

Spatial public goods games on any population structure

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ABSTRACT

Understanding the emergence of cooperation in spatially structured populations has advanced significantly in the context of pairwise games, but the fundamental theory of group-based public goods games (PGGs) remains less explored. Here, we provide theoretical conditions under which cooperation thrive in spatial PGGs on any population structure, which are accurate under weak selection. We find that PGGs can support cooperation across all kinds of model details and on almost all network structures in contrast to pairwise games. For example, a class of networks that would otherwise fail to produce cooperation, such as star graphs, are particularly conducive to cooperation in spatial PGGs. This fundamental advantage of spatial PGGs derives from reciprocity through second-order interactions, allowing local structures such as the clustering coefficient to play positive roles. We also verify the robustness of spatial PGGs on empirical networks where pairwise games cannot support cooperation, which implies that PGGs could be a universal interaction mode in real-world systems.

Cooperation is essential for the emergence of complex systems to a higher level^{1–3}. To answer the question of how individual selfishness leads to selfless cooperation in evolution, many theories have been developed, such as evolutionary games on spatial structures (also known as networks or graphs). When individuals interact with their neighbors and learn the strategy with high payoffs, the prosocial cooperation strategy can emerge through spatial reciprocity⁴. Over the past three decades, agent-based simulations of spatial evolutionary game theory have revealed numerous mechanisms that can promote cooperation^{5,6}. On the other hand, the fundamental theory of pairwise games, initially on the regular graphs^{7–9}, has developed to identify the conditions for cooperation success on any spatial structure^{10–12}—some network structures are more conducive to cooperation than others^{13,14}.

However, pairwise games were limited in capturing diverse natural and social phenomena such as the nonlinear mechanism^{15,16}. Real-world interactions may involve more than two individuals. The evolution of cooperation in such group interactions is better described by multiplayer games¹⁷. Applying the framework of spatial evolutionary dynamics, a natural approach is that individuals organize groups with their neighbors and play multiplayer games within such groups. In this way, individuals participate not only in the game organized by themselves but also in the games organized by their neighbors. Individuals take averaged or accumulated payoffs obtained in these games for comparison in strategy updates¹⁸. This spatial principle can be applied to any multiplayer game¹⁹, including the public goods game²⁰ and others^{21,22}.

The public goods game (PGG) is among the most fundamental multiplayer games, originating from the tragedy of the commons²³. Players choose whether to contribute to the common pool. All contributions are multiplied by a synergy factor and then evenly distributed among all players. From a group perspective, the amplification of contributions ensures they are rewarded. However, from an individual perspective, one can still receive the equal share without contributing. This results in higher payoffs for non-contributors and incentivizes individuals not to contribute. Apart from human experiments^{24–27}, previous research on PGGs primarily relies on agent-based simulations^{20,28}. Although the agent-based simulation allows for great flexibility in studying new mechanisms, it also requires intensive computational resources and is difficult to identify the underlying principles behind the phenomena. Therefore, people also attempted to analyze the numerous proposed mechanisms at a theoretical level^{29–34}. The feasibility of this large body of potential work depends on the support that the fundamental mathematical theory can provide.

The most advanced fundamental theory for spatial PGGs still remains on regular graphs. There is no efficient algorithm for general selection strength due to computational complexity³⁵, but a feasible way is to study the case in the weak selection limit³⁶. On this basis, Li et al.^{37,38} proposed the theory of PGGs in infinite structured populations through pair approximation, although

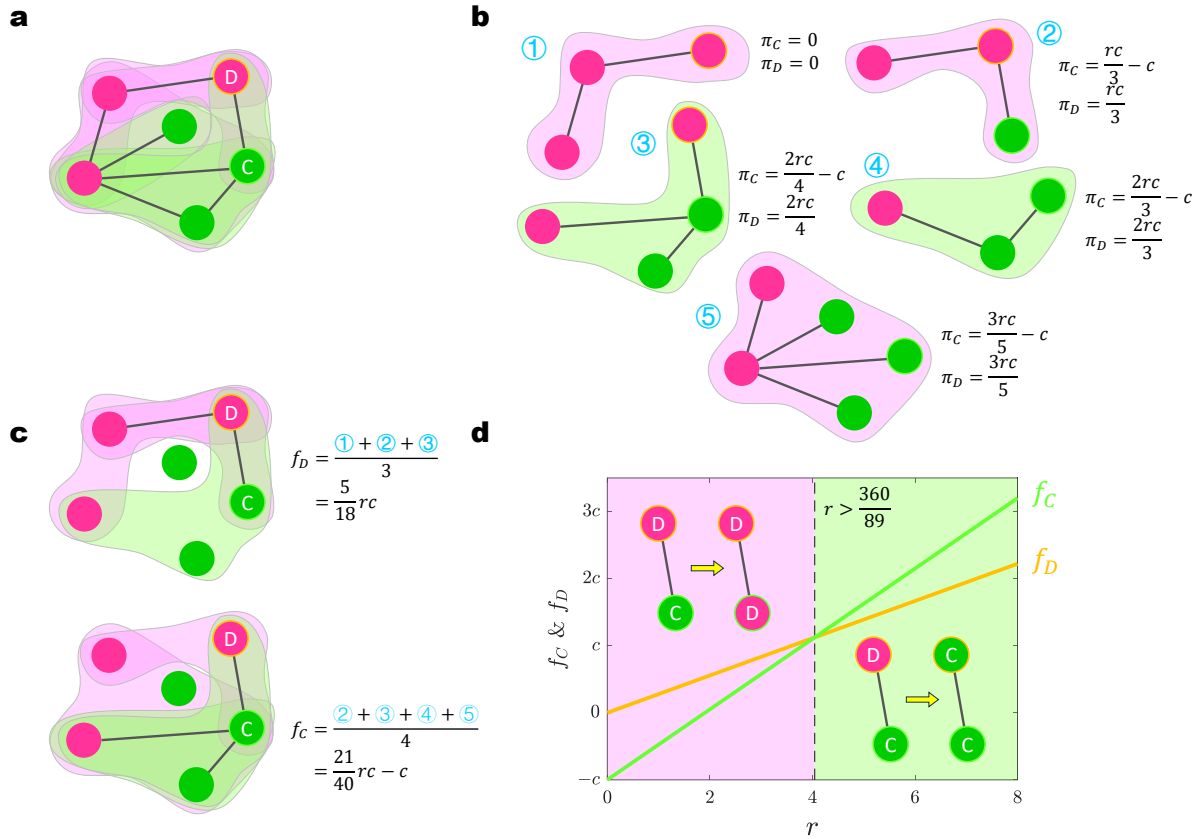


Figure 1. The spatial public goods game (PGG) on a general network. **a**, Each agent organizes a PGG in the group of itself and its neighbors. **b**, In each PGG, payoffs for cooperation and defection are calculated by Eq. (1). Obviously, $\pi_D > \pi_C$, defectors always have higher payoffs than cooperators, seemingly driving cooperation towards defection. **c**, Since each agent organizes a PGG, an agent plays not only the PGG organized by itself, but also the PGGs organized by its neighbors. We average the payoffs from these PGGs as an agent's actual payoff. **d**, The emergence of spatial reciprocity. For the presented two agents, their actual payoffs $f_C > f_D$ when $r > 360/89$, driving defection towards cooperation.

this approximation was unable to capture the effect of clustering coefficients and higher-order interactions. Su et al.^{39,40} addressed this limitation and further identified the theory of PGGs in finite structured populations. Both of these theories were confined to homogeneous network structures, where all individuals have the same number of neighbors. The most general results on heterogeneous networks were still lacking.

Here, we develop the fundamental theory for the evolution of cooperation in spatial PGGs on any population structure. We identify the critical synergy factor for cooperation success on different network structures, which is accurate under weak selection. With the proposal theory, we examine a large number of networks, finding that a class of structures, especially the star graph, significantly facilitates cooperation in spatial PGGs. We also explore spatial PGGs on a series of random networks, from random regular, small-world, to scale-free, verifying the general effects of local structures, such as the clustering coefficient, on cooperation. Finally, we analyze all small networks and four empirical networks from the Gahuku–Gama alliance structure to body contact interactions among North American barn swallows, where cooperation consistently emerge on these structures across various model details in spatial PGGs, while in pairwise games it cannot. The results imply that spatial PGGs are the possible universal interaction modes in the real world compared to pairwise games.

Results

PGGs on any population structure

In a public goods game (PGG) of G players, one can choose either cooperation (C) or defection (D). A cooperator pays a cost c and contributes to the common pool, while a defector does not pay or contribute. Suppose there are g_C ($0 \leq g_C \leq G$) cooperators, then the total contributions to the common pool are $g_C c$. These contributions are multiplied by a synergy factor r ($r > 1$) to produce the public goods $rg_C c$, which are evenly redistributed among all players, with each player sharing $rg_C c/G$.

Therefore, the payoffs for cooperation and defection, π_C and π_D , are

$$\pi_C = \frac{rg_{CC}}{G} - c, \quad (1a)$$

$$\pi_D = \frac{rg_{CC}}{G}. \quad (1b)$$

On the one hand, since the synergy factor $r > 1$, cooperation brings more benefits from the group perspective. On the other hand, defection can also share the public goods produced by cooperators, so the payoff of defectors is higher than that of cooperators. The social dilemma thus emerges in this scenario.

In this work, we study the PGG on general indirect and unweighted network structures. Suppose a population of size N , with the node set denoted by $\mathcal{N} = \{1, 2, \dots, N\}$. Each node represents an agent. The relation between agents i and j is represented by k_{ij} : if they are neighbors, $k_{ij} = 1$; otherwise, $k_{ij} = 0$. The number of agent i 's neighbors is thus $k_i = \sum_{j \in \mathcal{N}} k_{ij}$. For convenience, we denote the neighbor set of agent i as \mathcal{N}_i : if j is i 's neighbor ($k_{ij} = 1$), then $j \in \mathcal{N}_i$.

On such a network structure, each agent i organizes a group of $G_i = k_i + 1$ members, involving its neighbors and itself (Fig. 1a). A PGG is played in this group, and the payoffs are calculated according to Eq. (1) (Fig. 1b). Also, agent i participates in k_i PGGs organized by its k_i neighbors. In summary, the agent i plays $1 + k_i = G_i$ PGGs organized by itself and its neighbors. We take the averaged payoffs that agent i receives from these G_i PGGs as the actual payoff, $f_i = (1/G_i) \sum_{j \in \mathcal{G}_i} \pi_i^j$ (Fig. 1c), where π_i^j denotes the payoff that agent i receives in the PGG organized by agent j and $\mathcal{G}_i = \{i\} \cup \mathcal{N}_i$ denotes the group organized by agent i . The actual payoffs f_i have an influence on strategy evolution (Fig. 1d).

In each elementary step, a random focal agent i is selected to update its strategy. The actual payoff f_i is calculated and transformed to fitness, $F_i = \exp(\delta f_i)$ ^{14,19}. Here, $0 < \delta \ll 1$ is a weak selection strength since the explored game dynamics play only marginal roles in the complex real world. The neighbors of agent i also have their actual payoffs and fitnesses calculated for comparison. Commonly used update rules, such as pairwise comparison (PC)⁴¹, death-birth (DB)⁷, or birth-death (BD)⁴², vary in details but follow the same principle that strategies with higher payoffs have an advantage to propagate. We present the PC rule here as an example and have other update rules in [Supplementary Note 1](#). The focal agent i selects a random neighbor $j \in \mathcal{N}_i$ and adopts the strategy of agent j with a probability

$$W_{i \leftarrow j} = \frac{1}{1 + \exp(-\delta(f_j - f_i))}. \quad (2)$$

Otherwise, agent i keeps the current strategy unchanged. The probability in Eq. (2) can also be interpreted as $W_{i \leftarrow j} = F_j / (F_i + F_j)$, with the probability of keeping the strategy understood as $F_i / (F_i + F_j)$.

We move to the next elementary step, where another random focal agent i is selected to update the strategy, and this process continues (Methods). We track the fraction of cooperators ρ_C in the population, which changes over time and may reach steady states after sufficient steps.

