Supplementary Information: Punishment Induces Secondary Cooperation within Structured Populations Facing Social Dilemmas

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Contents

1 Stochastic dynamics of higher-order interactions in finite populations

We consider a finite population system consisting of Z players who participate simultaneously in M distinct games. Each game may involve pairwise (low-order) or multi-player (higher-order) interactions. Each player adopts a strategy from a finite set $S = \{S_1, S_2, \ldots, S_N\}$. Let $X_k \in \mathbb{N}$ represent the number of players choosing strategy S_k, with the constraint $\sum_{i=1}^{N} X_i = Z$. To model these interactions, we consider the hypergraph $\mathcal{H}(\mathcal{V}, \mathcal{E})$, where the vertex set $\mathcal{V}$, with $|\mathcal{V}| = Z$, represents the Z players, and the hyperedge set $\mathcal{E}$, with $|\mathcal{E}| = M$ corresponds to the M games. Each hyperedge e_g, for $g \in \{1, \ldots, M\}$, specifies a distinct game involving two or more participants. And the size of each hyperedge e_g is $q_g = |e_g| = \sum_{i=1}^{Z} b_{ig}$, which captures the number of participants in the game g. This hypergraph structure is encoded by a $Z \times M$ incidence matrix $\mathcal{B} = (b_{ig})$, where $b_{ig} = 1$ if the player i participates in the game g, and $b_{ig} = 0$ otherwise. The hyperdegree of a player i is defined as $k_i = \sum_{g=1}^{M} b_{ig}$, representing the number of games that the player joins. Accordingly, the average hyperdegree in the population is given by $\langle k \rangle = \frac{1}{Z} \sum_{i=1}^{Z} k_i$.

Specifically, in contexts characterized by frequent interactions among individuals, cumulative payoffs depend predominantly on the frequency distribution of strategies within the population. For instance, considering a well-mixed population composed of j cooperators and $N - j$ defectors in social dilemmas, the cumulative payoffs for cooperators (π_C) and defectors (π_D) are given respectively by

$$\pi_C = (j-1)R + (N-j)S \text{ and } \pi_D = jT + (N-j-1)P,$$

where $R,\ S,\ T$, and P are the standard payoff parameters defining the underlying game dynamics [1, 2]. However, in scenarios with higher-order interactions, cumulative payoffs for individuals in such high-order structures must incorporate contributions from group interactions beyond pairs, considering the frequency and size of interaction groups (hyperedges). Thus, under higher-order interactions, cumulative payoffs become explicitly dependent on the proportion and composition of hyperedges, and can be generalized as

$$\pi_{S_i} = \sum_{k} \rho_k \sum_{e_g \in \mathcal{G}_k} \Pi_{S_i}(e_g),$$

where ρ_k denotes the proportion of hyperedges of order k, $\mathcal{G}_k$ represents the set of all hyperedges of size k involving the focal player, and $\Pi_{S_i}(e_g)$ denotes the payoff of the focal player when interacting within the hyperedge e_g.

1.1 Evolutionary process Modeling

At each time step, an individual is randomly selected from the population as the focal player. Subsequently, another individual is randomly chosen from among the neighbors of the focal player in a hypergraph, where connections are defined by hyperedges of varying sizes. During each interaction, the focal player's payoff depends on its own strategy as well as the strategies of the other participants in the relevant hyperedge.

Following this interaction, the focal player updates its strategy according to the following rule. With probability μ, the focal player's current strategy, denoted by S_i, undergoes a mutation process, whereby it is replaced by an alternative strategy selected randomly from the set of all available strategies. With probability $1-\mu$, the focal player attempts to imitate the neighbor's strategy S_j, adopting it with the probability given by the Fermi function:

$$p = \frac{1}{1+\exp\left[-\omega\left(\pi_{S_j}-\pi_{S_i}\right)\right]}.$$

Here, π_{S_i} and π_{S_j} represent the cumulative payoffs obtained by the focal player and the selected neighbor, respectively, while $\omega \geq 0$ characterizes the intensity of selection. Under strong selection ($\omega \to \infty$), the imitation probability p converges to a deterministic outcome: it becomes $p=1$ or $p=0$, depending on the sign of the payoff difference. In contrast, under weak selection ($\omega \to 0$), the probability of imitation converges to $1/2$, reflecting an unbiased and random decision.

We define $T_i^{\pm}(\mathbf{X})$ as the probability that the number of players employing strategy S_i increases $(+)$ or decreases $(-)$ by one when the system is in state $\mathbf{X}=(X_1, X_2, \ldots, X_N)$. It should be noted that, as previously defined, each X_i denotes the number of individuals who select the strategy S_i. Specifically, the probability of an increase in the number of players adopting S_i is given by the sum

$$T_i^{+}(\mathbf{X}) = \sum_{j,\, j\neq i} T_{ij}^{+}(\mathbf{X}),$$

where $T_{ij}^{+}(\mathbf{X})$ denotes the probability that the number of players adopting S_i increases by one while that of players adopting S_j decreases by one. This probability is expressed as

$$T_{ij}^{+}(\mathbf{X}) = (1-\mu)\frac{1}{1+\exp\left[-\omega\left(\pi_{S_i}-\pi_{S_j}\right)\right]}\frac{X_i}{Z}\frac{X_j}{Z} + \mu\frac{X_j}{(N-1)Z}.$$

Similarly, the probability that the number of players adopting S_i decreases by one is given by

$$T_i^{-}(\mathbf{X}) = \sum_{j,\, j\neq i} T_{ij}^{-}(\mathbf{X}),$$

with

$$T_{ij}^{-}(\mathbf{X}) = (1-\mu)\frac{1}{1+\exp\left[\omega\left(\pi_{S_i}-\pi_{S_j}\right)\right]}\frac{X_i}{Z}\frac{X_j}{Z}+\mu\frac{X_i}{(N-1)Z}.$$

Indeed, the probability density function, $P^{\tau}(\mathbf{X})$, i.e. the prevalence of each state at time τ, evolves in time according to the master equation [3]

$$\begin{aligned}
&P^{\tau+1}(\mathbf{X})-P^{\tau}(\mathbf{X})\\
=&\sum_{i}\sum_{j,\,j\neq i}P^{\tau}(X_1,\ldots,X_i-1,\ldots,X_j+1,\ldots,X_N)T_{ij}^{+}(X_1,\ldots,X_i-1,\ldots,X_j+1,\ldots,X_N)\\
+&\sum_{i}\sum_{j,\,j\neq i}P^{\tau}(X_1,\ldots,X_i+1,\ldots,X_j-1,\ldots,X_N)T_{ij}^{-}(X_1,\ldots,X_i+1,\ldots,X_j-1,\ldots,X_N)\\
-&\sum_{i}\sum_{j,\,j\neq i}P^{\tau}(\mathbf{X})T_{ij}^{-}(\mathbf{X})-\sum_{i}\sum_{j,\,j\neq i}P^{\tau}(\mathbf{X})T_{ij}^{+}(\mathbf{X})
\end{aligned} \tag{1}$$

Introducing the notation $x_i=\frac{X_i}{Z}$, $t=\frac{\tau}{Z}$ and the probability density $\rho(\mathbf{x},t)=ZP^{\tau}(\mathbf{X})$, we have

$$\begin{aligned}
&\rho(\mathbf{x},t+Z^{-1})-\rho(\mathbf{x},t)\\
=&\sum_{i}\sum_{j,\,j\neq i}\rho(x_1,\ldots,x_i-Z^{-1},\ldots,x_j+Z^{-1},\ldots,x_N,t)T_{ij}^{+}(x_1,\ldots,x_i-Z^{-1},\ldots,x_j+Z^{-1},\ldots,x_N)\\
+&\sum_{i}\sum_{j,\,j\neq i}\rho(x_1,\ldots,x_i+Z^{-1},\ldots,x_j-Z^{-1},\ldots,x_N,t)T_{ij}^{+}(x_1,\ldots,x_i+Z^{-1},\ldots,x_j-Z^{-1},\ldots,x_N)\\
-&\sum_{i}\sum_{j,\,j\neq i}\rho(\mathbf{x},t)T_{ij}^{-}(\mathbf{x})-\sum_{i}\sum_{j,\,j\neq i}\rho(\mathbf{x},t)T_{ij}^{+}(\mathbf{x}).
\end{aligned}$$

Here $\mathbf{x}=(x_1,x_2,\ldots,x_N)$ and $\sum_{i=1}^{N}x_i=1$. For $Z\gg 1$, applying Taylor expansion to the probability densities and the transition probabilities yields

$$\frac{\mathrm{d}\rho(\mathbf{x},t)}{\mathrm{d}t}=-\sum_{i=1}^{N}\frac{\partial}{\partial x_i}\left(A_i(\mathbf{x})\rho(\mathbf{x},t)\right)+\frac{1}{2}\sum_{i,j=1}^{N}\frac{\partial^2}{\partial x_i\partial x_j}\left(B_{ij}(\mathbf{x})\rho(\mathbf{x},t)\right). \tag{2}$$

The drift vector $A(\mathbf{x})$, which characterizes the deterministic component of evolutionary dynamics, is defined as

$$A_i(\mathbf{x})=\sum_{j,\,j\neq i}\left(T_{ij}^{+}(\mathbf{x})-T_{ij}^{-}(\mathbf{x})\right). \tag{3}$$

Correspondingly, the diffusion matrix $B(\mathbf{x})$, which captures the stochastic fluctuations inherent in evolutionary dynamics, is expressed as

$$B_{ij}(\mathbf{x})=\frac{1}{Z}\left[\delta_{ij}\sum_{k}\left(T_{ik}^{+}(\mathbf{x})+T_{ik}^{-}(\mathbf{x})\right)-(T_{ij}+T_{ji})\right]. \tag{4}$$

Here, the Kronecker delta δ_{ij} denotes the identity indicator (with $\delta_{ij}=1$ if $i=j$, and 0 otherwise). For large but finite Z, Eq. (2) has the form of a Fokker-Planck equation, which has an equivalent Langevin equation

$$\dot{\mathbf{x}} = A(\mathbf{x}) + \Sigma(\mathbf{x})\xi$$

where $B = \Sigma\Sigma^T$ and ξ is Gaussian noise. In fact, this is a coupled system, and the evolution equations can be described by the first $N-1$ equations.

