for different population size  $N$  and intensity of selection  $\beta$ . Figure 6 also confirms the second part of



**Figure 5.** Compare the total costs  $E$  for reward and punishment as a function of  $\theta$ , for different values of  $N$  and  $\beta$ . Reward is less costly than punishment ( $E_r < E_p$ ) for small  $\theta$  and vice versa otherwise. The threshold of  $\theta$  for this change was obtained analytically (see Theorem 1), which is exactly equal to  $-\delta$ . Results are obtained for DG with  $b = 2$ ,  $c = 1$ .



**Figure 6.** Compare the total costs  $E$  for reward and punishment at the optimal value  $\theta^*$  (obtained using Algorithm 3.1), for varying the minimum required level of cooperation,  $\omega$ . Reward is more cost efficient for small  $\omega$ , while punishment is more cost efficient when  $\omega$  is larger. In both cases, the threshold is around  $\omega = 0.5$ . Other parameters:  $\beta = 1$ , DG with  $b = 2$ ,  $c = 1$ .

the theorem, where for small  $\beta$ , if one can choose the type of incentive to use, either reward or punishment, then the former can provide a lower cost when requiring less than 50% cooperation at minimum and the later otherwise. This is in line with previous work showing that reward mechanisms work very well to promote cooperation in environments in which it is rare, while punishment mechanisms are better at maintaining high levels of cooperation (see e.g., (Chen et al., 2015; Sasaki et al., 2012; Wang et al., 2019)).

## 4. Discussion

Institutional incentives such as punishment and reward provide an effective tool for promoting the evolution of cooperation in social dilemmas. Both theoretical and experimental analysis

has been made (Baldassarri and Grossman, 2011; Bardhan, 2005; Dong et al., 2019; García and Traulsen, 2019; Gülerk et al., 2006; Sasaki et al., 2012; Wu et al., 2014). However, past research usually ignores the question of how institutions' overall spending, i.e. the total cost of providing these incentives, can be minimized, while at the same time guaranteeing a minimum desired level of cooperation over time. Answering this question allows one to estimate exactly how incentives should be provided, that is how much to reward a cooperator and how severely to punish a wrongdoer. Existing works that consider this question usually omit the stochastic effects that drive population dynamics, namely, when the intensity of selection varies.

Resorting to a stochastic evolutionary game approach for finite, well-mixed populations, we have provided theoretical results for the optimal cost of incentives that ensure a desired level of cooperation while minimizing the total budget, for a given intensity of selection,  $\beta$ . We show that this cost strongly depends on the value of  $\beta$ , due to the existence of a phase transition in the cost functions when  $\beta$  varies. This behavior is missing in works that consider a deterministic evolutionary approach (Wang et al., 2019). The intensity of selection plays an important role in evolutionary processes. Its value differs depending on the payoff structure (i.e., scaling game payoff matrix by a factor is equivalent to dividing  $\beta$  by that factor) and is usually found to be specific for a given population, which can be estimated through behavioral experiments (Domingos et al., 2020; Rand et al., 2013; Traulsen et al., 2010; Zisis et al., 2015). Thus, our analysis provides a way to calculate the optimal incentive cost for a given population and game payoff matrix at hand.

As of theoretical importance, we characterized asymptotic behaviors of the total cost functions for both reward and punishment (namely, in the limits of large population, weak selection and strong selection) and compared these functions for the two types of incentive. We show that punishment is always more costly for a small (individual) incentive cost ( $\theta$ ) but less so when this cost is above a certain threshold. We provided an exact formula for this threshold. This result provides insights into the choice of which type of incentives to use.

In the context of institutional incentives modelling, a crucial issue is the question of how to maintain the budget of incentives providing (Hilbe et al., 2014; Sigmund et al., 2010b). The problem of who pays or contributes to the budget is a social dilemma itself, and how to escape this dilemma is critical research question. In this work we focus on the question of how to optimize the budget used for provided incentives.

There are several simplifications made for the theoretical analysis to be possible. First, in order to derive analytical formula for the frequency of cooperation, we assumed the small mutation limit. Despite the simplified assumption, this small mutation limit approach has been shown to be widely applicable to scenarios which go well beyond the strict limit of very small mutation rates (Rand et al., 2013; Sigmund et al., 2010b; Zisis et al., 2015). Relaxing this assumption would make the derivation of a close form for the frequency of cooperation intractable.

Second, we focused in this paper on two important cooperation dilemmas, the DG and the PGG. They have in common a useful property that the difference in (average) payoff between a cooperator and a defector,  $\delta = \Pi_C(i) - \Pi_D(i)$ , does not depend on  $i$ , the number of cooperators in the population. This property allows us to simplify the fundamental matrix to a tridiagonal form and apply techniques matrix analysis to obtain a close form of its inverse matrix (see SI). In games with more complex payoff matrices such as the Prisoner's dilemma in its general form and the collective risk game (Santos and Pacheco, 2011), the difference  $\delta$  depends on  $i$  and our technique in this paper can not be directly applied. We might consider other approaches to approximate the inverse matrix exploiting its block structure.

**Data Accessibility.** The article contains supporting information.

**Authors' Contributions.** MHD and TAH designed the researched, performed the research and wrote the paper. All authors gave final approval for publication and agree to be held accountable for the work performed therein

**Competing Interests.** We declare we have no competing interests.

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