Conditions for cooperation success

Although the cooperation fraction could fluctuate in non-equilibrium intermediate states for a very long time under a non-marginal selection¹⁸, it often quickly reaches a fixation state under weak selection. There are only two fixation states, full cooperation ($\rho_C = 1$) and full defection ($\rho_C = 0$).

To define when natural selection favors cooperation, we first consider the case where selection is absent, i.e., neutral drift ($\delta = 0$), where the two strategies are indistinguishable. In a full defection population, a random mutant cooperator has a certain probability to propagate and flip the population to full cooperation, and vice versa. This probability is called the fixation probability. On heterogeneous networks, the fixation probability may vary for different initial mutant nodes, despite equal chances for each node to start as the mutant. The average fixation probability over all nodes is $1/N$ ¹¹. In this way, we can define selection favoring cooperation (or evolution favoring cooperation): On the basis of neutral drift, if a marginal effect of spatial PGGs through a weak selection strength ($0 < \delta \ll 1$) has a tendency to increase the average fixation probability of a mutant cooperator (i.e., make it exceeds $1/N$), then evolution favors cooperation.

We find that evolution favors cooperation in spatial PGGs once the synergy factor r exceeds a critical value r^* . The critical synergy factor r^* depends on the network structure and model details. Under the PC update rule, the condition for cooperation success on any network structure is

$$r > \frac{\tau^{(1)}}{\Upsilon^{(1)}}. \quad (3)$$

Here, $\tau^{(n)} = \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \tau_{ij}$ and $\Upsilon^{(n)} = \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \Upsilon_{ij}$ can be obtained on the given network structure. First, $p_{ij}^{(n)}$ is the probability of arriving at node j after n -step random walks starting from node i . Second, the values of τ_{ij} between nodes i and j

can be determined by solving the following linear equations with $\tau_{ji} \equiv \tau_{ij}$:

$$\begin{cases} \tau_{ij} = 1 + \frac{1}{2k_i} \sum_{l \in \mathcal{N}_i} \tau_{jl} + \frac{1}{2k_j} \sum_{l \in \mathcal{N}_j} \tau_{il}, & \text{if } j \neq i, \\ \tau_{ij} = 0, & \text{if } j = i. \end{cases} \quad (4)$$

Third, the values of Υ_{ij} between nodes i and j can be calculated by these τ_{ij} values:

$$\Upsilon_{ij} = \frac{1}{G_i} \left(\frac{\tau_{ij} + \sum_{l \in \mathcal{N}_i} (\tau_{jl} - \tau_{il})}{G_i} + \sum_{l \in \mathcal{N}_i} \frac{(\tau_{jl} - \tau_{il}) + \sum_{\ell \in \mathcal{N}_i} (\tau_{j\ell} - \tau_{i\ell})}{G_l} \right). \quad (5)$$

Note that $\Upsilon_{ii} = 0$ because $\tau_{ii} = 0$. However, usually $\Upsilon_{ij} \neq \Upsilon_{ji}$ due to the various group sizes on heterogeneous networks.

We are thus able to determine the cooperation condition for spatial PGGs on all network structures. Similar to Eq. (3), we also identify the condition under the DB rule, which is $r > \tau^{(2)}/\Upsilon^{(2)}$. See [Supplementary Note 1](#) for the conditions under the BD rule and all theoretical deductions for other model details.

Theoretical networks

We start the discussion from theoretical networks, which are uniquely determined by their network parameters. The conditions for cooperation success in spatial PGGs can be expressed as a function of these network parameters.

A simple example is the star graph, composed of one hub and n leaves (Fig. 2a). We find that star graphs consistently promote cooperation in spatial PGGs for $r > 4$ under all update rules (and in the infinite population limit $n \rightarrow \infty$). This differs from the previous conclusion in pairwise donation games (DGs), where cooperation cannot emerge on star graphs¹⁰, and the so-called graph surgery, such as connecting the hubs of two stars, was a way to rescue cooperation in pairwise games. Here, if we further connect two hubs, we get a super structure to support cooperation in spatial PGGs: With a variation of model details (accumulated instead of averaged payoffs), the condition for cooperation success is $r > 1$, that is, cooperation is maximally favored.

The intuition of $r^* = 4$ for star graphs can be interpreted as 2×2 , two groups for a leaf times two players in the group organized by the leaf. We explain this under the DB update rule, which has $r^* \equiv 4$ regardless of population size. Since the focal agent's payoff does not influence strategy updates (only neighbors compete for the focal vacant position), a focal leaf always takes the strategy of the hub neighbor. On the other hand, when the hub updates, the competition happens among all leaves and is independent of the hub. Therefore, the hub's payoff does not work, and we only need to discuss the competition among all leaves. A leaf participates in 2 PGGs, organized by itself and the hub neighbor. In the PGG organized by itself, the payoff is $r(1 + x_H)c/2 - c$ if cooperating or $rx_Hc/2$ if defecting ($x_H = 1$ if the hub cooperates and $x_H = 0$ if it defects), where the overlapping term $rx_Hc/2$ can be eliminated. In the PGG organized by the hub, the payoff is $rg_{CC}/(n+1) - c$ or $rg_{CC}/(n+1)$, where the overlapping term $rg_{CC}/(n+1)$ can be eliminated. In this way, a cooperator leaf has a higher payoff than a defector leaf if and only if $(rc/2 - 2c)/2 > 0$ or $r/2 - 2 > 0$. That is, $r > r^* = 2 \times 2 = 4$.

On the $L \times L$ square lattices of different neighborhoods ($G = 5$ and $G = 9$) with periodic boundary conditions, our results meet with the previous work on regular networks^{31,40} (Fig. 2b). Observing these results, we notice that cooperation conditions on star graphs could be even more advantageous than regular graphs, as the critical synergy factor rises with group size on regular graphs but remains constant on star graphs. For example, the square lattice of $G = 9$ has $r^* \approx 5.79$ under death-birth, which is worse than the constant $r^* = 4$ of the star graph.

Fig. 2b also shows results on more heterogeneous networks. For m fully connected hubs with n leaves on each, we have $r^* = 4m/(2m-1)$ (PC update) and $r^* = (12m-4)/(9m-7)$ (DB update) for large n , which are $r^* = 2$ and $r^* = 4/3$ for large m . As another minor extension, for ceiling fans with n fans (each has 2 leaves), we have $r^* = 21/4$ for PC update and $r^* = 27/8$ for DB update. The DB update promotes cooperation on ceiling fans, while the PC rule inhibits it (compared to the original star graph). This is because the DB rule can utilize the clustering coefficient to promote cooperation in spatial PGGs, which will be explained in the next section. Our predictions for these theoretical networks are also validated by agent-based simulations under different update rules (Fig. 2c).

General roles of local structures

Next, we investigate the general roles of local structures on classic random networks, from random regular (ER), small-world (SW), and scale-free (BA) by Fig. 3a-c. These networks are randomly generated by given parameters, hence the need of studying a lot of random structures under the same network parameters.

Random regular networks reflect the effect of average degree (Fig. 3a). We use the Erdős-Rényi (ER) algorithm⁴³ to generate random regular networks. Among $N = 100$ nodes, there can be at most $N(N-1)/2$ edges. Let the probability of an

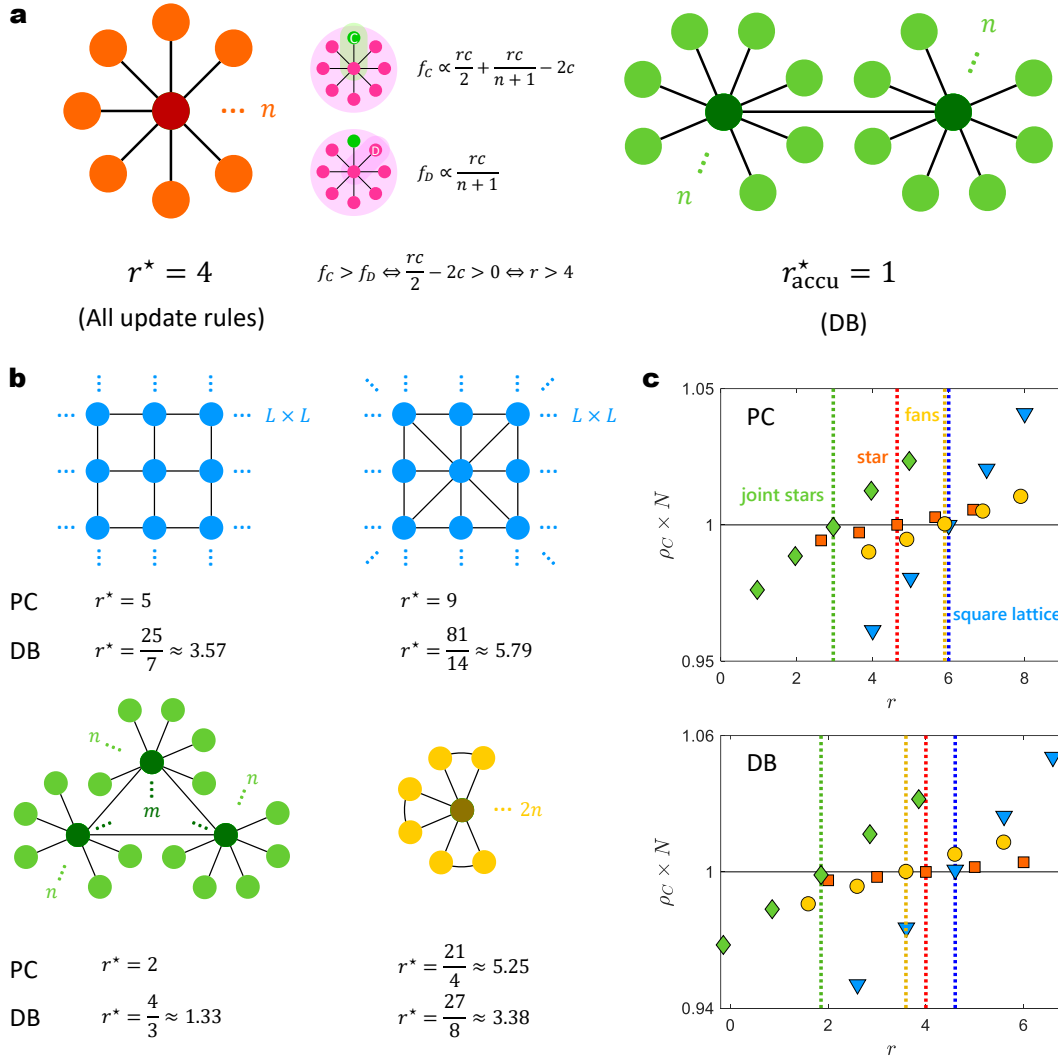


Figure 2. Cooperation conditions for spatial PGGs on homogeneous and heterogeneous networks. **a**, Star graphs support cooperation in PGGs as simple as when $r > 4$, and the essence of which is 2×2 : There are 2 groups for a leaf, with 2 players in its own group. When using accumulated payoffs, connecting the hubs of two or more star graphs leads to $r_{\text{accu}}^* = 1$ under the DB rule, which maximally supports cooperation. **b**, Comparison with other networks, including square lattices with von Neumann (left) and Moore (right) neighborhoods, joint stars with any number of hubs, and ceiling fans. The r^* values reported here are for infinite population size; see [Supplementary Note 2](#) for finite size. **c**, Agent-based simulations confirm the theoretical predictions on $L = 5$ square lattice with von Neumann neighborhood, $n = 9$ star, $m = 3$ & $n = 9$ joint stars, and $n = 9$ ceiling fans. The dots represent the average cooperation fraction in the steady states (Methods), while the dashed lines are theoretical r^* over which $\rho_C > 1/N$.

edge existing be p , then the average degree of the network is approximately $\langle k \rangle \approx p(N - 1)$, which increases with p . We find that the critical synergy factor in spatial PGGs increases with p , which indicates that an average degree increase is detrimental to cooperation. This is consistent with the conclusions in pairwise games^{7,10}.