1.2 Applications in three strategies

In this subsection, we investigate evolutionary dynamics on random hypergraphs consisting of both pairwise and three-player interactions. Specifically, we consider hypergraphs of size Z, comprising n_1 two-player interactions and n_2 three-player group interactions. The hypergraph structure is characterized by the average hyperdegree $\langle k \rangle = \frac{1}{Z}\sum_{i=1}^{Z} k_i$, indicating the average number of hyperedges each node participates in. Consequently, a randomly chosen focal player engages in a three-player interaction with probability $\delta = \frac{n_2}{Z\langle k \rangle}$, and participates in a pairwise interaction with probability $1-\delta$. Here, the total number of interactions satisfies $Z\langle k \rangle = n_1 + n_2$, with $n_1 = \sum_i \sum_{g|q_g=2} b_{ig}$ representing the sum of elements of the incidence matrix restricted to hyperedges of size two, and $n_2 = \sum_i \sum_{g|q_g=3} b_{ig}$ is hyperedges of size three [4].

In order to extend the traditional social dilemma game framework, we incorporate peer punishment as an additional strategic dimension. Thus, players may select among three strategies: cooperation (C), defection (D), and peer punishment (P). A player adopting the punishment strategy incurs a personal cost $\alpha > 0$ each time they punish a defector. In contract, the punished defective player is charged with a fine $\beta > 0$.

At each time step, a randomly selected focal player participates either in a 3-person (namely 3-game) or a 2-person (2-game) interaction, according to the probabilities defined above. For the pairwise interaction scenario, the payoff matrix is explicitly given by:

$$\begin{array}{c|ccc} & C & D & P \\ \hline C & 1 & S & 1 \\ D & T & 0 & T-\beta \\ P & 1 & S-\alpha & 1 \end{array} . \tag{5}$$

In this matrix, the parameters S and T represent the classic payoff structures for social dilemmas. Specifically, the Snowdrift game corresponds to payoff rankings $T > 1 > S > 0$, the Stag-Hunt game to $1 > T > 0 > S$, and the Prisoner's Dilemma to $T > 1 > 0 > S$ [1].

For three-person interactions, the payoff structure expands due to multiple co-players, denoted as

$$
\begin{array}{c|cccccc}
 & CC & CD & CP & DD & DP & PP \\
\hline
C & 1 & G & 1 & S & G & 1 \\
D & T & W & T-\beta & 0 & W-\beta & T-2\beta \\
P & 1 & G-\alpha & 1 & S-2\alpha & G-\alpha & 1
\end{array}. \tag{6}
$$

We consider a finite population of size Z, partitioned into three discrete strategic types: cooperators (C, $X_C = i$), defectors (D, $X_D = j$) and peer punishers (P, $X_P = Z - i - j$). The relative frequencies of these strategies are defined as

$$x_C = \frac{i}{Z},\ x_D = \frac{j}{Z},\ \text{and}\ x_P = \frac{Z-i-j}{Z} = 1 - x_C - x_P.$$

The state of the system is represented by the vector $\boldsymbol{X} = (i,\ j,\ Z-i-j)$ where $i,\ j \in \mathbb{N}$, with the transition $\boldsymbol{X} \to \boldsymbol{X}' = (i+\delta_1,\ j+\delta_2,\ Z-i-j+\delta_3)$ following a death-birth process: components exchange unit mass via vectors

$$(\delta_1,\ \delta_2,\ \delta_3) \in \{(\pm 1,\ \mp 1,\ 0),\ (\pm 1,\ 0,\ \mp 1),\ (0,\ \pm 1,\ \mp 1)\},$$

yielding six transitions per interior state. Then the cumulative payoffs for cooperators (π_C), defectors (π_D) and punishers (π_P), respectively, are given respectively by

$$\pi_C = \langle k\rangle \left\{(1-\delta)\left(x_C + x_D S + x_P\right) + \delta\left[(x_C + x_P)^2 + 2(x_C+x_P)x_D G + x_D^2 S\right]\right\}, \tag{7a}$$

$$\begin{aligned}\pi_D &= \delta\langle k\rangle\left[(x_C+x_P)^2 T + 2(x_C+x_P)x_D W - 2x_P\beta\right] \\ &\quad + (1-\delta)\langle k\rangle\left[x_C T + x_P\left(T-\beta\right)\right],\end{aligned} \tag{7b}$$

$$\begin{aligned}\pi_P &= \delta\langle k\rangle\left[(x_C+x_P)^2 + 2(x_C+x_P)x_D G + x_D^2 S - 2x_D\alpha\right] \\ &\quad + (1-\delta)\langle k\rangle\left[x_C + x_D\left(S-\alpha\right) + x_P\right].\end{aligned} \tag{7c}$$

Thus, as described in subsection 1.1, we have

$$\begin{aligned}
T_{13}^{+}(\boldsymbol{X}) &= T_{P\to C}(\boldsymbol{X}) = (1-\mu)\frac{1}{1+\exp\left[-\omega\left(\pi_C - \pi_P\right)\right]}x_C x_P + \mu\frac{x_P}{N-1}, \\
T_{12}^{+}(\boldsymbol{X}) &= T_{D\to C}(\boldsymbol{X}) = (1-\mu)\frac{1}{1+\exp\left[-\omega\left(\pi_C - \pi_D\right)\right]}x_C x_D + \mu\frac{x_D}{N-1}, \\
T_{23}^{+}(\boldsymbol{X}) &= T_{P\to D}(\boldsymbol{X}) = (1-\mu)\frac{1}{1+\exp\left[-\omega\left(\pi_D - \pi_P\right)\right]}x_D x_P + \mu\frac{x_P}{N-1}.
\end{aligned}$$

In a similar manner, expressions for T_{12}^{-}, T_{13}^{-} and T_{23}^{-} can be obtained. The drift vector A and diffusion matrix B in Eq. (2) are specifically defined as

$$A = \begin{pmatrix} (1-\mu)\left[x_C x_P \tanh\frac{\omega}{2}(\pi_C - \pi_P) + x_C x_D \tanh\frac{\omega}{2}(\pi_C - \pi_D)\right] + \frac{\mu}{2}\left(1 - 3x_C\right) \\ (1-\mu)\left[x_D x_P \tanh\frac{\omega}{2}(\pi_D - \pi_P) - x_C x_D \tanh\frac{\omega}{2}(\pi_C - \pi_D)\right] + \frac{\mu}{2}\left(1 - 3x_D\right) \\ (1-\mu)\left[-x_C x_P \tanh\frac{\omega}{2}(\pi_C - \pi_P) - x_D x_P \tanh\frac{\omega}{2}(\pi_D - \pi_P)\right] + \frac{\mu}{2}\left(1 - 3x_P\right) \end{pmatrix},$$

and

$$B = \frac{(1-\mu)}{Z}\begin{pmatrix} x_C(1-x_C) & -x_C x_D & -x_C x_P \\ -x_C x_D & x_D(1-x_D) & -x_D x_P \\ -x_C x_P & -x_D x_P & x_P(1-x_P) \end{pmatrix} + \frac{\mu}{2Z}\begin{pmatrix} 1+x_C & x_C+x_D & x_C+x_P \\ x_C+x_D & 1+x_D & x_D+x_P \\ x_C+x_P & x_D+x_P & 1+x_P \end{pmatrix}.$$

Taking the limit $Z \to \infty$, the diffusion term vanishes as $\mathcal{O}(Z^{-1})$, giving deterministic dynamics

$$\dot{x}_C = (1-\mu)\left[x_C x_P \tanh\frac{\omega}{2}(\pi_C - \pi_P) + x_C x_D \tanh\frac{\omega}{2}(\pi_C - \pi_D)\right] + \frac{\mu}{2}\left(1 - 3x_C\right), \tag{8a}$$

$$\dot{x}_D = (1-\mu)\left[x_D x_P \tanh\frac{\omega}{2}(\pi_D - \pi_P) - x_C x_D \tanh\frac{\omega}{2}(\pi_C - \pi_D)\right] + \frac{\mu}{2}\left(1 - 3x_D\right), \tag{8b}$$

$$\dot{x}_P = (1-\mu)\left[-x_C x_P \tanh\frac{\omega}{2}(\pi_C - \pi_P) - x_D x_P \tanh\frac{\omega}{2}(\pi_D - \pi_P)\right] + \frac{\mu}{2}\left(1 - 3x_P\right). \tag{8c}$$

1.3 Stationary Distribution Analysis

We still consider Z players who simultaneously engage in M games, with each player selecting a strategy from a set comprising N distinct strategies. The stationary distribution $\bar{P}$ can be derived by setting the left-hand side of Eq. (1) to zero, thus the equation reduces to an eigenvector problem. Specifically, this involves solving the eigenvalue equation $\mathcal{T}^\top \bar{P} = \bar{P}$, where $\mathcal{T}$ is the stochastic matrix that encodes the permissible state transitions. The state space $\mathcal{S}$ consists of configurations $\mathbf{X} = (X_1,\ X_2, \ldots X_N)\,,\ \sum_{i=1}^{N} X_i = Z$. Consequently, the cardinality of this state space is $|\mathcal{S}| = \binom{Z+N-1}{N-1}$.

Each off-diagonal element $\mathcal{T}_{\mathbf{X}\to\mathbf{X}'}$ corresponds to transitions between adjacent states $\mathbf{X}' = \mathbf{X} + \boldsymbol{\delta}$, where the vector $\boldsymbol{\delta} = (\delta_1,\ \ldots,\ \delta_N)$ contains exactly two nonzero entries, specifically $\delta_i = +1$ and $\delta_j = -1$, representing a shift of one individual from strategy S_j to strategy S_i. The corresponding transition probability from state $\mathbf{X}$ to $\mathbf{X}'$ is determined by the given rule

$$\mathcal{T}_{\mathbf{X}\to\mathbf{X}'} = T_{ij}^{+}(\mathbf{X}) = (1-\mu)\frac{1}{1+\exp\left[-\omega\left(\pi_{S_i} - \pi_{S_j}\right)\right]}\frac{X_i}{Z}\frac{X_j}{Z} + \mu\frac{X_j}{(N-1)Z}.$$

It is evident that diagonal elements of the matrix $\mathcal{T}$, denoted by $\mathcal{T}_{\mathbf{X}\to\mathbf{X}}$, satisfy the condition $\mathcal{T}_{\mathbf{X}\to\mathbf{X}} = 1 - \sum_{\mathbf{X}'\neq\mathbf{X}} \mathcal{T}_{\mathbf{X}\to\mathbf{X}'}$. For example, in the case of $Z = 2$ and $N = 3$, the system exhibits six distinct states, each represented by an ordered triplet $(i,\ j,\ k)$ satisfying $i + j + k = 2$.

Here, the non-negative integers $i,\ j$, and k correspond to the number of individuals adopting cooperation (C), defection (D), and punishment (P) strategies, respectively. The corresponding state transition matrix is given by

	$(0,\ 0,\ 2)$	$(0,\ 1,\ 1)$	$(0,\ 2,\ 0)$	$(1,\ 1,\ 0)$	$(1,\ 0,\ 1)$	$(2,\ 0,\ 0)$
$(0,\ 0,\ 2)$	$1-\mu$	$\frac{\mu}{2}$	0	0	$\frac{\mu}{2}$	0
$(0,\ 1,\ 1)$	$\mathcal{F}(\pi_D-\pi_P)$	0	$\mathcal{F}(\pi_P-\pi_D)$	$\frac{\mu}{4}$	$\frac{\mu}{4}$	0
$(0,\ 2,\ 0)$	0	$\frac{\mu}{2}$	$1-\mu$	$\frac{\mu}{2}$	0	0
$(1,\ 1,\ 0)$	0	$\frac{\mu}{4}$	$\mathcal{F}(\pi_C-\pi_D)$	0	$\frac{\mu}{4}$	$\mathcal{F}(\pi_D-\pi_C)$
$(1,\ 0,\ 1)$	$\mathcal{F}(\pi_C-\pi_P)$	$\frac{\mu}{4}$	0	$\frac{\mu}{4}$	0	$\mathcal{F}(\pi_P-\pi_C)$
$(2,\ 0,\ 0)$	0	0	0	$\frac{\mu}{2}$	$\frac{\mu}{2}$	$1-\mu$

,

where $\mathcal{F}(x)$ is given by

$$\mathcal{F}(x) = (1-\mu)\frac{1}{1+\exp(\omega x)} + \frac{\mu}{4}.$$

The payoffs π_C, π_D, and π_P for cooperation, defection, and punishment strategies, respectively, are analytically determined through Eq. (7) under the condition $\delta = 0$, where δ represents the probability of interaction with three players.

2 Replicator dynamics in higher-order interactions with punishment mechanisms

2.1 Governing equation derivation

We consider evolutionary dynamics in an infinite population limit ($Z \to \infty$). Under the condition of weak selection ($\omega \ll 1$) and in the absence of mutation ($\mu = 0$), the evolutionary process (8) can be accurately captured by the replicator equation. Given the payoffs π_C, π_D, and π_P previously defined in equations (7), the temporal evolution of the frequency of each strategy in a well-mixed population is described by

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = x_i\left(\pi_i - \langle\pi\rangle\right), \quad i = C,\ D,\ P, \tag{9}$$

where $\langle\pi\rangle = x_C\pi_C + x_D\pi_D + x_P\pi_P$ represents the average payoff of the entire population. By explicitly substituting the average payoff $\langle\pi\rangle$ into Eq. (9), we obtain the detailed expressions governing the temporal evolution of each frequency of the strategy as follows:

$$\frac{\mathrm{d}x_C}{\mathrm{d}t} = x_C\left(1-x_C\right)\left(\pi_C-\pi_D\right)+x_C x_P\left(\pi_D-\pi_P\right), \tag{10a}$$

$$\frac{\mathrm{d}x_D}{\mathrm{d}t} = x_D\left(1-x_D\right)\left(\pi_D-\pi_C\right)+x_D x_P\left(\pi_C-\pi_P\right), \tag{10b}$$

$$\frac{\mathrm{d}x_P}{\mathrm{d}t} = x_P\left(1-x_P\right)\left(\pi_P-\pi_C\right)+x_D x_P\left(\pi_C-\pi_D\right). \tag{10c}$$

Let $a := 2\left(G-W\right)$, $b := T-S-1$ and $c := a+b$. In the case of the Prisoner's Dilemma, it is given that for this game $S<0,\ a>0$ and $b+S=T-1>0$. Therefore, we conclude that $c>0$. Substituting Eq. (7) into Eq. (10), we obtain the following expressions:

$$\begin{aligned}\frac{\mathrm{d}x_C}{\mathrm{d}t} =& \langle k\rangle\left\{-\delta x_C x_D^3 c+\delta x_C x_D\left[x_D c+x_P\left(\alpha+\beta\right)\right]+x_C x_D^2\left(b+2S-\alpha-\beta\right)\right.\\ &\left.+x_C x_D\left(-b-S+\alpha+\beta\right)-x_C^2 x_D\left(\alpha+\beta\right)\right\},\end{aligned} \tag{11a}$$

$$\begin{aligned}\frac{\mathrm{d}x_D}{\mathrm{d}t} =& \langle k\rangle\left\{\delta x_D^3\left(1-x_D\right)c+\delta x_D\left(1-x_D\right)\left[-x_D\left(c-\alpha\right)-x_P\beta\right]-\delta x_C x_D^2\alpha-x_D^2 x_C\alpha\right.\\ &\left.+x_D^2\left(1-x_D\right)\left(-b-2S+\alpha+\beta\right)+x_C x_D\left(1-x_D\right)\beta+x_D\left(1-x_D\right)\left(b+S-\beta\right)\right\},\end{aligned} \tag{11b}$$

$$\begin{aligned}\frac{\mathrm{d}x_P}{\mathrm{d}t} =& \langle k\rangle\left\{-\delta x_D^3 x_P c+\delta x_D x_P\left[x_D c+x_P\left(\alpha+\beta\right)-\alpha\right]+x_P x_D^2\left(b+2S\right)\right.\\ &\left.+x_D x_P^2\left(\alpha+\beta\right)+x_D x_P\left(-b-S-\alpha\right)\right\}.\end{aligned} \tag{11c}$$

2.2 Stability criteria and phase transitions

We denote the state of the system $\boldsymbol{x}=\left(x_C,x_D,x_P\right)$. Solving $\frac{\mathrm{d}x_i}{\mathrm{d}t}=0,\ i=C,\ D,\ P$, we obtain equilibrium points which can be divided into three categories:

(i) $x_D=0$, $x_C+x_P=1$, i.e., a point on the CP-edge, $x^{(CP)}=\left(x_C^{(CP)},0,x_P^{(CP)}\right)$.

(ii) $x_P=0$, $x_C+x_D=1$, i.e., a point on the CD-edge, $x^{(CD)}=\left(x_C^{(CD)},x_D^{(CD)},0\right)$.

(iii) $x_C=0$, $x_D+x_P=1$, i.e., a point on the DP-edge, $x^{(DP)}=\left(0,x_D^{(DP)},x_P^{(DP)}\right)$.

Proposition 1. *Let $\delta\in(0,1]$ denote the probability of a three-player interaction and let $\alpha>0$ represent the cost incurred for peer punishment. Then, the dynamical system described by Eq. (11) does not admit interior equilibria within the strategy simplex $x_C+x_D+x_P=1$.*

Proof. Assuming $x_C,\ x_D,\ x_P\neq 0$, for $\frac{\mathrm{d}\rho}{\mathrm{d}t}=0$, the right-hand sides of Eq. $(11)_a$ and Eq. $(11)_c$

can be reduced to

$$-\delta x_D^2 c + \delta \left[x_D c + x_P (\alpha+\beta)\right] + x_D (b + 2S - \alpha - \beta) - b - S + \alpha + \beta - x_C (\alpha+\beta) = 0, \tag{12a}$$

$$-\delta x_D^2 c + \delta \left[x_D c + x_P (\alpha+\beta) - \alpha\right] + x_D (b + 2S) + x_P (\alpha+\beta) - b - S - \alpha = 0. \tag{12b}$$