Small-world networks (SW) reflect the role of network cohesion, measured by clustering coefficients (Fig. 3b). We use the Watts–Strogatz algorithm⁴⁴ to generate small-world networks. Starting from a ring network of $N = 100$ where each node has $2d$ neighbors within distance $d = 2$ on both sides. Then, each node rewires the other end of each edge with probability p (the same edge cannot rewire twice; no self-loops or duplicate edges). The clustering coefficient, measuring network cohesion, is approximately $\frac{3(d-1)}{2(2d-1)}(1-p)^3$ (accurate in large populations)⁴⁷, which decreases as p increases. The critical synergy factor r^* decreases with p , which indicates that network cohesion promotes cooperation. This result is consistent with the previous conclusions on regular graphs⁴⁰ ([Supplementary Note 2](#)), which can be understood as an impact of “higher-order interactions”⁴⁸.

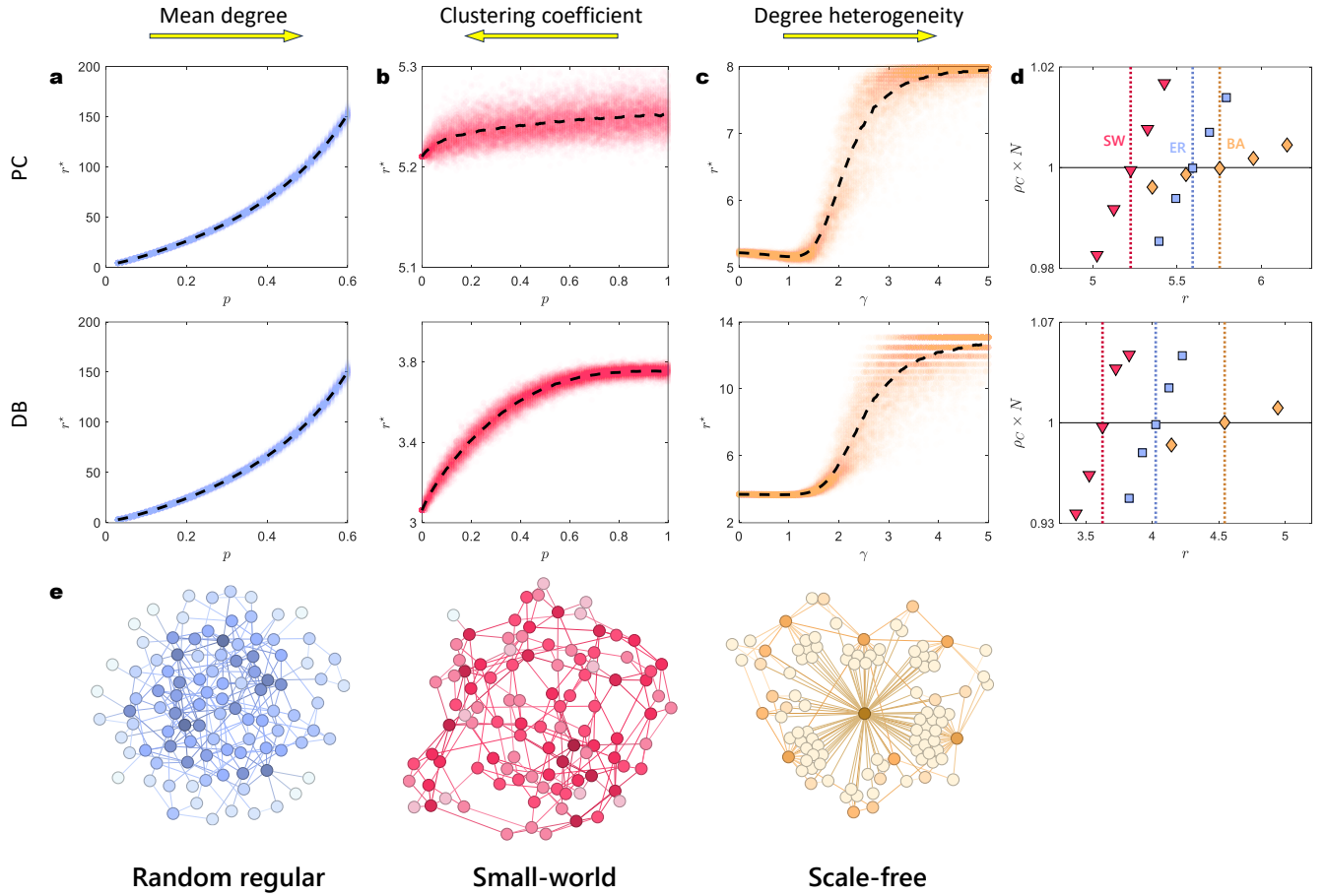


Figure 3. Effects of local structures on cooperation in spatial PGGs. **a**, Critical synergy factor r^* as a function of connecting probability p on random regular graphs (ER)⁴³. The increasing average degree inhibits cooperation. **b**, r^* as a function of rewiring probability p on small-world networks (SW)⁴⁴ with $d = 2$. The increasing clustering coefficient promotes cooperation. **c**, r^* as a function of generated degree distribution heterogeneity γ on scale-free networks (BA)^{45,46} with $m = 2$. The increasing degree heterogeneity initially promotes but ultimately inhibits cooperation. In **a–c**, each point on dashed lines is the average result of 1,000 randomly generated networks (totaling 58,000 in **a**, 101,000 in **b**, 101,000 in **c**). All networks are of size $N = 100$ and are connected. **d**, Agent-based simulations on selected sample networks confirm theoretical predictions. For ER, $p = 4/99$; for SW, $d = 2$, $p = 0.5$; for BA, $m = 2$, $\gamma = 2$. **e**, Visualization of the sample network structures in agent-based simulations.

Notably, network cohesion only significantly promotes cooperation under the DB rule. On the one hand, agents interact with second-order neighbors in spatial PGGs (while pairwise games only involve first-order neighbors). On the other hand, the essence of DB update is competition with second-order neighbors, while the PC rule is with first-order neighbors⁹. The combination of second-order game interactions and strategy competitions provides enough reach to be influenced by triangle motifs and network cohesion.

Scale-free networks reflect the impact of degree heterogeneity on cooperation (Fig. 3c). We use the algorithm proposed by Krapivsky et al.⁴⁶, which is an improvement of the Barabási–Albert (BA)⁴⁵, to generate scale-free networks. We start with $m = 2$ isolated initial nodes. The remaining $N - m = 98$ nodes then join the existing network one by one. Each new node selects m existing nodes (hence the approximate average degree $\langle k \rangle = 2m(1 - m/N)$). The probability of selecting node i is proportional to k_i^γ , where γ is the strength of preferential attachment, determining the degree heterogeneity. When $\gamma = 1$, we reduce to the standard BA scale-free network. We find that increasing degree heterogeneity γ initially slightly promotes cooperation but ultimately hinders cooperation. In other words, a moderate network heterogeneity is most conducive to cooperation⁴⁹, which is more pronounced under the DB rule. This is different from some previous studies on pairwise games^{50,51}

The conclusions are robust and could be more subtle across other model details (Fig. S2). The theoretical results on these

random networks are also supported by agent-based simulations (Fig. 3d) on selected structures as shown in Fig. 3d. According to these simulations with consistent average degrees, the small-world network ($\langle k \rangle = 4$) is most conducive to cooperation, the random regular ($\langle k \rangle \approx 4$) is secondary, and the scale-free ($\langle k \rangle = 3.84$) is least conducive.

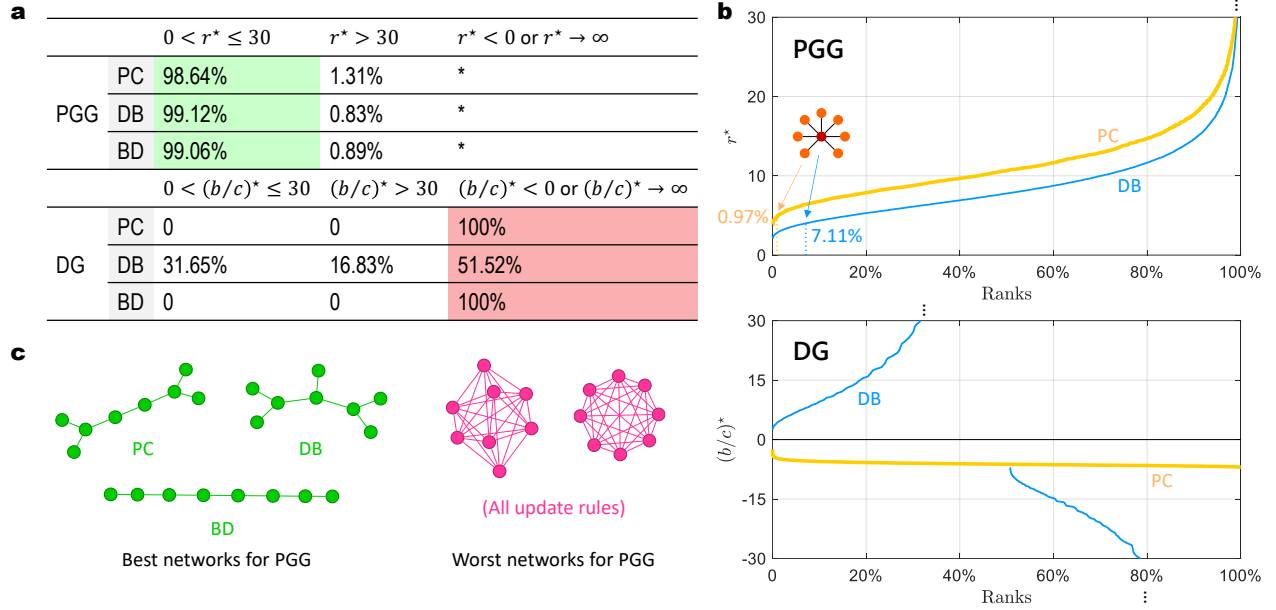


Figure 4. Cooperation emerges consistently in spatial PGGs on almost all networks under different update rules, outperforming pairwise DGs. **a**, Among all 12,111 networks of sizes $3 \leq N \leq 8$, the fraction of networks classified by their critical synergy factors. Almost all networks have $0 < r^* \leq 30$ in supporting cooperation. The symbol * means that the only structure that does not support cooperation is the fully connected network. In contrast, for pairwise DGs, cooperation is only possible under DB update, with more than half of networks not supporting cooperation. **b**, The ranks of all 11,117 networks of size $N = 8$ in supporting cooperation for PGGs and DGs under PC and DB update rules. The star graph ranks the top 0.97% (PC) and 7.11% (DB). The results in spatial PGGs are consistent under different update rules, while in pairwise DGs they are quite different. **c**, The best and worst networks of size $N = 8$ for cooperation in spatial PGGs. The best networks differ with update rules. The worst two networks are consistent under all update rules, which are the fully connected (right) and a similar network (left).

Fundamental advantages of PGGs

We further investigate the cooperation conditions of spatial PGGs on all small networks. For population sizes $3 \leq N \leq 8$, there are 2 ($N = 3$), 6 ($N = 4$), 21 ($N = 5$), 112 ($N = 6$), 853 ($N = 7$), and 11,117 ($N = 8$) possible network structures, respectively. The critical synergy factors on these 12,111 networks are summarized in Fig. 4a. There are 98.64% (PC), 99.12% (DB), and 99.06% (BD) networks where the critical synergy factors are $0 < r^* \leq 30$. The conditions for cooperation success are relaxed on almost all network structures under various update rules. There are only a few networks (1.31% for PC, 0.83% for DB, and 0.89% for BD) with strict cooperation conditions of $r^* > 30$. The last category is $r^* < 0$ or $r^* \rightarrow \infty$ (we also numerically categorize $r > 10^3$ as $r \rightarrow \infty$ here). When $r^* < 0$, the cooperation condition becomes $r < r^*$ and cooperation is impossible for meaningful $r > 1$. The symbol * means that the only network structure that does not support cooperation in spatial PGGs is the fully connected network.