To admit a solution where all variables are strictly positive under the constraint $x_C + x_D + x_P = 1$, the system must satisfy

$$(1+\delta)\,\alpha = 0,$$

which is in contradiction with the definition of α. □

Case (i): The stability of $x^{(CP)} = \left(x_C^{(CP)}, 0, x_P^{(CP)}\right)$. When $x_D = 0$, it follows that $\frac{\mathrm{d}x_C}{\mathrm{d}t} = \frac{\mathrm{d}x_P}{\mathrm{d}t}$, implying that strategies C and P are indistinguishable. Under this condition, it is appropriate to consider the combined proportion $x_C + x_P$ as a single state variable. Thus, the system can be effectively analyzed by examining the dynamics of $\frac{\mathrm{d}x_D}{\mathrm{d}t}$ and $\frac{\mathrm{d}(x_C+x_P)}{\mathrm{d}t}$. Since $x_C + x_P = 1 - x_D$, substituting this identity directly yields

$$\begin{aligned}\frac{\mathrm{d}x_D}{\mathrm{d}t} = \langle k\rangle \big\{ &\delta x_D^3 (1-x_D)\, c + \delta x_D (1-x_D)\left[-x_D (c-\alpha) - x_P\beta\right] - \delta x_C x_D^2 \alpha - x_D^2 x_C \alpha \\ &+ x_D^2 (1-x_D)(-b - 2S + \alpha + \beta) + x_C x_D (1-x_D)\,\beta + x_D (1-x_D)(b + S - \beta)\big\}.\end{aligned}$$

The element of the single-order Jacobian matrix is

$$\begin{aligned}\frac{\mathrm{d}\dot{x}_D}{\mathrm{d}x_D} = \langle k\rangle \big\{ &3\delta x_D^2 (1-x_D)\, c - \delta x_D^3 c - 2\delta x_D (1-x_D)(c-\alpha) + \delta x_D^2 (c-\alpha) + \delta x_D x_P \beta \\ &- \delta (1-x_D)\, x_P \beta - 2(1+\delta)\, x_C x_D \alpha + \left[2x_D (1-x_D) - x_D^2\right](-b - 2S + \alpha + \beta) \\ &+ x_C (1-x_D)\,\beta - x_C x_D \beta + (1-x_D)(b + S - \beta) - x_D (b + S - \beta)\big\}.\end{aligned} \tag{13}$$

By substituting the expression for $x^{(CP)}$ into Eq. (13), we have

$$\left.\frac{\mathrm{d}\dot{x}_D}{\mathrm{d}x_D}\right|_{x^{(CP)}} = \langle k\rangle \left[-(1+\delta)\, x_P^{(CP)} \beta + b + S\right]. \tag{14}$$

Therefore, the equilibrium state $x^{(CP)}$ is stable if and only if $x_C^{(CP)} < x_{C,*}^{(CP)}$ (or equivalently, $x_P^{(CP)} > x_{P,*}^{(CP)}$), where

$$x_{C,*}^{(CP)} = 1 - \frac{b+S}{(1+\delta)\,\beta}, \tag{15}$$

and correspondingly,

$$x_{P,*}^{(CP)} = \frac{b+S}{(1+\delta)\,\beta}.$$

Although every point on the CP-edge is an equilibrium, only those points satisfying $x_C^{(CP)} <$

$x_{C,*}^{(CP)}$ exhibit stability. Through direct calculation, we derive the following explicit conditions:

- If inequality $b + S < 0$ holds, it necessarily follows that $x_{C,*}^{(CP)} > 1$. Consequently, all points on the CP-edge are stable.
- If condition $b + S > (1+\delta)\beta$ is satisfied, it implies $x_{C,*}^{(CP)} < 0$. Thus, all points on the CP-edge are unstable.
- If inequality $0 < b+S < (1+\delta)\beta$ holds, we have $0 < x_{C,*}^{(CP)} < 1$. In this case, the points on the CP-edge that satisfy $x_C^{(CP)} < x_{C,*}^{(CP)}$ are stable.

Case (*ii*): The stability of $x^{(CD)} = \left(x_C^{(CD)}, x_D^{(CD)}, 0\right)$. We cancel $x_P = 1 - x_C - x_D$ and study the dynamics depicted by $\frac{\mathrm{d}x_C}{\mathrm{d}t}$ and $\frac{\mathrm{d}x_D}{\mathrm{d}t}$,

$$\begin{aligned}\frac{\mathrm{d}x_C}{\mathrm{d}t} &= \langle k\rangle \left\{-\delta x_C x_D^3 c + \delta x_C x_D \left[x_D c + (1 - x_C - x_D)(\alpha+\beta)\right]\right. \\ &\left.+ x_C x_D^2 (b + 2S - \alpha - \beta) + x_C x_D (-b - S + \alpha + \beta) - x_C^2 x_D (\alpha+\beta)\right\}, \quad (16a)\\ \frac{\mathrm{d}x_D}{\mathrm{d}t} &= \langle k\rangle \left\{\delta x_D^3 (1 - x_D) c + \delta x_D (1 - x_D)\left[-x_D (c - \alpha) - (1 - x_C - x_D)\beta\right]\right. \\ &- \delta x_C x_D^2 \alpha - x_D^2 x_C \alpha + x_D^2 (1 - x_D)(-b - 2S + \alpha + \beta) \\ &\left.+ x_C x_D (1 - x_D)\beta + x_D (1 - x_D)(b + S - \beta)\right\}. \quad (16b)\end{aligned}$$

For $0 < x_D^{(CD)} < 1$, it satisfies

$$-\delta c x_D^2 + x_D (\delta c + b + 2S) - b - S = 0. \quad (17)$$

Then the Jacobian matrix of the system (16) at $x^{(CD)}$ is

$$J|_{x^{(CD)}} = \begin{pmatrix} m\langle k\rangle & n\langle k\rangle \\ -m\langle k\rangle - x_D^{(CD)}(1+\delta)\langle k\rangle\alpha & -n\langle k\rangle - x_D^{(CD)}(1+\delta)\langle k\rangle\alpha \end{pmatrix}, \quad (18)$$

where

$$\begin{aligned} m &= (1+\delta)(\alpha+\beta)\left(x_D^{(CD)} - 1\right) x_D^{(CD)}, \\ n &= \left(x_D^{(CD)}\right)^2 \left[b + 2S + (1+\delta)(\alpha+\beta)\right] - x_D^{(CD)}\left[2(b+S) + (1+\delta)(\alpha+\beta)\right] + b + S. \end{aligned}$$

The matrix has two eigenvalues, denoted as

$$\begin{aligned} \lambda_1 &= -(1+\delta)\langle k\rangle x_D^{(CD)}\alpha, \\ \lambda_2 &= (m-n)\langle k\rangle = \left[-\left(x_D^{(CD)}\right)^2 S - (b+S)\left(x_D^{(CD)} - 1\right)^2\right]\langle k\rangle. \end{aligned}$$

Besides, $0 < x_C^{(CD)} < 1$ satisfies

$$-\delta c x_C^2 + x_C\left(\delta c - b - 2S\right) + S = 0. \tag{19}$$

Then we deduce that

$$\begin{aligned}
\lambda_2 &= -\left(x_C^{(CD)}\right)^2 \langle k\rangle \left(b+2S\right) + 2x_C^{(CD)}\langle k\rangle S - \langle k\rangle S \\
&= -x_C^{(CD)}\langle k\rangle \left[-c\delta\left(x_C^{(CD)}\right)^2 + c\delta x_C^{(CD)} + S\right] + 2x_C^{(CD)}\langle k\rangle S - S\langle k\rangle \\
&= \left(1 - x_C^{(CD)}\right)\langle k\rangle \left[-c\delta\left(x_C^{(CD)}\right)^2 - S\right],
\end{aligned}$$

which implies that λ_2 is negative when $\left(x_C^{(CD)}\right)^2 > -\frac{S}{c\delta}$. Then we will determine the value of $x_C^{(CD)}$. By solving equation (19), we have the non-trivial stationary solutions:

$$x_{C,\pm}^* = \frac{c\delta - b - 2S \pm \sqrt{\left(c\delta - b\right)^2 + 4S\left(b+S\right)}}{2c\delta}. \tag{20}$$

It follows that when $\Delta = \left(c\delta - b\right)^2 + 4S\left(b+S\right) \geq 0$, then $x_{C,\pm}^*$ is real valued for every $b,\ c,\ ,\delta,\ S$. Since $c > 0$, $\Delta \geq 0$ requires the following conditions:

$$\delta \geq \delta_+ := \frac{b + \sqrt{-4S\left(b+S\right)}}{c}, \tag{21a}$$

$$\delta \leq \delta_- := \frac{b - \sqrt{-4S\left(b+S\right)}}{c}. \tag{21b}$$

It can also be verified that if $c\delta - b - 2S < 0$, then $x_{C,\pm}^* < 0$. Conversely, if $c\delta - b - 2S > 0$, or equivalently, if

$$\delta > \delta_* := \frac{b+2S}{c}, \tag{22}$$

then $x_{C,\pm}^* > 0$. Since $2S < \sqrt{-4S(b+S)}$, it follows directly that $\delta_- < \delta_* < \delta_+$. Therefore, for $\delta \geq \delta_+$, there exist positive real-valued stationary solutions $0 < x_{C,\pm}^* < 1$, while for $\delta \leq \delta_- < \delta_*$, the solutions are real but negative. We also observe that for the appearance of the non-trivial stationary solution $x_{C,+}^*$ at $\delta = \delta_+$ is always abrupt. Meanwhile, we have the following claim.

Proposition 2. *Suppose* $0 < x_{C,\pm}^* < 1$ *and* $x_{C,+}^* \neq x_{C,-}^*$. *Then, the stationary solution* $x^{(CD)} = \left(x_{C,+}^*, 1 - x_{C,+}^*, 0\right)$ *is stable, while the stationary solution* $x^{(CD)} = \left(x_{C,-}^*, 1 - x_{C,-}^*, 0\right)$ *is unstable.*

Proof. Note that λ_1 is always negative. Moreover, we recall that λ_2 is negative in the case of $\left(x_C^{(CD)}\right)^2 > -\frac{S}{c\delta}$. Let $c\delta - b - 2S = M > 0$. Then, we have $M^2 + 4c\delta S = \Delta > 0$. Next, we investigate the condition $\left(x^*_{C,+}\right)^2 > -\frac{S}{c\delta}$. This is equivalent to

$$\begin{aligned}\left(x^*_{C,+}\right)^2 > -\frac{S}{c\delta} &\iff \left(M+\sqrt{\Delta}\right)^2 > -4c\delta S\\ &\iff M^2+4c\delta S+M\sqrt{\Delta}>0\\ &\iff \Delta+M\sqrt{\Delta}>0.\end{aligned}$$

The last inequality always holds, since $\Delta > 0$ and $M\sqrt{\Delta} > 0$. Thus, we conclude that the stationary solution $x^{(CD)} = \left(x^*_{C,+}, 1-x^*_{C,+}, 0\right)$ is stable. Similarly, we have

$$\begin{aligned}\left(x^*_{C,-}\right)^2 > -\frac{S}{c\delta} &\iff \left(M-\sqrt{\Delta}\right)^2 > -4c\delta S\\ &\iff M^2+4c\delta S-M\sqrt{\Delta}>0\\ &\iff \sqrt{\Delta}\left(\sqrt{\Delta}-M\right)>0.\end{aligned}$$

This leads to a contradiction, as $S < 0$ and $\sqrt{\Delta} < M$. Therefore, the stationary solution $x^{(CD)} = \left(x^*_{C,-}, 1-x^*_{C,-}, 0\right)$ is unstable. □

For $x_D = 0$, it has $x^{(CD)} = (1,0,0)$. Then the Jacobian matrix of the system (16) at $x^{(CD)}$ is

$$J|_{x^{(CD)}} = \begin{pmatrix}0 & (-b-S)\langle k\rangle\\ 0 & (b+S)\langle k\rangle\end{pmatrix}, \tag{23}$$

with eigenvalues $\lambda_1 = 0$ and $\lambda_2 = (b+S)\langle k\rangle$. Since $b+S>0$, $x^{(CD)}$ is unstable.

Case (iii): The stability of $x^{(DP)} = \left(0, x_D^{(DP)}, x_P^{(DP)}\right)$. We cancel $x_C = 1-x_D-x_P$ and study the dynamics depicted by $\frac{\mathrm{d}x_D}{\mathrm{d}t}$ and $\frac{\mathrm{d}x_P}{\mathrm{d}t}$,

$$\begin{aligned}\frac{\mathrm{d}x_D}{\mathrm{d}t} &= \langle k\rangle\left\{\delta x_D^3\left(1-x_D\right)c+\delta x_D\left(1-x_D\right)\left[-x_D\left(c-\alpha\right)-x_P\beta\right]\right.\\ &\quad -x_D^2\left(1-x_D\right)\left(b+2S-\alpha-\beta\right)-\left(1+\delta\right)\left(1-x_D-x_P\right)x_D^2\alpha\\ &\quad \left.+x_D\left(1-x_D\right)\left[\left(1-x_D-x_P\right)\beta+\left(b+S-\beta\right)\right]\right\}, \qquad (24a)\\ \frac{\mathrm{d}x_P}{\mathrm{d}t} &= \langle k\rangle\left\{-\delta x_D^3 x_P c+\delta x_D x_P\left[x_D c+x_P\left(\alpha+\beta\right)-\alpha\right]+x_P x_D^2\left(b+2S\right)\right.\\ &\quad \left.+x_D x_P^2\left(\alpha+\beta\right)+x_D x_P\left(-b-S-\alpha\right)\right\}. \qquad (24b)\end{aligned}$$

For $0 < x_D^{(CD)} < 1$, it satisfies

$$\delta c x_D^2 + x_D\left[\delta\left(\alpha+\beta-c\right)+\left(\alpha+\beta-b-2S\right)\right]+b+S-\left(1+\delta\right)\beta = 0. \tag{25}$$

Then the Jacobian matrix of the system (24) at $x^{(DP)}$ is

$$J|_{x^{(DP)}} = \begin{pmatrix} m\langle k\rangle & n\langle k\rangle \\ -m\langle k\rangle + x_D^{(DP)}(1+\delta)\langle k\rangle\alpha & -n\langle k\rangle + x_D^{(DP)}(1+\delta)\langle k\rangle\alpha \end{pmatrix}, \tag{26}$$

where

$$\begin{aligned} m &= \left(x_D^{(DP)}\right)^2 [2(1+\delta)(\alpha+\beta) - (b+2S)] + x_D^{(DP)} [2(b+S) - 3(1+\delta)\beta] \\ &\quad - b - S + (1+\delta)\beta, \\ n &= \left(x_D^{(DP)}\right)^2 (1+\delta)(\alpha+\beta) - x_D^{(DP)}(1+\delta)\beta. \end{aligned}$$

The matrix has two eigenvalues, denoted as

$$\begin{aligned} \lambda_1 &= x_D^{(DP)}(1+\delta)\langle k\rangle\alpha, \\ \lambda_2 &= \left(x_D^{(DP)}\right)^2 \langle k\rangle [(1+\delta)(\alpha+\beta) - (b+2S)] + 2x_D^{(DP)}\langle k\rangle [(b+S) - (1+\delta)\beta] \\ &\quad - b\langle k\rangle - S\langle k\rangle + (1+\delta)\langle k\rangle\beta. \end{aligned}$$

Since λ_1 is always positive, $x^{(DP)}$ is unstable. Note that, when considering only the points on the DP-edge, we return to the case where only the two strategies D and P are present. In this case,

$$\begin{aligned} \frac{\mathrm{d}x_P}{\mathrm{d}t} &= x_P(1-x_P)(\pi'_P - \pi'_D) \\ &= x_P(1-x_P)\langle k\rangle \left\{-c\delta x_P^2 + x_P[c\delta - b - 2S + (1+\delta)(\alpha+\beta)] + S - (1+\delta)\alpha\right\}, \end{aligned} \tag{27}$$

where

$$\begin{aligned} \pi'_P &= (1-\delta)\langle k\rangle [x_D(S-\alpha) + x_P] + \delta\langle k\rangle \left[x_P^2 + x_D^2(S-2\alpha) + 2x_Dx_P(G-\alpha)\right], \\ \pi'_D &= (1-\delta)\langle k\rangle x_P(T-\beta) + \delta\langle k\rangle \left[x_P^2(T-2\beta) + 2x_Dx_P(W-\beta)\right]. \end{aligned}$$

In the following, we need to consider the solution of equation $\pi'_P - \pi'_D = 0$. In other words, we consider the quadratic equation

$$-c\delta x_P^2 + x_P[c\delta - b - 2S + (1+\delta)(\alpha+\beta)] + S - (1+\delta)\alpha = 0 \tag{28}$$

and obtain the following result.

Proposition 3. *If $(1+\delta)\beta > b+S$, then the equation (28) admits two real solutions*

$$x^*_{P,\pm} = \frac{c\delta - b - 2S + (1+\delta)(\alpha+\beta) \pm \sqrt{\Delta}}{2c\delta},$$

where $\Delta = [c\delta - b - 2S + (1+\delta)(\alpha+\beta)]^2 + 4c\delta[S - (1+\delta)\alpha]$*. Moreover, these solutions satisfy the inequalities* $0 < x^*_{P,-} < 1$ *and* $x^*_{P,+} > 1$*. In addition,* $x^*_{P,-}$ *is unstable.*

Proof. Since $(1+\delta)\beta > b + S$, it follows that

$$\begin{aligned}\Delta &= [c\delta - b - 2S + (1+\delta)(\alpha+\beta)]^2 + 4c\delta[S - (1+\delta)\alpha]\\ &> [c\delta - S + (1+\delta)\alpha]^2 + 4c\delta[S - (1+\delta)\alpha]\\ &= [c\delta + S - (1+\delta)\alpha]^2\\ &> 0.\end{aligned}$$

Therefore, the equation has real solutions. Moreover, it is straightforward to verify that both solutions, $x^*_{P,\pm}$, are positive.

Next, we find that $x^*_{P,-} < 1$ is equivalent to

$$-c\delta - b - 2S + (1+\delta)(\alpha+\beta) < \sqrt{\Delta}. \tag{29}$$

Now we consider two cases:

(i) If $c\delta + b + 2S \geq (1+\delta)(\alpha+\beta)$, the inequality (29) always holds.

(ii) If $c\delta + b + 2S < (1+\delta)(\alpha+\beta)$, the inequality (29) is equivalent to

$$[-c\delta - b - 2S + (1+\delta)(\alpha+\beta)]^2 < \Delta \iff 4c\delta[b + S - (1+\delta)\beta] < 0$$

And the last line always holds under the condition $(1+\delta)\beta > b + S$.

Furthermore, we find that $x^*_{P,+} > 1$ is equivalent to

$$\sqrt{\Delta} > c\delta + b + 2S - (1+\delta)(\alpha+\beta). \tag{30}$$

Similar to $x^*_{P,-}$, we consider two cases as follows:

(i) If $c\delta + b + 2S \leq (1+\delta)(\alpha+\beta)$, the inequality (30) always holds.

(ii) If $c\delta + b + 2S > (1+\delta)(\alpha+\beta)$, the inequality (30) is also equivalent to

$$4c\delta[b + S - (1+\delta)\beta] < 0,$$

which, once again, holds in the case of $(1+\delta)\beta > b + S$.