In comparison, cooperation cannot thrive well in pairwise interactions, with the donation game (DG)¹⁰ as an example. A cooperator donates b to the other player by paying c , where $b > c$. The studied quantity here is the benefit-to-cost ratio, b/c , which has a critical value $b/c > (b/c)^*$ over which cooperation is favored. We find the critical values $(b/c)^*$ fall within unfavorable intervals. Under PC and BD updates, no network can support cooperation ($(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$ for 100%). Under the DB update, more than half networks (51.52%) cannot support cooperation, with only 31.65% of structures having relaxed cooperation conditions. These conclusions on group PGGs and pairwise DGs remain valid if we use accumulated payoffs (Figs. S3 and S4).

From these insights, we see a fundamental advantage of spatial PGGs, that cooperation can emerge on all network structures (excepted fully connect) and under various update rules, which outperforms pairwise DGs. In the emergence of cooperation, two-step random walks play a key role because the second step may loop back and generate personal benefits. The essence

of PC and BD updates is the competition between first-order neighbors ($r^* = \tau^{(1)}/\Gamma^{(1)}$), while DB update is the competition between second-order neighbors⁹ ($r^* = \tau^{(2)}/\Gamma^{(2)}$). This is the reason why only the DB rule can produce cooperation in pairwise DGs. However, in spatial PGGs, agents have already interacted with second-order neighbors by playing the games organized by neighbors. Being one order higher in payoff calculation, it compensates for the deficiency of the single order under the PC and BD updates in strategy competition. This compensation effect by second-order group organizations explains the fundamental advantage of spatial PGGs that cooperation can emerge under all update rules with even the minimal order of competition.

We show the ranks of all 11,117 networks of size $N = 8$ under PC and DB rules in Fig. 4b. Networks with smaller critical synergy factors r^* are more advantageous for cooperation success and rank earlier. We see that PC and DB updates show consistency in their rank trends, with the DB rule slightly more favorable for cooperation. In contrast, the ranks in pairwise DGs are quite different under PC and DB rules. This is curious, since there is no qualitative difference between these update rules, which consistently assume the advantages of high payoffs in strategy evolution. Here, spatial PGGs show another fundamental advantage, that they perform consistently across various details in update rules.

Additionally, it is worth mentioning that the star graph ranks in the top 0.97% and 7.11% for the PC and DB updates, which agrees with our previous conclusion that star graphs are among the most useful networks for cooperation in spatial PGGs. More generally, we present the best and worst networks of size $N = 8$ as shown in Fig. 4c. The best networks vary in different update rules, but they all have low degrees. From BD, PC, to DB rules, the best networks shift from linear to star-like in shape. The worst networks are consistent across all update rules, which have high degrees, from fully connected to similar structures.

Robustness of PGGs in the real world

The fundamental advantages of spatial PGGs were presented on small networks of sizes $N \leq 8$, but we are also interested in the robustness of these advantages in large real-world systems. Here, we utilize four empirical network datasets and calculate the critical synergy factors for cooperation success on these real network structures (Fig. 5). The results are presented across various model details, including three update rules (PC, DB, and BD) and two payoff calculations (averaged (ave) and accumulated (accu)).

The first two scenarios are human societies, including a pre-modern and a modern social structure. The pre-modern example is 16 tribes of the Gahuku–Gama alliance structure of the Eastern Central Highlands of New Guinea^{52,53} (Fig. 5a), with normalized critical synergy factors $r^*/\langle k \rangle = 1.83 \sim 2.33$ in PGGs and benefit-to-cost ratios $(b/c)^*/\langle k \rangle < 0$ & $(b/c)^*/\langle k \rangle \geq 23.26$ in DGs. The modern social structure is 29 seventh-grade students in Australia, connected by whom they would prefer to work with⁵⁴ (Fig. 5b), with normalized critical synergy factors $r^*/\langle k \rangle = 1.44 \sim 2.13$ and benefit-to-cost ratios $(b/c)^*/\langle k \rangle < 0$ & $(b/c)^*/\langle k \rangle \geq 12.28$. The third scenario is an ecological structure, the trophic interactions among 69 major taxonomic groups of the various everglades habitats in South Florida ecosystems^{52,55,56} (Fig. 5c), which has $r^*/\langle k \rangle = 1.37 \sim 2.03$ and $(b/c)^*/\langle k \rangle < 0$ & $(b/c)^*/\langle k \rangle \geq 17.44$. The last scenario is an animal social network, constructed with edges of body contact interactions among 17 North American barn swallows^{52,57} (Fig. 5d), with $r^*/\langle k \rangle = 1.58 \sim 2.24$ and $(b/c)^*/\langle k \rangle < 0$ & $(b/c)^*/\langle k \rangle \geq 8.94$. Since the cooperation conditions increase with average degrees, we mentioned the corresponding normalized conditions above for comparison.

According to these real data, we verify that spatial PGGs can support cooperation on these real-world population structures with relaxed conditions and are robust across all model details. In contrast, pairwise DGs do not support cooperation on these real structures. This contradicts the empirical fact that cooperation can evolve from various natural and social systems, where the strategy evolution mechanisms could be diverse and not limited to death-birth. Yet, pairwise DGs only support cooperation under special model details (death-birth) and the cooperation conditions are strict, which cannot explain the consistent emergence of cooperation in these real-world systems. From this perspective, spatial PGGs could instead be one of the universal interaction modes in the real world, across human society, ecological and animal social systems, where cooperation emerge consistently.

We also see that accumulated payoffs are slightly more conducive to cooperation in spatial PGGs (the only exceptions are the DB update in “classmates” and “swallows”). This is also consistent with our intuition that payoffs from different groups are physically accumulated in the real world. In contrast, the averaged payoffs serve normalization and theoretical analysis, which are less conducive to cooperation on the studied real-world networks.

Discussion

The instinct of selfish organisms seems to contradict the ubiquity of cooperation. Previous mathematical models have been developed to explain this in the framework of pairwise games^{10,42}, which were unable to provide consistent support for cooperation on diverse network structures and model details. As a complement, PGGs reflects the common pattern of group interactions in both nature and human systems. Importantly, spatial PGGs capture the empirical fact that individuals not only interact with their direct friends, but also with their second-order neighbors in the circle organized by the direct friends^{58–60}.

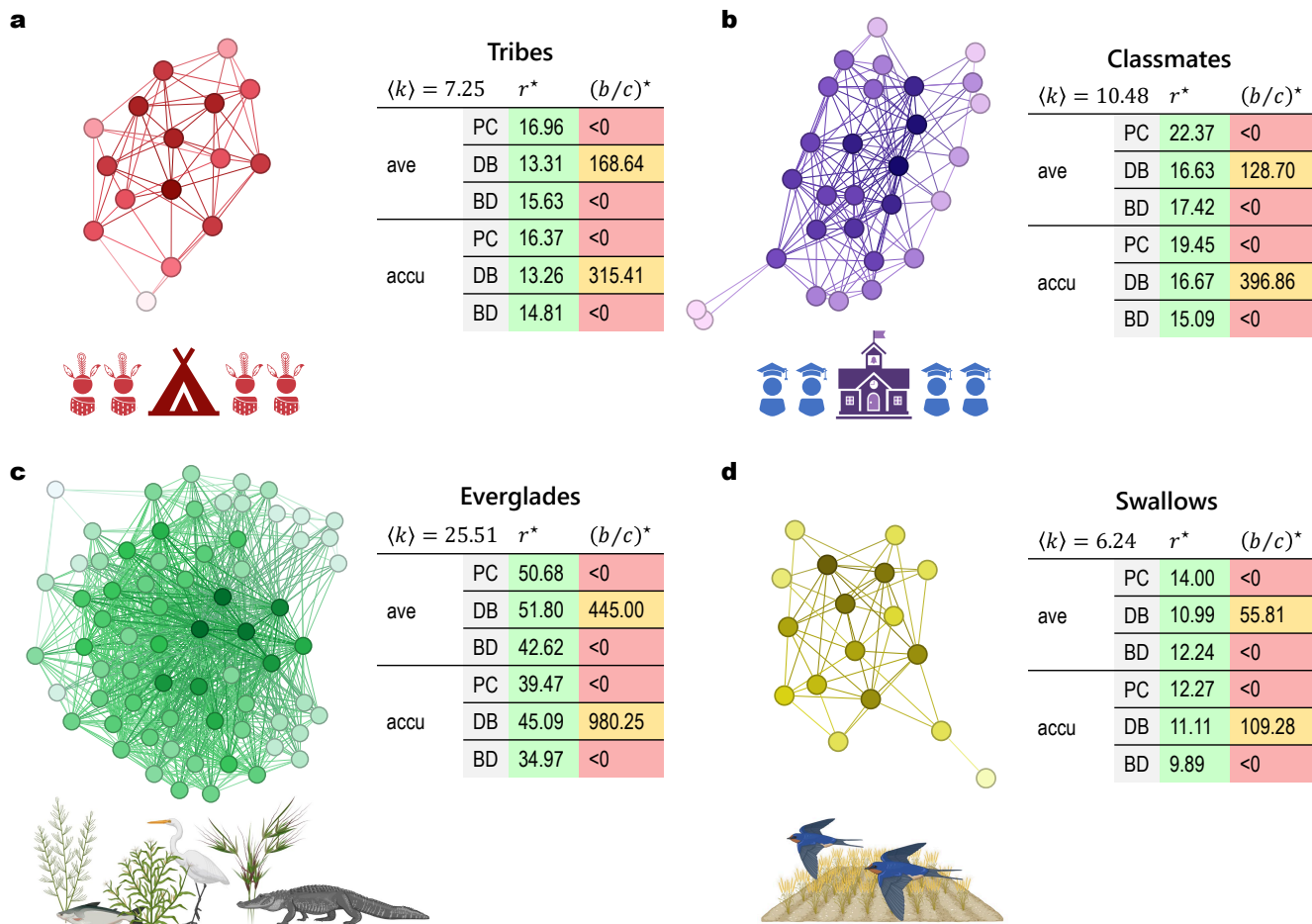


Figure 5. Spatial PGGs could be a universal interaction mode for cooperation in the real world. We analyze spatial PGGs on four empirical network structures, where the cooperation conditions are consistently relaxed across various model details in spatial PGGs. In contrast, the conditions for cooperation are strict and inconsistent across different model details in pairwise DGs. The examined empirical systems include: **a**, 16 tribes of the Gahuku–Gama alliance structure of the Eastern Central Highlands of New Guinea^{52,53}. **b**, 29 seventh-grade students in Victoria, Australia, connected by whom they would prefer to work with⁵⁴. **c**, The networks of trophic interactions that occur among the 69 major taxonomic groups of everglades habitats in South Florida ecosystems^{52,55,56}. **d**, The network of body contact interactions among 17 North American barn swallows^{52,57}.

Here, we provide a fundamental theory for the evolution of cooperation in spatial PGGs on arbitrary network structures. Cooperation emerge in the population as the synergy factor increases, with the efficiency varying depending on network structures. We obtain the formulas of the critical synergy factor for the emergence of cooperation on any network structure and across all model details. The formulas are accurate in the weak selection limit. Using the proposed fundamental theory, we find that a class of networks, including the star graph, which were considered unfavorable for cooperation in pairwise games^{10,13}, can significantly promote cooperation in spatial PGGs. On the star graph, cooperation only requires a simple condition $r > 4$, which could be even more advantageous than regular graphs. When two or more stars are connected by their hubs, we obtain an ultimate cooperation supporter: the condition for cooperation is $r > 1$ when using accumulated payoffs.

We examine the general roles of local structures by studying 260,000 classic random networks, from random-regular, small-world, to scale-free. Similar to the pairwise game, increasing the average degree or its heterogeneity is detrimental to cooperation in spatial PGGs. However, small-world networks reveal the positive effect of network cohesion (measured by clustering coefficient) on cooperation in spatial PGGs. This can be explained by second-order interactions: individuals play games organized by neighbors and therefore interact with second-order neighbors⁶¹. Similar phenomena about were also observed in parallel studies on higher-order networks^{48,62,63}. Our conclusions remain robust and could be more subtle under other model details, from payoff calculations to strategy updates (Fig. S2).