In conclusion, we have $0 < x^*_{P,-} < 1$ and $x^*_{P,+} > 1$. We then prove that $x^*_{P,-}$ is unstable. Let

$$f(x_P) = x_P(1 - x_P)\left\{-c\delta x_P^2 + x_P[c\delta - b - 2S + (1+\delta)(\alpha+\beta)] + S - (1+\delta)\alpha\right\}.$$

Then, we compute the derivative of $f(x_P)$ at $x^*_{P,-}$:

$$f'(x^*_{P,-}) = x^*_{P,-}\left(1 - x^*_{P,-}\right)\left[-2c\delta x^*_{P,-} + c\delta - b - 2S + (1+\delta)(\alpha+\beta)\right] > 0,$$

where $-2c\delta x^*_{P,-} + c\delta - b - 2S + (1+\delta)(\alpha+\beta) = \sqrt{\Delta} > 0$. Hence, $x^*_{P,-}$ is unstable. □

We now analyze the stable stationary solutions on the DP-edge under the condition $b + S \geq (1+\delta)\beta$. Specifically, we examine the real-valued roots within the interval $(0,1)$ of equation (28). Suppose that this equation has two distinct solutions $x_1,\ x_2 \in (0,1)$. This implies that the discriminant Δ must satisfy

$$\Delta = \left[c\delta - b - 2S + (1+\delta)(\alpha+\beta)\right]^2 + 4c\delta\left[S - (1+\delta)\alpha\right] > 0.$$

Under this condition, the two distinct solutions are explicitly given by

$$x_{1,2} = \frac{c\delta - b - 2S + (1+\delta)(\alpha+\beta) \pm \sqrt{\Delta}}{2c\delta}. \tag{31}$$

Based on direct calculations, we will identify three scenarios in the following.

(A1) When

$$\begin{cases} c\delta - b - 2S + (1+\delta)(\alpha+\beta) > 0, \\ c\delta + b + 2S - (1+\delta)(\alpha+\beta) > 0, \end{cases}$$

both solutions $x_1,\ x_2$ lie within (0,1). Among them, the solution x_1 is unstable, while the solution x_2 is stable.

(A2) When

$$\begin{cases} c\delta - b - 2S + (1+\delta)(\alpha+\beta) > 0, \\ c\delta + b + 2S - (1+\delta)(\alpha+\beta) < 0, \end{cases}$$

both solutions $x_1,\ x_2$ are greater than 1.

(A3) When $c\delta - b - 2S + (1+\delta)(\alpha+\beta) < 0$, both solutions x_1 and x_2 are negative.

We proceed by analyzing case **(A1)**. Combining condition $b + S \geq (1+\delta)\beta$ with the case **(A1)**, we define three critical parameters as

$$\delta_1 = \frac{b+S}{\beta} - 1,\ \delta_2 = \frac{b + 2S - \alpha - \beta}{c + \alpha + \beta} \text{ and } \delta_3 = \frac{\alpha + \beta - b - 2S}{c - \alpha - \beta}.$$

If condition $c - \alpha - \beta > 0$ holds, the signs of δ_2 and δ_3 are strictly opposite. Specifically, if $\delta_2 > 0$, then it necessarily follows that $\delta_3 < 0$. In contrast, under the condition $c - \alpha - \beta < 0$, combined with the assumptions outlined in **(A1)**, we must simultaneously have $\delta < \delta_3$ and $\delta > \delta_2$. This scenario warrants further consideration in two distinct cases:

- If $\alpha + \beta > b + 2S$, it implies that both $\delta_3 < 0$ and $\delta_2 < 0$, thereby making it impossible to satisfy the simultaneous inequalities, resulting in a contradiction.
- If $\alpha + \beta < b + 2S$, noting that $c = a + b < \alpha + \beta$, together with the imposed constraints $S < 0,\ a > 0,\ b > 0$, it is a contradiction to $\alpha + \beta < b + 2S$.

Hence, under the condition $c - \alpha - \beta < 0$, both cases inevitably lead to logical contradictions, thus demonstrating that the initial assumptions are invalid in this scenario. Next, we analyze the condition $\Delta > 0$. Let $f(\delta)$ denote

$$\begin{aligned} f(\delta) = \Delta = \delta^2 \left[(c-\alpha-\beta)^2 + 4c\beta\right] + 2\delta \left\{c(\beta-\alpha-b) + (\alpha+\beta)\left[(\alpha+\beta)-(b+2S)\right]\right\} \\ + (b+2S-\alpha-\beta)^2 . \end{aligned} \tag{32}$$

Notice that $f(\delta)$ is a quadratic function in δ with a positive leading coefficient and satisfies $f(0) > 0$. Therefore, if the quadratic does not admit real roots, then $f(\delta) > 0$ holds for all $\delta \in (0, 1)$. If, on the other hand, $f(\delta) = 0$ has two distinct real solutions (that is, its discriminant $\Delta' > 0$), denoted by $x_{\delta,-}$ and $x_{\delta,+}$ with $x_{\delta,-} < x_{\delta,+}$. If both roots lie within the interval $(0, 1)$, then by the upward-opening nature of $f(\delta)$, it follows that $f(\delta) > 0$ precisely for

$$0 < \delta < x_{\delta,-} \quad \text{or} \quad x_{\delta,+} < \delta < 1.$$

Define

$$\delta_4 = \begin{cases} x_{\delta,-} & \text{if } x_{\delta,-} \text{ exists} \\ 1 & \text{otherwise} \end{cases} \quad \text{and} \quad \delta_5 = \begin{cases} x_{\delta,+} & \text{if } x_{\delta,+} \text{ exists} \\ 0 & \text{otherwise} \end{cases},$$

and it is obvious that $\delta_4 < \delta_5$. Specifically, if the corresponding root lies in the interval $(0, 1)$, δ takes that value; otherwise (or if no such root exists), we set $\delta_4 = 1$ and $\delta_5 = 0$. Based on the preceding discussion, we now state the following proposition.

Proposition 4. *Let $\alpha,\ \beta,\ c, b$ and S be parameters that satisfy $c - \alpha - \beta > 0$. If*

$$\max\{\delta_2,\ \delta_3\} < \delta < \min\{\delta_1,\ \delta_4,\ 1\} \quad \textit{or} \quad \max\{\delta_2,\ \delta_3,\ \delta_5\} < \delta < \min\{\delta_1,\ 1\},$$

then the DP-edge admits two fixed points, x_1 and x_2, with $x_1,\ x_2 \in (0, 1)$ as defined in Eq. (31). Moreover, x_1 is unstable, while x_2 is stable.

Let $\delta_6 = \delta_+ = \frac{b+\sqrt{-4S(b+S)}}{c}$ and $\delta_7 = \max\{\delta_2,\ \delta_3\}$. We analyze the order of stable equilibrium points by comparing the magnitudes of critical thresholds $\delta_1,\ \delta_4,\ \delta_5,\ \delta_6$ and δ_7. Given the multi-parametric nature of the system, accurate determination of these critical thresholds inherently depends on parameter selection. Based on the preceding analysis, we choose the appropriate parameter values to provide a clear illustration.

With the parameters $\alpha,\ \beta,\ b,\ c$, and S fixed appropriately, we explore the relationship between the sequential emergence of stable equilibrium points and the probability of third-order interactions δ. The relationships can be broadly classified into several distinct categories when $\delta_5 > \delta_1$, as shown in Fig. 1. Here, δ_1 characterizes the emergence of a stable equilibrium on the CP-edge, while the relationship between δ_4 and δ_7 governs the formation of a stable equilibrium on the DP-edge. Similarly, δ_6 determines the stability condition for the equilibria along the CD-edge. The schematic representation is conceptual rather than quantitative; data points illustrate the relative ordering (non-strict inequality) of the parameters $\delta_1,\ \delta_4,\ \delta_5,\ \delta_6,\ \delta_7$, without implying specific numerical values.

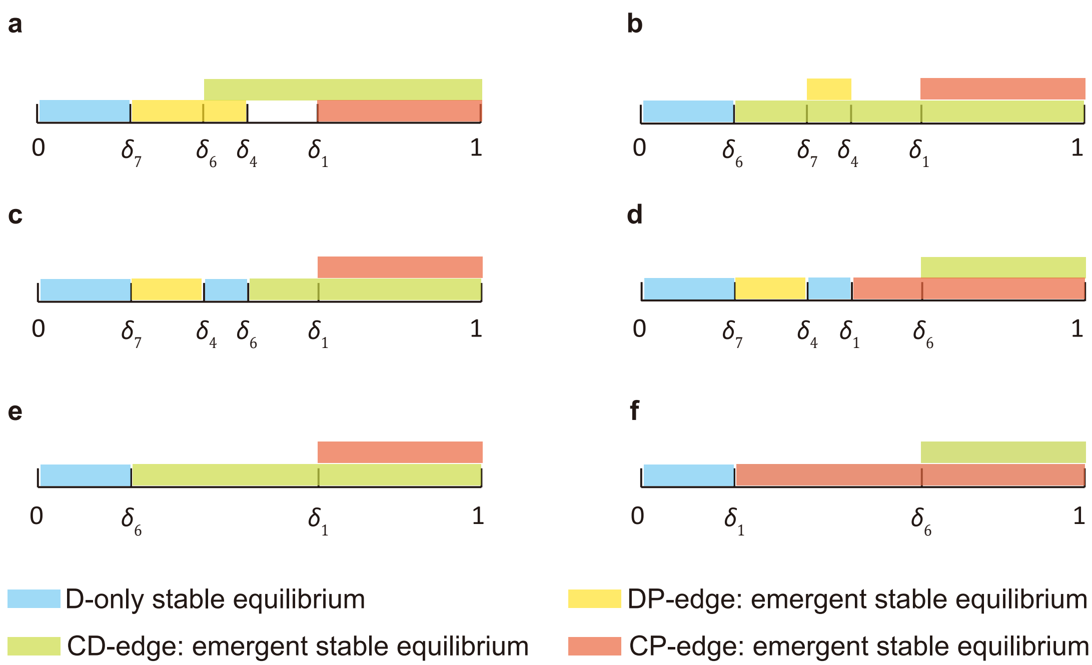

Figure 1: Hierarchical emergence of stable equilibria as governed by the third-order interaction probability δ with all other parameters suitably fixed. Panels **a-d** show the bifurcation sequences and resulting equilibrium types when stable points arise at the DP-edge. In contrast, **e-f** illustrate scenarios in which no stable equilibria persist at the DP-edge.