More generally, we test all 12,111 networks of sizes $3 \leq N \leq 8$. We find that spatial PGGs consistently produce cooperation on all network structures under the investigated update rules (the only exception is the fully connected network). In contrast, pairwise games fail to produce cooperation on most networks¹⁰. The PC and BD rules, which follow the same assumptions of individual selfishness, even fail to produce cooperation on any structured populations (Figs. 4, S3, and S4). This contrasts the common sense that cooperation is ubiquitous in natural and social systems where the evolutionary details may vary. Instead, the consistent results in spatial PGGs meet with our common sense.

To verify the robustness of spatial PGGs in the real world, we further examined four empirical networks, with scenarios from primitive tribes, junior students, everglades, and barn swallows. It is found that cooperation cannot emerge effectively on these real networks through pairwise games. Instead, the spatial PGG can produce consistent cooperation across all kinds of evolutionary details on these real networks. Our results thus imply that spatial PGGs could be a universal interaction mode for the emergence of cooperation in real-world systems.

Our ground-breaking theory lays the foundation for exploring a large number of extended mechanisms⁶ in spatial PGGs, such as inertia^{31,33}, on general population structures. One can investigate the additional effects of different network structures on these mechanisms. One can also study the evolutionary dynamics of spatial PGGs on multi-layer⁶⁴ and dynamic networks⁶⁵, which were only studied in pairwise games previously. More fundamentally, one can generalize our results to weighted networks and also study the outcomes with arbitrary initial conditions¹². The algorithm for group interactions based on second-order neighbors can also be used to study other multiplayer games, which bear unknown complexity^{66,67}.

Methods

Theoretical analysis of cooperation success

Here, we briefly summarize the mathematical derivations of the cooperation condition in spatial PGGs. The system state is denoted by $\mathbf{x} = (x_1, x_2, \dots, x_N)$, where $x_i = 1$ if agent i cooperates and $x_i = 0$ if it defects. In this way, we can formalize the payoff calculation on networks. The actual payoff of agent i at system state \mathbf{x} , denoted by $f_i(\mathbf{x})$, is expressed as

$$\begin{aligned} f_i(\mathbf{x}) &= \frac{1}{G_i} \sum_{l \in \mathcal{G}_i} \left(\frac{r \sum_{\ell \in \mathcal{G}_l} x_\ell c}{G_l} - x_i c \right) \\ &= \frac{1}{1+k_i} \left[\left(\frac{r(x_i + \sum_{l \in \mathcal{N}_i} x_l) c}{k_i + 1} - x_i c \right) + \sum_{l \in \mathcal{N}_i} \left(\frac{r(x_l + \sum_{\ell \in \mathcal{N}_l} x_\ell) c}{k_l + 1} - x_i c \right) \right]. \end{aligned} \quad (6)$$

Agent i plays $G_i = 1 + k_i$ games, organized by itself and its k_i neighbors $l \in \mathcal{N}_i$, which form the group $\mathcal{G}_i = \{i\} \cup \mathcal{N}_i$. In the game organized by agent l , there are G_l players in the group.

In the weak selection limit ($0 < \delta \ll 1$), the dynamics of strategy evolution almost reduces to the Voter model⁶⁸, where the marginal role of games does not influence strategy distributions. Therefore, in previous literature^{10,11} (or [Supplementary Note 1](#)), the conditions for cooperation success were obtained under neutral drift ($\delta = 0$) and remain unchanged for different payoff calculations.

In other words, the key difference in analyzing spatial PGGs is the payoff calculation. We only need to substitute the payoffs of spatial PGGs, i.e., Eq. (6), into the previously obtained cooperation conditions, which (under the PC rule) is

$$\frac{1}{4N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij} \mathbb{E}_{\text{RMC}}^\circ [(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0. \quad (7)$$

Applying $f_i(\mathbf{x})$ ($f_j(\mathbf{x})$) of Eq. (6) and considering

$$\tau_{ij} = \frac{\frac{1}{2} - \mathbb{E}_{\text{RMC}}^\circ [x_i x_j]}{K/4}, \quad (8)$$

we can calculate the condition of Eq. (7) as

$$\begin{aligned} & \sum_{i,j \in \mathcal{N}} k_i p_{ij} \left\{ \left(\frac{rc}{(k_i + 1)^2} - c \right) \tau_{ij} + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (-\tau_{il} + \tau_{jl}) \right. \\ & \left. + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) - \left(\frac{rc}{(k_j + 1)^2} - c \right) (-\tau_{ij}) \right\} \end{aligned}$$

$$\begin{aligned}
& -\frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j+1} + \frac{1}{k_l+1} \right) (-\tau_{il} + \tau_{jl}) - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) \Big\} > 0 \\
\Leftrightarrow r & > \frac{2 \sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij} (\Upsilon_{ij} + \Upsilon_{ji})}, \tag{9}
\end{aligned}$$

which is equivalent to Eq. (3) in the main text, with τ_{ij} and Υ_{ij} obtained through Eqs. (4) and (5), respectively. See [Supplementary Note 1](#) for the meaning of mathematical symbols in Eqs. (7)–(9) and their detailed deductions.

The results under the DB and BD update rules, including those with accumulated payoffs, follow the same idea. We have the cooperation conditions (Eq. (S41) for DB and Eq. (S53) for BD) which are independent of payoff calculations. Applying $f_i(\mathbf{x})$ ($f_j(\mathbf{x})$) of Eq. (6) (or the ones for accumulated payoffs) and their respect τ_{ij} values leads to the resultant cooperation conditions, as detailed in [Supplementary Note 1](#).

Agent-based simulations

We conduct the agent-based simulations using the standard Monte Carlo method. The selection strength δ is between 0.01^{31,40} and 0.025^{10,69}, which is considered numerically weak. The cost of cooperation c is set to 1²⁰. In the initial state, there is one random cooperator and $N - 1$ defectors. Each full Monte Carlo step (MCS) contains N elementary time steps where a random focal agent is selected to update the strategy, so that every agent is updated once on average. We allow for up to 4×10^5 full MCS, which is theoretically infinite¹⁰. If the fraction of cooperators hits a fixation state ($\rho_C = 1$ or $\rho_C = 0$), we end the current run and record the result. If a fixation state is not reached within the maximally allowed MCS, we take the actual ρ_C at the last step as the result. We repeat the simulations 10^6 – 10^9 times independently under the given game parameters and network structure, averaging the final fraction of cooperators ρ_C in these runs as the actual result of ρ_C . If the average cooperation fraction $\rho_C > 1/N$, then evolution favors cooperation.

Data availability

All data generated or analysed during this study are included within the paper and its supplementary information file.

Author contributions

C.W. conceived and designed the research with contributions from Q.S; C.W. performed the calculations; C.W. and Q.S. wrote the paper and approved the submission.

Competing interests

The authors declare no competing interests.

Supplementary Information for Spatial public goods games on any population structure

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Contents

Supplementary Note 1: Conditions for cooperation success in spatial PGGs	13
1.1 Payoff calculation for PGGs on any network	13
1.2 General conditions for cooperation success	13
1.3 Pairwise comparison (PC)	15
1.4 Death-birth (DB)	19
1.5 Beath-dirth (BD)	22
1.6 Variation of the model: Accumulated payoff	26
1.6.1 Modified payoff calculation	27
1.6.2 Pairwise comparison	27
1.6.3 Death-birth	28
1.6.4 Birth-death	28
Supplementary Note 2: Applications to specific network structures	29
2.1 Regular graphs	29
2.2 Star graph	32
2.3 Hub-to-hub star	35
2.4 m -hub star	39
2.5 Ceiling fan	43
Supplementary Note 3: Some extensions to the donation game (DG)	46
3.1 Pairwise comparison	47
3.2 Death-birth	47
3.3 Birth-death	48
3.4 Variation of the model: Accumulated payoff	48
3.4.1 Pairwise comparison	48
3.4.2 Death-birth	49
3.4.3 Birth-death	49

Supplementary Note 1: Conditions for cooperation success in spatial PGGs

1.1 Payoff calculation for PGGs on any network

According to the description in the main text, agents participate in the PGGs organized by themselves and their neighbors, taking the averaged payoffs obtained in these games as the actual payoff. To formally express this algorithm, we denote the system state (i.e., the strategies of all agents) by $\mathbf{x} = (x_1, x_2, \dots, x_N)$, in a population of size N . If agent i cooperates, $x_i = 1$. If agent i defects, $x_i = 0$. The full cooperation state can be written by $\mathbf{C} = \mathbf{1} = (1, 1, \dots, 1)$ and the full defection state is $\mathbf{D} = \mathbf{0} = (0, 0, \dots, 0)$. The set consisting of all possible system states is denoted by \mathbf{X} .

We denote $f_i(\mathbf{x})$ as the averaged payoff that agent i obtains from the PGGs organized by itself and its neighbors at system state \mathbf{x} . Literally, $f_i(\mathbf{x})$ follows the calculation in Eq. (S1):

$$\begin{aligned} f_i(\mathbf{x}) &= \frac{1}{G_i} \sum_{l \in \mathcal{G}_i} \left(\frac{r \sum_{\ell \in \mathcal{G}_l} x_\ell c}{G_l} - x_i c \right) \\ &= \frac{1}{1+k_i} \left[\left(\frac{r(x_i + \sum_{l \in \mathcal{N}_i} x_l) c}{k_i + 1} - x_i c \right) + \sum_{l \in \mathcal{N}_i} \left(\frac{r(x_l + \sum_{\ell \in \mathcal{N}_l} x_\ell) c}{k_l + 1} - x_l c \right) \right] \\ &= \left(\frac{rc}{(k_i + 1)^2} - c \right) x_i + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) x_l + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} x_\ell. \end{aligned} \quad (\text{S1})$$

In the first line, $\mathcal{G}_i = \{i\} \cup \mathcal{N}_i$ is the group containing oneself and its neighbors. In the second line, the former item is the PGG organized by agent i , and the latter item is the PGGs organized by its neighbors $l \in \mathcal{N}_i$. The third line is a simplification of the second line for later use.

1.2 General conditions for cooperation success

According to Ref.¹¹, the general condition for cooperation success on arbitrary network structures is

$$\mathbb{E}_{\text{RMC}}^\circ [\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0, \quad (\text{S2})$$

where, the upper-right corner label \circ of a quantity is to take the value of this quantity at $\delta = 0$ (neutral drift). The upper-right corner label $'$ of a quantity is to calculate the first-order derivative of this quantity with respect to δ at $\delta = 0$.

$\hat{\Delta}_{\text{sel}}(\mathbf{x})$ is the change in the cooperation fraction within an elementary Monte Carlo step (MCS) due to strategy learning (i.e., selection, abbreviated as “sel”), weighted by reproduction numbers, at system state \mathbf{x} . The expression of $\hat{\Delta}_{\text{sel}}(\mathbf{x})$ is⁷⁰

$$\hat{\Delta}_{\text{sel}}(\mathbf{x}) = \frac{1}{N} \sum_{i \in \mathcal{N}} x_i (\hat{b}_i(\mathbf{x}) - \hat{d}_i(\mathbf{x})), \quad (\text{S3})$$

where $\hat{b}_i(\mathbf{x})$ and $\hat{d}_i(\mathbf{x})$ represent the birth and death probabilities of agent i , weighted by reproduction numbers, respectively.

Before weighted by reproduction numbers, $\hat{b}_i(\mathbf{x})$ and $\hat{d}_i(\mathbf{x})$ are given by $b_i(\mathbf{x}) = \sum_{j \in \mathcal{N}} e_{ij}(\mathbf{x})$ and $d_i(\mathbf{x}) = \sum_{j \in \mathcal{N}} e_{ji}(\mathbf{x})$. An agent's strategy reproduces if learned by other agents, or dies if the agent adopts the strategy of others. Here, $e_{ij}(\mathbf{x})$ is the probability that agent i transmits its strategy to agent j , determined by specific strategy update rules.

The birth and death probabilities of agent i weighted by reproduction numbers, $\hat{b}_i(\mathbf{x})$ and $\hat{d}_i(\mathbf{x})$, take the following form:

$$\hat{b}_i(\mathbf{x}) = \sum_{j \in \mathcal{N}} e_{ij}(\mathbf{x}) v_j, \quad (\text{S4a})$$

$$\hat{d}_i(\mathbf{x}) = \sum_{j \in \mathcal{N}} e_{ji}(\mathbf{x}) v_i, \quad (\text{S4b})$$

where, v_i and v_j represent the reproduction numbers of agents i and j , respectively. The reproduction numbers $\{v_i\}_{i \in \mathcal{N}}$ of all agents in the population are defined based on the fact that under neutral drift, natural selection does not influence the change in strategy proportions ($\hat{\Delta}_{\text{sel}}^\circ(\mathbf{x}) = 0$). Additionally, considering normalization, the average reproduction number for each agent is set to 1. Therefore, the following equation holds¹¹:

$$\hat{d}_i^\circ(\mathbf{x}) = \hat{b}_i^\circ(\mathbf{x}) \Leftrightarrow \sum_{j \in \mathcal{N}} e_{ji}^\circ(\mathbf{x}) v_i = \sum_{j \in \mathcal{N}} e_{ij}^\circ(\mathbf{x}) v_j, \quad (\text{S5a})$$

$$\sum_{i \in \mathcal{N}} v_i = N. \quad (\text{S5b})$$

The first line results from $\hat{\Delta}'_{\text{sel}}(\mathbf{x}) = 0$, while the second line is for normalization. From Eqs. (S5), the reproduction numbers of all agents can be solved given the network structure and update rules.

Since there is no expected change in $\hat{\Delta}_{\text{sel}}(\mathbf{x})$ caused by natural selection under neutral drift, we can study the first derivative of $\hat{\Delta}_{\text{sel}}(\mathbf{x})$ with respect to δ at $\delta = 0$ in order to quantitatively analyze $\hat{\Delta}_{\text{sel}}(\mathbf{x})$. Substituting Eqs. (S4) into Eq. (S3) and taking the derivative, we obtain

$$\begin{aligned}\hat{\Delta}'_{\text{sel}}(\mathbf{x}) &= \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i (e'_{ij}(\mathbf{x}) v_j - e'_{ji}(\mathbf{x}) v_i) \\ &= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) (e'_{ij}(\mathbf{x}) v_j - e'_{ji}(\mathbf{x}) v_i).\end{aligned}\quad (\text{S6})$$

Taking the equivalent form in the second line (based on the symmetry between i and j) can facilitate subsequent calculations. At this point, by calculating the strategy reproduction probabilities $\{e_{ij}(\mathbf{x})\}_{i,j \in \mathcal{N}, \mathbf{x} \in \mathbf{X}}$ and reproduction numbers $\{v_i\}_{i \in \mathcal{N}}$ under the given update rule, we can obtain the corresponding value of $\hat{\Delta}'_{\text{sel}}(\mathbf{x})$.

Another concept that appears in Eq. (S2) is $\mathbb{E}_{\text{RMC}}[\cdot]$, where RMC stands for the rare-mutation conditional distribution. Before defining RMC, it is necessary to define MSS: the mutation-selection stationary distribution. This distribution describes the system's state when a mutation mechanism is present. The introduction of the mutation mechanism is intended to construct a mathematically tractable, complete Markov chain. Suppose that in each elementary Monte Carlo step, the focal agent mutates with probability u (i.e., mutation): it switches to either cooperation or defection with probability $1/2$ respectively. With the remaining probability $1 - u$, the agent update the strategy (i.e., selection) according to the given update rule. The weak mutation limit $u \rightarrow 0$ leads to the model we study in the main text, where strategy updates depend solely on the strategy update rule.

$\Pi_{\text{MSS}}(\mathbf{x})$ represents the probability that the system stabilizes at state \mathbf{x} under the mutation-selection stationary distribution. The sum of probabilities for all possible stationary states is 1, i.e., $\sum_{\mathbf{x} \in \mathbf{X}} \Pi_{\text{MSS}}(\mathbf{x}) = 1$. Obviously, in the weak mutation limit $u \rightarrow 0$, the system has only two stable states: full cooperation ($\mathbf{x} = \mathbf{C}$) and full defection ($\mathbf{x} = \mathbf{D}$): $\Pi_{\text{MSS}}(\mathbf{C}) \rightarrow \rho_C / (\rho_C + \rho_D)$, $\Pi_{\text{MSS}}(\mathbf{D}) \rightarrow \rho_D / (\rho_C + \rho_D)$ ^{71,72}. For $\mathbf{x} \notin \{\mathbf{C}, \mathbf{D}\}$, $\Pi_{\text{MSS}}(\mathbf{x}) \rightarrow 0$.

On this basis, the rare-mutation conditional (RMC) distribution describes the distribution of system states among possible states other than full cooperation and full defection as $u \rightarrow 0$. $\Pi_{\text{RMC}}(\mathbf{x})$ represents the probability that the system is in state \mathbf{x} under the RMC distribution, satisfying the normalization condition $\sum_{\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}} \Pi_{\text{RMC}}(\mathbf{x}) = 1$ (note that here \mathbf{x} is restricted to $\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}$, i.e., $\mathbf{x} \notin \{\mathbf{C}, \mathbf{D}\}$). By this definition, $\Pi_{\text{RMC}}(\mathbf{x})$ can be derived from $\Pi_{\text{MSS}}(\mathbf{x})$,

$$\Pi_{\text{RMC}}(\mathbf{x}) = \lim_{u \rightarrow 0} \frac{\Pi_{\text{MSS}}(\mathbf{x})}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})}. \quad (\text{S7})$$

$\mathbb{E}_{\text{MSS}}[\cdot]$ and $\mathbb{E}_{\text{RMC}}[\cdot]$ represent the expected value under the corresponding distribution, i.e., the sum of the products of all possible state variables in $[\cdot]$ and their respective probabilities. For example, given a function $f(\mathbf{x})$ of the system state \mathbf{x} , we have

$$\mathbb{E}_{\text{MSS}}[f(\mathbf{x})] = \sum_{\mathbf{x} \in \mathbf{X}} \Pi_{\text{MSS}}(\mathbf{x}) f(\mathbf{x}), \quad (\text{S8})$$

$$\mathbb{E}_{\text{RMC}}[f(\mathbf{x})] = \sum_{\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}} \Pi_{\text{RMC}}(\mathbf{x}) f(\mathbf{x}). \quad (\text{S9})$$

Later, we will need the following property: in the limit $u \rightarrow 0$, for any agent $i \in \mathcal{N}$, we have $\mathbb{E}_{\text{MSS}}^\circ[x_i] = 1/2$ and $\mathbb{E}_{\text{RMC}}^\circ[x_i] = 1/2$. To prove, under neutral drift, strategies C and D are indistinguishable and thus interchangeable. From $\rho_C = \rho_D$ and $\rho_C + \rho_D = 1$, we can solve for $\rho_C = \rho_D = 1/2$. Therefore, based on $\Pi_{\text{MSS}}(\mathbf{C}) \rightarrow \rho_C / (\rho_C + \rho_D)$ and $\Pi_{\text{MSS}}(\mathbf{D}) \rightarrow \rho_D / (\rho_C + \rho_D)$, we have $\Pi_{\text{MSS}}(\mathbf{C}), \Pi_{\text{MSS}}(\mathbf{D}) \rightarrow 1/2$. Consequently, $\mathbb{E}_{\text{MSS}}^\circ[x_i] = 1/2 \times 1 + 1/2 \times 0 = 1/2$. Similarly, due to the interchangeability of C and D , we have $\Pi_{\text{RMC}}(\mathbf{x}) = \Pi_{\text{RMC}}(\mathbf{1} - \mathbf{x})$, and we can calculate $\mathbb{E}_{\text{RMC}}^\circ[x_i] = (1/2) \sum_{\mathbf{x} \notin \{\mathbf{C}, \mathbf{D}\}} (\Pi_{\text{RMC}}(\mathbf{x}) x_i + \Pi_{\text{RMC}}(\mathbf{1} - \mathbf{x})(1 - x_i)) = (1/2) \sum_{\mathbf{x} \notin \{\mathbf{C}, \mathbf{D}\}} \Pi_{\text{RMC}}(\mathbf{x})(x_i + 1 - x_i) = 1/2$.

We define a quantity K ,

$$K = \lim_{u \rightarrow 0} \frac{u}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})}. \quad (\text{S10})$$

Ref.¹¹ has shown that K exists and is positive.

Later, we will need another property: let $\phi(\mathbf{x})$ be a function that satisfies $\phi(\mathbf{C}) = \phi(\mathbf{D}) = 0$, then we can calculate and find that $\mathbb{E}_{\text{RMC}}[\phi(\mathbf{x})]$ and $\mathbb{E}_{\text{MSS}}[\phi(\mathbf{x})]$ are related by Eq. (S11):

$$\mathbb{E}_{\text{RMC}}[\phi(\mathbf{x})] = \sum_{\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}} \Pi_{\text{RMC}}(\mathbf{x}) \phi(\mathbf{x})$$

$$\begin{aligned}
&= \sum_{\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}} \lim_{u \rightarrow 0} \frac{\Pi_{\text{MSS}}(\mathbf{x})}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})} \phi(\mathbf{x}) \\
&= \lim_{u \rightarrow 0} \frac{\sum_{\mathbf{x} \in \mathbf{X} \setminus \{\mathbf{C}, \mathbf{D}\}} \Pi_{\text{MSS}}(\mathbf{x}) \phi(\mathbf{x})}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})} \\
&= \lim_{u \rightarrow 0} \frac{\sum_{\mathbf{x} \in \mathbf{X}} \Pi_{\text{MSS}}(\mathbf{x}) \phi(\mathbf{x})}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})} \\
&= \lim_{u \rightarrow 0} \frac{\mathbb{E}_{\text{MSS}}[\phi(\mathbf{x})]}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})} \\
&= \left(\lim_{u \rightarrow 0} \frac{u}{1 - \Pi_{\text{MSS}}(\mathbf{C}) - \Pi_{\text{MSS}}(\mathbf{D})} \right) \left(\lim_{u \rightarrow 0} \frac{\mathbb{E}_{\text{MSS}}[\phi(\mathbf{x})]}{u} \right) \\
&= K \left(\lim_{u \rightarrow 0} \frac{\mathbb{E}_{\text{MSS}}[\phi(\mathbf{x})]}{u} \right) \\
&= K \left. \frac{d\mathbb{E}_{\text{MSS}}[\phi(\mathbf{x})]}{du} \right|_{u=0}. \tag{S11}
\end{aligned}$$

The final step in Eq. (S11) employs L'Hôpital's Rule, which allows for the calculation of the limit when both the numerator and denominator approach zero by taking the derivative of the numerator and denominator separately.

By utilizing the relationship between $\mathbb{E}_{\text{MSS}}[\cdot]$ and $\mathbb{E}_{\text{RMC}}[\cdot]$, we can start from the MSS distribution and, using stability, derive a recurrence relation by strategy updates within an elementary MCS under the given update rule. Then, by taking the weak mutation limit, we can obtain the results needed for the evolutionary dynamics (RMC distribution) as discussed in the main text (see details below).