For $x_D = 0$, it has $x^{(DP)} = (0,0,1)$. The Jacobian matrix of the system (24) at $x^{(DP)}$ is

$$J|_{x^{(DP)}} = \begin{pmatrix} [b+S-(1+\delta)\beta]\langle k\rangle & 0 \\ [(1+\delta)\beta-(b+S)]\langle k\rangle & 0 \end{pmatrix}, \tag{33}$$

with eigenvalues $\lambda_1 = 0$ and $\lambda_2 = [b+S-(1+\delta)\beta]\langle k\rangle$. The stability condition for the equilibrium point $x^{(DP)} = (0,0,1)$ is determined by the sign of the expression $b+S-(1+\delta)\beta$.

For $x_P = 0$, it has $x^{(DP)} = (0, 1, 0)$. The Jacobian matrix of the system (24) at $x^{(DP)}$ is

$$J|_{x^{(DP)}} = \begin{pmatrix} S\langle k\rangle & (1+\delta)\langle k\rangle\alpha \\ 0 & -(1+\delta)\langle k\rangle\alpha + S\langle k\rangle \end{pmatrix}, \tag{34}$$

with eigenvalues $\lambda_1 = S\langle k\rangle$ and $\lambda_2 = -(1+\delta)\langle k\rangle\alpha + S\langle k\rangle$. Since $\alpha > 0$ and $S < 0$, $x^{(DP)}$ is stable.

3 Replicator Dynamics in Two-Population Games under Higher-Order Interactions and Punishment Mechanisms

In this section, we consider a theoretical model involving two distinct roles, each associated with two strategies, in a population where individuals participate concurrently in both pairwise and three-player interactions. Our primary objective is to determine how the proportion of these two roles affects the prevalence of cooperation in the population.

We denote the two roles by M_1 and M_2, with η representing the proportion of individuals in role M_1, and $1-\eta$ the proportion in role M_2. The set of strategies for M_1 is $S_{M_1} = \{C,\ D_1\}$, while the set of strategies for M_2 is $S_{M_2} = \{P,\ D_2\}$. Let $x_C \in [0, \eta]$ and $x_{D_1} \in [0, \eta]$ denote the proportions of the population adopting strategies C and D_1 respectively, constrained by $x_C + x_{D_1} = \eta$. Similarly, define $x_P \in [0, 1-\eta]$ and $x_{D_2} \in [0, 1-\eta]$ as the proportions for strategies P and D_2, satisfying $x_P + x_{D_2} = 1-\eta$. Moreover, by direct computation, $x_1 = \frac{x_C}{\eta}$ is the proportion of M_1 individuals using strategy C, which implies that the proportion of M_1 individuals using strategy D_1 is $1 - x_1$. Similarly, $x_2 = \frac{x_P}{1-\eta}$ is the proportion of M_2 individuals using strategy P, while $1 - x_2$ is the proportion of M_2 individuals using strategy D_2. For the pairwise interaction scenario, the payoff matrix is explicitly given by

M_1	P	D_2	C	D_1
C	1	S	1	S
D_1	$T-\beta$	0	T	0

and

M_2	C	D_1	P	D_2
P	1	$S-\alpha$	1	$S-\alpha$
D_2	T	0	$T-\beta$	0

.

For three-person interactions, the payoff structure expands due to multiple co-players, denoted as

M_1	CC	CD_1	CD_2	CP	D_1D_2	D_1D_1	D_2D_2	D_1P	D_2P	PP
C	1	G	G	1	S	S	S	G	G	1
D_1	T	W	W	$T-\beta$	0	0	0	$W-\beta$	$W-\beta$	$T-2\beta$

,

and

M_2	CC	CD_1	CD_2	CP	D_1D_2	D_1D_1	D_2D_2	D_1P	D_2P	PP
P	1	$G-\alpha$	$G-\alpha$	1	$S-2\alpha$	$S-2\alpha$	$S-2\alpha$	$G-\alpha$	$G-\alpha$	1
D_2	T	W	W	$T-\beta$	0	0	0	$W-\beta$	$W-\beta$	$T-2\beta$

The expected payoffs for each strategy are given by

$$\begin{aligned}\pi_C &= (1-\delta)\langle k\rangle\left[(1-x_C-x_P)S+x_C+x_P\right]+\delta\langle k\rangle\left[(1-x_C-x_P)^2 S\right.\\ &\quad\left.+2(x_C+x_P)(1-x_C-x_P)G+(x_C+x_P)^2\right], \qquad (35a)\\ \pi_{D_1} &= \pi_{D_2} = (1-\delta)\langle k\rangle\left[(x_C+x_P)T-x_P\beta\right]+\delta\langle k\rangle\left[(x_C+x_P)^2T-2x_P\beta\right.\\ &\quad\left.+2(x_C+x_P)(1-x_C-x_P)W\right], \qquad (35b)\\ \pi_P &= (1-\delta)\langle k\rangle\left[(1-x_C-x_P)(S-\alpha)+x_P+x_C\right]+\delta\langle k\rangle\left[(1-x_C-x_P)^2S\right.\\ &\quad\left.+2(x_C+x_P)(1-x_C-x_P)G-2(1-x_C-x_P)\alpha+(x_C+x_P)^2\right]. \qquad (35c)\end{aligned}$$

The mean payoff of the population M_1 is then calculated by $\langle\pi_1\rangle = x_1\pi_C+(1-x_1)\pi_{D_1}$, while the mean payoff of the population M_2 is $\langle\pi_2\rangle = x_2\pi_P+(1-x_2)\pi_{D_2}$. Then the evolution in time of the proportion of x_1 and x_2 is given by the replicator equation

$$\begin{cases}\dot{x}_1 = x_1(\pi_C-\langle\pi_1\rangle)\\ \dot{x}_2 = x_2(\pi_P-\langle\pi_2\rangle)\end{cases}. \qquad (36)$$

Substituting the expression for $\langle\pi_1\rangle$ and $\langle\pi_2\rangle$ into Eq. (10), we have

$$\begin{cases}\dot{x}_1 = x_1(1-x_1)(\pi_C-\pi_{D_1}),\\ \dot{x}_2 = x_2(1-x_2)(\pi_P-\pi_{D_2}),\end{cases} \qquad (37)$$

where

$$\begin{aligned}\pi_C-\pi_{D_1} &= \delta\langle k\rangle(x_C+x_P)^2(1-T+2W-2G+S)+(x_C+x_P)\langle k\rangle(1-S-T)+S\langle k\rangle\\ &\quad+x_P\langle k\rangle\beta+\delta\langle k\rangle\left[(x_C+x_P)(T-1+2G-2W-S)+x_P\beta\right]\end{aligned}$$

and

$$\pi_P-\pi_{D_2} = \pi_C-\pi_{D_1}-(1+\delta)\langle k\rangle(1-x_C-x_P)\alpha.$$

We also denote $a=2(G-W),\ b=T-1-S$ and $c=a+b$. We define the payoff difference functions $f(x_C,x_P)=\pi_C-\pi_{D_1}$ and $g(x_C,x_P)=\pi_P-\pi_{D_2}$ as

$$f(x_C,x_P)=\left[(x_C+x_P)(c\delta-b-2S)-c\delta(x_C+x_P)^2+(1+\delta)x_P\beta+S\right]\langle k\rangle$$

and

$$g(x_C, x_P) = f(x_C, x_P) - (1+\delta)\langle k\rangle(1 - x_C - x_P)\alpha,$$

respectively. Assuming that $\dot{x}_1 = 0$ and $\dot{x}_2 = 0$, the equilibrium points in Eq. (37) classified into three distinct categories:

(i) **Vertex equilibrium points.** Four vertex equilibrium points are given by $V_1 = (0,0),\ V_2 = (0,1),\ V_3 = (1,0),$ and $V_4 = (1,1)$.

(ii) **Interior equilibrium point.** There exists one interior equilibrium point $V_5 = (x_1^*, x_2^*)$, where

$$x_1^* = \frac{(1+\delta)\beta - (T-1)}{(1+\delta)\beta\eta} \text{ and } x_2^* = \frac{T-1}{(1-\eta)(1+\delta)\beta}.$$

This equilibrium is meaningful if and only if the condition $T - 1 = b + S < (1+\delta)\beta$ is satisfied.

(iii) **Boundary equilibrium points.** There are four boundary equilibrium points defined as follows:

- $V_6 = (1, x_2')$, with $x_2' \in (0,1)$ satisfying $g(\eta, (1-\eta)x_2') = 0$;
- $V_7 = (0, x_2')$, with $x_2' \in (0,1)$ satisfying $g(0, (1-\eta)x_2') = 0$;
- $V_8 = (x_1', 0)$, with $x_1' \in (0,1)$ satisfying $f(\eta x_1', 0) = 0$;
- $V_9 = (x_1', 1)$, with $x_1' \in (0,1)$ satisfying $f(\eta x_1', 1-\eta) = 0$.

We turn to studying the stability of these equilibrium points. The Jacobian matrix of the system (37) is

$$J = \begin{pmatrix} (1-2x_1)f(\eta x_1, (1-\eta)x_2) + x_1(1-x_1)\frac{\partial f}{\partial x_1} & x_1(1-x_1)\frac{\partial f}{\partial x_2} \\ x_2(1-x_2)\frac{\partial g}{\partial x_1} & (1-2x_2)g(\eta x_1, (1-\eta)x_2) + x_2(1-x_2)\frac{\partial g}{\partial x_2} \end{pmatrix}. \tag{38}$$

Case (i): The stability of vertex equilibrium points. Substituting the value of $V_1 = (0,0)$ into Eq. (38), we have

$$J|_{V_1} = \begin{pmatrix} S\langle k\rangle & 0 \\ 0 & S\langle k\rangle - (1+\delta)\langle k\rangle\alpha \end{pmatrix}.$$

We know that V_1 is stable if and only if $S < 0$. Similarly, substituting $V_2 = (0,1),\ V_3 = (1,0),$ and $V_4 = (1,1)$ into Eq. (38), we obtain

$$J|_{V_2} = \begin{pmatrix} f(0, 1-\eta) & 0 \\ 0 & -g(0, 1-\eta) \end{pmatrix}, \quad J|_{V_3} = \begin{pmatrix} -f(\eta, 0) & 0 \\ 0 & g(\eta, 0) \end{pmatrix},$$

and

$$J|_{V_4} = \begin{pmatrix} -f(\eta, 1-\eta) & 0 \\ 0 & -g(\eta, 1-\eta) \end{pmatrix}.$$

For the equilibrium point V_2:

- If $f(0, 1-\eta) < 0$, it follows that $g(0, 1-\eta) = f(0, 1-\eta) - (1+\delta)\langle k\rangle\eta\alpha < 0$, implying that V_2 is a saddle point.

- If $f(0, 1-\eta) > 0$, then V_2 is a saddle when $g(0, 1-\eta) > 0$ and unstable when $g(0, 1-\eta) < 0$.

For the equilibrium point V_3:

- If $f(\eta, 0) < 0$, then $g(\eta, 0) = f(\eta, 0) - (1+\delta)\langle k\rangle(1-\eta)\alpha < 0$, indicating that V_2 is a saddle point.

- If $f(\eta, 0) > 0$, then V_2 is a saddle when $g(\eta, 0) > 0$ and stable when $g(\eta, 0) < 0$.

For the equilibrium point V_4:

- Since $f(\eta, 1-\eta) = g(\eta, 1-\eta) = (1+\delta)\langle k\rangle(1-\eta)\beta - b - S$, V_4 is stable when $f(\eta, 1-\eta) > 0$ and unstable when $f(\eta, 1-\eta) < 0$.

Case (ii): The stability of the interior equilibrium point. Substituting $V_5 = (x_1^*, x_2^*)$ into Eq. (38), since $\eta x_1^* + (1-\eta)x_2^* = 1$ and $f(\eta x_1^*, (1-\eta)x_2^*) = g(\eta x_1^*, (1-\eta)x_2^*) = 0$, we have

$$J|_{V_5} = \begin{pmatrix} -QM\langle k\rangle & -Q\langle k\rangle\left[M - (1+\delta)\beta\right] \\ -R\langle k\rangle\left[M - (1+\delta)\alpha\right] & -R\langle k\rangle\left[M - (1+\delta)(\alpha+\beta)\right] \end{pmatrix},$$

where $M = c\delta + b + 2S$, $Q = \eta x_1^*(1 - x_1^*)$ and $R = (1-\eta)x_2^*(1 - x_2^*)$. Then we obtain

$$\begin{aligned} \det(\lambda I - J|_{V_5}) &= \begin{vmatrix} \lambda + MQ\langle k\rangle & Q\langle k\rangle\left[M - (1+\delta)\beta\right] \\ R\langle k\rangle\left[M - (1+\delta)\alpha\right] & \lambda + R\langle k\rangle\left[M - (1+\delta)(\alpha+\beta)\right] \end{vmatrix} \\ &= \lambda^2 + \left[(Q+R)M - R(1+\delta)(\alpha+\beta)\right]\langle k\rangle\lambda - QR(1+\delta)^2\langle k\rangle^2\alpha\beta. \end{aligned}$$

Given that

$$\Delta = \left[(Q+R)M - R(1+\delta)(\alpha+\beta)\right]^2\langle k\rangle^2 + 4QR(1+\delta)^2\langle k\rangle^2\alpha\beta > 0,$$

the characteristic equation $\det(\lambda I - J|_{V_5}) = 0$ has two distinct real roots, denoted λ_1 and λ_2. Furthermore, since

$$\lambda_1\lambda_2 = -QR(1+\delta)^2\langle k\rangle^2\alpha\beta < 0,$$

it follows that λ_1 and λ_2 have opposite signs. This indicates that V_5 is a saddle point.

Case (iii): The stability of boundary equilibrium points. Substituting $V_6 = (1, x_2')$ into Eq. (38), and noting that

$$g(\eta, (1-\eta)x_2') = f(\eta, (1-\eta)x_2') - (1+\delta)(1-\eta)(1-x_2')\alpha = 0,$$

yields

$$J|_{V_6} = \begin{pmatrix} -f(\eta, (1-\eta)x_2') & 0 \\ x_2'(1-x_2')\frac{\partial g}{\partial x_1}|_{V_6} & x_2'(1-x_2')\frac{\partial g}{\partial x_2}|_{V_6} \end{pmatrix}.$$

Here, the term $\frac{\partial g}{\partial x_2}|_{V_6}$ satisfies that

$$\frac{\partial g}{\partial x_2}|_{V_6} = (1-\eta)\langle k\rangle \left\{-2c\delta\left[\eta + x_2'(1-\eta)\right] + c\delta - (b+2S) + (1+\delta)(\alpha+\beta)\right\}.$$

Moreover, x_2' satisfies the quadratic equation

$$\begin{aligned} &-c\delta(1-\eta)^2(x_2')^2 + x_2'\left[(1-\eta)c\delta + (1+\delta)(1-\eta)(\alpha+\beta) - 2c\delta\eta(1-\eta)\right. \\ &\left.-(1-\eta)(b+2S)\right] - c\delta\eta^2 + c\delta\eta - \eta(b+2S) - (1-\eta)(1+\delta)\alpha + S = 0. \end{aligned}$$

Since $f(\eta, (1-\eta)x_2') = (1+\delta)\langle k\rangle(1-\eta)(1-x_2')\alpha > 0$, if one selects appropriate values for $\alpha,\ \beta,\ c,\ S,\ \eta$ and δ so that the roots $x_{2,\pm}'$ with $x_{2,-}' < x_{2,+}'$, lie within the interval (0,1), it follows that $\frac{\partial g}{\partial x_2}|_{(1,x_{2,+}')} < 0$ and $\frac{\partial g}{\partial x_2}|_{(1,x_{2,-}')} > 0$. Consequently, the equilibrium point $(1, x_{2,+}')$ is stable and $(1, x_{2,-}')$ is a saddle point.

By substituting $V_7 = (0, x_2')$ into Eq. (38), and noting that

$$g(0, (1-\eta)x_2') = f(0, (1-\eta)x_2') - (1+\delta)\langle k\rangle\left[1-(1-\eta)x_2'\right]\alpha = 0,$$

we obtain

$$J|_{V_7} = \begin{pmatrix} f(0, (1-\eta)x_2') & 0 \\ x_2'(1-x_2')\frac{\partial g}{\partial x_1}|_{V_7} & x_2'(1-x_2')\frac{\partial g}{\partial x_2}|_{V_7} \end{pmatrix}.$$

Here, the term $\frac{\partial g}{\partial x_2}|_{V_7}$ satisfies that

$$\frac{\partial g}{\partial x_2}|_{V_7} = (1-\eta)\langle k\rangle\left\{-2c\delta x_2'(1-\eta) + c\delta - (b+2S) + (1+\delta)(\alpha+\beta)\right\}.$$

Since $f(0, (1-\eta)x_2') = (1+\delta)\langle k\rangle\left[1-(1-\eta)x_2'\right]\alpha > 0$, V_7 is unstable when $\frac{\partial g}{\partial x_2}|_{V_7} > 0$ and becomes a saddle point when $\frac{\partial g}{\partial x_2}|_{V_7} < 0$.

Similarly, substituting $V_8 = (x_1', 0)$ into Eq. (38), and noting that $f(\eta x_1', 0) = 0$, we have

$$J|_{V_8} = \begin{pmatrix} x_1'(1-x_1')\frac{\partial f}{\partial x_1}\big|_{V_8} & x_1'(1-x_1')\frac{\partial f}{\partial x_2}\big|_{V_8} \\ 0 & g(\eta x_1', 0) \end{pmatrix}.$$

Since $g(\eta x_1', 0) = -(1+\delta)\langle k\rangle(1-x_1'\eta)\alpha < 0$, the equilibrium point V_8 is stable when $\frac{\partial f}{\partial x_1}\big|_{V_8} < 0$ and becomes a saddle point when $\frac{\partial f}{\partial x_1}\big|_{V_8} > 0$.

Finally, we analyze the stability of the equilibrium point V_9. Since $f(x_1'\eta, 1) = 0$, the Jacobian evaluated at V_9 is given by

$$J|_{V_9} = \begin{pmatrix} x_1'(1-x_1')\frac{\partial f}{\partial x_1}\big|_{V_9} & x_1'(1-x_1')\frac{\partial f}{\partial x_2}\big|_{V_9} \\ 0 & -g(\eta x_1', 1) \end{pmatrix}.$$

Since $g(\eta x_1', 1) = -(1+\delta)\langle k\rangle\eta(1-x_1')\alpha < 0$, it follows that the equilibrium V_9 is unstable when $\frac{\partial f}{\partial x_1}\big|_{V_9} > 0$, and becomes a saddle point when $\frac{\partial f}{\partial x_1}\big|_{V_9} < 0$.

In fact, the behavior of $V_7,\ V_8$ and V_9 is analogous to that of V_6. The unknowns x_1' and x_2' are determined by a quadratic function with a negative leading coefficient. Setting this function equal to zero, the existence of roots within the interval (0,1) confirms the presence of the corresponding equilibria $V_7,\ V_8$ and V_9. Furthermore, analyzing the sign of the derivative at these roots determines the stability of each equilibrium.

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