1.3 Pairwise comparison (PC)

For the PC rule, the probability $e_{ij}(\mathbf{x})$ that agent i transmits its strategy to agent j can be calculated as follows. In each elementary MCS, agent j is selected as the focal agent with probability $1/N$ to update the strategy. Agent i is chosen as the reference by agent j with probability $k_{ji}/k_j = p_{ji}$ (i.e., $k_{ji}/k_j = 1/k_j$ if i neighbors j ; otherwise this probability is zero), and agent i 's strategy is learned by agent j with the learning probability $W_{j \leftarrow i}(\mathbf{x})$ (defined by Eq. (2) in the main text). That is,

$$e_{ij}(\mathbf{x}) = \frac{p_{ji}}{N} \times W_{j \leftarrow i}(\mathbf{x}) = \frac{p_{ji}}{N} \times \frac{1}{1 + \exp(-\delta(f_i(\mathbf{x}) - f_j(\mathbf{x})))}. \tag{S12}$$

Taking $\delta = 0$ in Eq. (S12), we have

$$e_{ij}^{\circ}(\mathbf{x}) = \frac{p_{ji}}{2N}. \tag{S13}$$

Taking the derivative of Eq. (S12) with respect to δ at $\delta = 0$, we have

$$e'_{ij}(\mathbf{x}) = \frac{p_{ji}}{4N} (f_i(\mathbf{x}) - f_j(\mathbf{x})). \tag{S14}$$

Substituting Eq. (S13) into Eqs. (S5), we obtain

$$\sum_{j \in \mathcal{N}} e_{ji}^{\circ}(\mathbf{x}) v_i = \sum_{j \in \mathcal{N}} e_{ij}^{\circ}(\mathbf{x}) v_j \Leftrightarrow \frac{v_i}{2N} = \sum_{j \in \mathcal{N}} \frac{p_{ji}}{2N} v_j, \tag{S15a}$$

$$\sum_{i \in \mathcal{N}} v_i = N. \tag{S15b}$$

Given that $p_{ji} = k_{ji}/k_j$, the solution to Eqs. (S15) is $v_i = k_i/\langle k \rangle$ for $i \in \mathcal{N}$, where $\langle k \rangle = (\sum_{j \in \mathcal{N}} k_j)/N$ represents the average degree of all nodes on the network.

Substituting $v_i = k_i/\langle k \rangle$ and Eq. (S14) into Eq. (S6), we can calculate $\hat{\Delta}'_{\text{sel}}(\mathbf{x})$ under the PC rule:

$$\begin{aligned}
\hat{\Delta}'_{\text{sel}}(\mathbf{x}) &= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) (e'_{ij}(\mathbf{x}) v_j - e'_{ji}(\mathbf{x}) v_i) \\
&= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) \left(\frac{p_{ji}}{4N} (f_i(\mathbf{x}) - f_j(\mathbf{x})) \frac{k_j}{\langle k \rangle} - \frac{p_{ij}}{4N} (f_j(\mathbf{x}) - f_i(\mathbf{x})) \frac{k_i}{\langle k \rangle} \right)
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) \frac{k_{ij}}{4N \langle k \rangle} (f_i(\mathbf{x}) - f_j(\mathbf{x}) - f_j(\mathbf{x}) + f_i(\mathbf{x})) \\
&= \frac{1}{4N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} (x_i - x_j) k_i p_{ij} (f_i(\mathbf{x}) - f_j(\mathbf{x})).
\end{aligned} \tag{S16}$$

Substituting Eq. (S16) into Eq. (S2), we obtain the condition for cooperation success under the PC rule:

$$\mathbb{E}_{\text{RMC}}^{\circ}[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0 \Leftrightarrow \frac{1}{4N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0. \tag{S17}$$

Note that quantities such as N , k_i , and p_{ij} are input parameters with constant expected values. Therefore, they can be factored out of $\mathbb{E}_{\text{RMC}}^{\circ}[\cdot]$.

We first calculate $\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ in Eq. (S17). Inserting the payoffs in spatial PGGs, $f_i(\mathbf{x})$ and $f_j(\mathbf{x})$, by using Eq. (S1) and notice that r and c are also input parameters that remain constant, we have

$$\begin{aligned}
&\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] \\
&= \mathbb{E}_{\text{RMC}}^{\circ} \left[\left(\frac{rc}{(k_i + 1)^2} - c \right) (x_i^2 - x_i x_j) + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (x_i x_l - x_j x_l) \right. \\
&\quad + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_i} (x_i x_{\ell} - x_j x_{\ell}) - \left. \left(\frac{rc}{(k_j + 1)^2} - c \right) (x_i x_j - x_j^2) \right. \\
&\quad \left. - \frac{rc}{k_j + 1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (x_i x_l - x_j x_l) - \frac{rc}{k_j + 1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_j} (x_i x_{\ell} - x_j x_{\ell}) \right] \\
&= \left(\frac{rc}{(k_i + 1)^2} - c \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i^2] - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]) + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_l]) \\
&\quad + \frac{rc}{k_i + 1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_i} (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_{\ell}] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_{\ell}]) - \left(\frac{rc}{(k_j + 1)^2} - c \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j^2]) \\
&\quad - \frac{rc}{k_j + 1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_l]) \\
&\quad - \frac{rc}{k_j + 1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_j} (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_{\ell}] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_{\ell}]).
\end{aligned} \tag{S18}$$

Since $x_i \in \{0, 1\}$, we have $x_i^2 = x_i$, and thus $\mathbb{E}_{\text{RMC}}^{\circ}[x_i^2] = \mathbb{E}_{\text{RMC}}^{\circ}[x_i] = 1/2$ for $i \in \mathcal{N}$. The remaining work is to calculate $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ for all $i, j \in \mathcal{N}$.

We begin with the MSS distribution. Since the MSS distribution is stationary, the expected system's state remains unchanged after strategy updates. We aim to derive a recurrence relation by working through the strategy update within an elementary MCS. For convenience of calculation, we study $\mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)]$, which has a useful property $\mathbb{E}_{\text{MSS}}^{\circ}[x_i - 1/2] = 0$ due to $\mathbb{E}_{\text{MSS}}^{\circ}[x_i] = 1/2$.

Integrating the mutation mechanism described in Section 1.2, the possible events that happen within an elementary MCS can be classified into the following categories based on their impact on x_i or x_j .

- Agent i is selected as the focal agent with probability $1/N$ to update its strategy:
 - (i) The focal agent i mutates with probability u , becoming cooperation ($x_i \leftarrow 1$) with probability $1/2$, or defection ($x_i \leftarrow 0$) with probability $1/2$;
 - (ii) Agent i updates its strategy under the PC rule with probability $1 - u$. With probability p_{il} , agent i chooses reference agent l ($l \in \mathcal{N}$), learning l 's strategy, $x_i \leftarrow x_l$, with probability $W_{i \leftarrow l}^{\circ}(\mathbf{x}) = 1/2$ (note that we are discussing neutral drift now), or keeping the current strategy x_i unchanged with probability $1 - W_{i \leftarrow l}^{\circ}(\mathbf{x}) = 1/2$. The probabilities summarized here are consistent with the strategy transmission probability $e_{ii}^{\circ} = p_{il}/(2N)$ in Eq. (S13), but the probability $1/N$ to select focal agent i is not repeatedly considered.
- Similarly, agent j is selected as the focal agent with probability $1/N$ to update its strategy:

(i) The focal agent j mutates with probability u , becoming cooperation ($x_j \leftarrow 1$) with probability $1/2$, or defection ($x_j \leftarrow 0$) with probability $1/2$;

(ii) Agent j updates its strategy under the PC rule with probability $1 - u$. With probability p_{jl} , agent j chooses reference agent l ($l \in \mathcal{N}$), learning l 's strategy, $x_j \leftarrow x_l$, with probability $W_{j \leftarrow l}^\circ(\mathbf{x}) = 1/2$, or keeping the current strategy x_j unchanged with probability $1 - W_{j \leftarrow l}^\circ(\mathbf{x}) = 1/2$.

- The focal agent is one of the remaining $N - 2$ agents other than i and j , with probability $1/N$. Since only the focal agent's strategy may update, both x_i and x_j remain unchanged.

Combining all the above possibilities of an elementary MCS, we can obtain the following recurrence relation under the MSS distribution:

$$\begin{aligned}
& \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
&= \frac{1}{N} \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(1 - 1/2)(x_j - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(0 - 1/2)(x_j - 1/2)] \right) \right. \\
&\quad \left. + (1 - u) \sum_{l \in \mathcal{N}} p_{il} \left(W_{i \leftarrow l}^\circ(\mathbf{x}) \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + (1 - W_{i \leftarrow l}^\circ(\mathbf{x})) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right) \right\} \\
&\quad + \frac{1}{N} \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(1 - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(0 - 1/2)] \right) \right. \\
&\quad \left. + (1 - u) \sum_{l \in \mathcal{N}} p_{jl} \left(W_{j \leftarrow l}^\circ(\mathbf{x}) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] + (1 - W_{j \leftarrow l}^\circ(\mathbf{x})) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right) \right\} \\
&\quad + (N - 2) \frac{1}{N} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
&= \frac{1}{N} \left\{ 0 + (1 - u) \sum_{l \in \mathcal{N}} \frac{p_{il}}{2} \left(\mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right) \right\} \\
&\quad + \frac{1}{N} \left\{ 0 + (1 - u) \sum_{l \in \mathcal{N}} \frac{p_{jl}}{2} \left(\mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] + \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right) \right\} \\
&\quad + (N - 2) \frac{1}{N} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]. \tag{S19}
\end{aligned}$$

We integrate $\mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]$ into the left-hand side and denote $\underline{x}_i = x_i - 1/2$ for convenience. Then, we have

$$\mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] = \frac{1 - u}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right). \tag{S20}$$

We define variables $\phi_{ij}(\mathbf{x})$,

$$\phi_{ij}(\mathbf{x}) = \underline{x}_i \underline{x}_j - \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \underline{x}_l \underline{x}_j + \sum_{l \in \mathcal{N}} p_{jl} \underline{x}_i \underline{x}_l \right), \tag{S21}$$

which satisfy the properties $\phi_{ij}(\mathbf{C}) = 1/4 - 1/2 \times (1/4 + 1/4) = 0$ and similarly, $\phi_{ij}(\mathbf{D}) = 0$. Therefore, $\phi_{ij}(\mathbf{x})$ can be used to relate the MSS and RMC distributions through Eq. (S11) as $u \rightarrow 0$.

We first calculate $\mathbb{E}_{\text{MSS}}^\circ[\phi_{ij}(\mathbf{x})]$. Writing down the expected value of Eq. (S21) and using Eq. (S20), we have

$$\begin{aligned}
\mathbb{E}_{\text{MSS}}^\circ[\phi_{ij}(\mathbf{x})] &= \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] - \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right) \\
&= \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] - \frac{1}{1 - u} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] \\
&= -\frac{u}{1 - u} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j]. \tag{S22}
\end{aligned}$$

According to Eq. (S11), we can calculate $\mathbb{E}_{\text{RMC}}^{\circ}[\phi_{ij}(\mathbf{x})]$ from $\mathbb{E}_{\text{MSS}}^{\circ}[\phi_{ij}(\mathbf{x})]$,

$$\begin{aligned}
\mathbb{E}_{\text{RMC}}^{\circ}[\phi_{ij}(\mathbf{x})] &= K \left. \frac{d\mathbb{E}_{\text{MSS}}^{\circ}[\phi_{ij}(\mathbf{x})]}{du} \right|_{u=0} \\
&= K \left. \frac{d}{du} \right|_{u=0} \left(-\frac{u}{1-u} \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] \right) \\
&= K \left(-\mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] \Big|_{u=0} + 0 \right) \\
&= -K \left(\frac{1}{2} \times \left(1 - \frac{1}{2}\right) \left(1 - \frac{1}{2}\right) + \frac{1}{2} \times \left(0 - \frac{1}{2}\right) \left(0 - \frac{1}{2}\right) \right) \\
&= -\frac{K}{4}.
\end{aligned} \tag{S23}$$

In the second-to-last step, we recalled that as $u \rightarrow 0$, there are only two stationary states under MSS, $\mathbf{x} = \mathbf{1}$ or $\mathbf{x} = \mathbf{0}$, each with probability 1/2 under neutral drift.

On the other hand, we write down the expected value of Eq. (S21) under the RMC distribution and obtain another expression of $\mathbb{E}_{\text{RMC}}^{\circ}[\phi_{ij}(\mathbf{x})]$:

$$\mathbb{E}_{\text{RMC}}^{\circ}[\phi_{ij}(\mathbf{x})] = \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{RMC}}^{\circ}[x_l x_j] + \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] \right). \tag{S24}$$

Substituting $\mathbb{E}_{\text{RMC}}^{\circ}[\phi_{ij}(\mathbf{x})] = -K/4$ (Eq. (S23)) into Eq. (S24), we have

$$\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{RMC}}^{\circ}[x_l x_j] + \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] \right) - \frac{K}{4}. \tag{S25}$$

We define variables τ_{ij} for $i, j \in \mathcal{N}$,

$$\tau_{ij} = \frac{\frac{1}{2} - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]}{K/4}. \tag{S26}$$

Obviously, $\tau_{ii} = 0$ when $i = j$, because $\mathbb{E}_{\text{RMC}}^{\circ}[x_i^2] = 1/2$. Also, $\tau_{ij} = \tau_{ji}$, because $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_i]$.

When $i \neq j$, we can solve for the values of τ_{ij} by the recurrence relation. We know that $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ and $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l]$ have the following relation:

$$\begin{aligned}
\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] &= \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - 1/2)(x_j - 1/2)] \\
&= \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \frac{1}{2} \mathbb{E}_{\text{RMC}}^{\circ}[x_i] - \frac{1}{2} \mathbb{E}_{\text{RMC}}^{\circ}[x_j] + \frac{1}{4} \\
&= \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \frac{1}{4},
\end{aligned} \tag{S27}$$

and therefore, Eq. (S26) can be written as

$$\tau_{ij} = \frac{\frac{1}{2} - \left(\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] + \frac{1}{4} \right)}{K/4} = \frac{1 - 4\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]}{K} \tag{S28}$$

or

$$\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \frac{1 - K\tau_{ij}}{4}. \tag{S29}$$

Substituting Eq. (S29) into Eq. (S25), we obtain the recurrence relation of τ_{ij} :

$$\frac{1 - K\tau_{ij}}{4} = \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \frac{1 - K\tau_{lj}}{4} + \sum_{l \in \mathcal{N}} p_{jl} \frac{1 - K\tau_{il}}{4} \right) - \frac{K}{4}$$

$$\Leftrightarrow \tau_{ij} = 1 + \frac{1}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \tau_{lj} + \sum_{l \in \mathcal{N}} p_{jl} \tau_{il} \right). \quad (\text{S30})$$

The recurrence relation Eq. (S30), together with $\tau_{ii} = 0$, form a system of linear equations, through which all τ_{ij} values ($i, j \in \mathcal{N}$) can be determined on a given network structure.

Back to the halfway calculation in Eq. (S18) of the cooperation success condition. Substituting all $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ into Eq. (S18) with computable τ_{ij} using Eq. (S26), and then substituting the result into Eq. (S17), where the positive factors $K/4$ and $1/(4N^2 \langle k \rangle)$ can be canceled out, we arrive at the following condition for cooperation success:

$$\begin{aligned} & \mathbb{E}_{\text{RMC}}^{\circ}[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0 \\ \Leftrightarrow & \sum_{i,j \in \mathcal{N}} k_i p_{ij} \left\{ \left(\frac{rc}{(k_i+1)^2} - c \right) \tau_{ij} + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i+1} + \frac{1}{k_l+1} \right) (-\tau_{il} + \tau_{jl}) \right. \\ & + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_i} (-\tau_{i\ell} + \tau_{j\ell}) - \left. \left(\frac{rc}{(k_j+1)^2} - c \right) (-\tau_{ij}) \right. \\ & \left. - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j+1} + \frac{1}{k_l+1} \right) (-\tau_{il} + \tau_{jl}) - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_j} (-\tau_{i\ell} + \tau_{j\ell}) \right\} > 0 \\ \Leftrightarrow & r > \frac{2 \sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij} (\Upsilon_{ij} + \Upsilon_{ji})}, \end{aligned} \quad (\text{S31})$$

where Υ_{ij} are defined by (equivalent to Eq. (5) in the main text)

$$\Upsilon_{ij} = \frac{1}{k_i+1} \left(\frac{\tau_{ij} + k_i \sum_{l \in \mathcal{N}} p_{il} (\tau_{jl} - \tau_{il})}{k_i+1} + k_i \sum_{l \in \mathcal{N}} p_{il} \frac{(\tau_{jl} - \tau_{il}) + k_l \sum_{\ell \in \mathcal{N}} p_{l\ell} (\tau_{j\ell} - \tau_{i\ell})}{k_l+1} \right). \quad (\text{S32})$$

And according to the previous discussion, τ_{ij} can be solved by the following system of linear equations (equivalent to Eq. (4) in the main text):

$$\begin{cases} \tau_{ij} = 1 + \frac{1}{2} \sum_{l \in \mathcal{N}} (p_{il} \tau_{jl} + p_{jl} \tau_{il}), & \text{if } j \neq i, \\ \tau_{ij} = 0, & \text{if } j = i. \end{cases} \quad (\text{S33})$$

Finally, although usually $\Upsilon_{ij} \neq \Upsilon_{ji}$, we can still infer that $\sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ji} = \sum_{i,j \in \mathcal{N}} k_{ij} \Upsilon_{ji} = \sum_{j,i \in \mathcal{N}} k_{ji} \Upsilon_{ij} = \sum_{j,i \in \mathcal{N}} k_{ij} \Upsilon_{ij} = \sum_{j,i \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij}$, such that $\sum_{i,j \in \mathcal{N}} k_i p_{ij} (\Upsilon_{ij} + \Upsilon_{ji}) = 2 \sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij}$. Therefore, $\sum_{i,j \in \mathcal{N}} k_i p_{ij} (\Upsilon_{ij} + \Upsilon_{ji}) = 2 \sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij}$. As a result, Eq. (S31) can be further simplified as

$$r > \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij}}. \quad (\text{S34})$$

The right-hand side is the r^* value under the PC rule, as mentioned in the main text.

1.4 Death-birth (DB)

For the DB rule, the probability $e_{ij}(\mathbf{x})$ that agent i transmits its strategy to agent j can be calculated as follows. In each elementary MCS, agent j is selected as the focal agent with probability $1/N$ to update the strategy. Agent j 's strategy "dies", and agent i 's strategy occupies the vacant position with probability $W_{j \leftarrow i}(\mathbf{x})$, which is proportional to its fitness among j 's neighbors (see Eq. (S35)). That is,

$$e_{ij}(\mathbf{x}) = \frac{1}{N} \times W_{j \leftarrow i}(\mathbf{x}) = \frac{1}{N} \times \frac{k_{ji} F_i(\mathbf{x})}{\sum_{l \in \mathcal{N}} k_{jl} F_l(\mathbf{x})}. \quad (\text{S35})$$

Taking $\delta = 0$ in Eq. (S35), we have

$$e_{ij}^{\circ}(\mathbf{x}) = \frac{k_{ji}}{N k_j} = \frac{p_{ji}}{N}. \quad (\text{S36})$$

Taking the derivative of Eq. (S35) with respect to δ at $\delta = 0$, we have

$$e'_{ij}(\mathbf{x}) = \frac{1}{N} \frac{k_{ji}f_i(\mathbf{x})k_j - k_{ji}\sum_{l \in \mathcal{N}} k_{jl}f_l(\mathbf{x})}{k_j^2} = \frac{p_{ji}}{N} \left(f_i(\mathbf{x}) - \sum_{l \in \mathcal{N}} p_{jl}f_l(\mathbf{x}) \right). \quad (\text{S37})$$

Substituting Eq. (S36) into Eqs. (S5), we obtain

$$\sum_{j \in \mathcal{N}} e'_{ji}(\mathbf{x})v_i = \sum_{j \in \mathcal{N}} e'_{ij}(\mathbf{x})v_j \Leftrightarrow \frac{v_i}{N} = \sum_{j \in \mathcal{N}} \frac{p_{ji}}{N} v_j, \quad (\text{S38a})$$

$$\sum_{i \in \mathcal{N}} v_i = N. \quad (\text{S38b})$$

Similar to the PC rule, the solution to Eqs. (S38) is also $v_i = k_i/\langle k \rangle$ for $i \in \mathcal{N}$, where $\langle k \rangle = (\sum_{j \in \mathcal{N}} k_j)/N$ represents the average degree of all nodes.

Substituting $v_i = k_i/\langle k \rangle$ and Eq. (S37) into Eq. (S6), we can calculate $\hat{\Delta}'_{\text{sel}}(\mathbf{x})$ under the DB rule. We start from the first line in Eq. (S6),

$$\begin{aligned} \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i (e'_{ij}(\mathbf{x})v_j - e'_{ji}(\mathbf{x})v_i) &= \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i \left(\frac{p_{ji}}{N} \left(f_i(\mathbf{x}) - \sum_{l \in \mathcal{N}} p_{jl}f_l(\mathbf{x}) \right) \frac{k_j}{\langle k \rangle} - \frac{p_{ij}}{N} \left(f_j(\mathbf{x}) - \sum_{l \in \mathcal{N}} p_{il}f_l(\mathbf{x}) \right) \frac{k_i}{\langle k \rangle} \right) \\ &= \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i \frac{k_i p_{ij}}{N \langle k \rangle} \left(f_i(\mathbf{x}) - \sum_{l \in \mathcal{N}} p_{jl}f_l(\mathbf{x}) - f_j(\mathbf{x}) + \sum_{l \in \mathcal{N}} p_{il}f_l(\mathbf{x}) \right) \\ &= \frac{1}{N} \sum_{i \in \mathcal{N}} x_i \frac{k_i}{N \langle k \rangle} \left(f_i(\mathbf{x}) - \sum_{j \in \mathcal{N}} p_{ij} p_{jl} f_l(\mathbf{x}) - \sum_{j \in \mathcal{N}} p_{ij} f_j(\mathbf{x}) + \sum_{l \in \mathcal{N}} p_{il} f_l(\mathbf{x}) \right) \\ &= \frac{1}{N} \sum_{i \in \mathcal{N}} x_i \frac{k_i}{N \langle k \rangle} \left(f_i(\mathbf{x}) - \sum_{l \in \mathcal{N}} p_{il}^{(2)} f_l(\mathbf{x}) \right) \\ &= \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i \frac{k_i p_{ij}^{(2)}}{N \langle k \rangle} (f_i(\mathbf{x}) - f_j(\mathbf{x})), \end{aligned} \quad (\text{S39})$$

where $p_{ij}^{(2)}$ is defined as $\sum_{l \in \mathcal{N}} p_{il} p_{lj}$. Then, by comparing Eq. (S39) and Eq. (S6), we know that

$$\begin{aligned} \hat{\Delta}'_{\text{sel}}(\mathbf{x}) &= \frac{1}{N} \sum_{i,j \in \mathcal{N}} x_i (e'_{ij}(\mathbf{x})v_j - e'_{ji}(\mathbf{x})v_i) \\ &= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) (e'_{ij}(\mathbf{x})v_j - e'_{ji}(\mathbf{x})v_i) \\ &= \frac{1}{2N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} (x_i - x_j) k_i p_{ij}^{(2)} (f_i(\mathbf{x}) - f_j(\mathbf{x})). \end{aligned} \quad (\text{S40})$$

Substituting Eq. (S40) into Eq. (S2), we obtain the condition for cooperation success under the DB rule:

$$\mathbb{E}_{\text{RMC}}^{\circ}[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0 \Leftrightarrow \frac{1}{2N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0. \quad (\text{S41})$$

Similarly, we first calculate $\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ in Eq. (S41), which is completely the same as the one under the PC rule (see Eq. (S18) for the same result).

The remaining work is to calculate $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ for all $i, j \in \mathcal{N}$ under the DB rule. Similarly, we begin with the MSS distribution and aim to derive a recurrence relation by working through the strategy update within an elementary MCS. Under the DB rule, the possible events that happen within an elementary MCS can be classified into the following categories based on their impact on x_i or x_j .

- Agent i is selected as the focal agent with probability $1/N$ to update its strategy:
 - (i) The focal agent i mutates with probability u , becoming cooperation ($x_i \leftarrow 1$) with probability $1/2$, or defection ($x_i \leftarrow 0$) with probability $1/2$;

(ii) Agent i learns the strategy of a neighbor under the DB rule with probability $1 - u$. With probability $W_{i \leftarrow l}^\circ(\mathbf{x}) = p_{il}$, agent i learns the strategy of agent l , $x_i \leftarrow x_l$. Note that under the DB rule, $\sum_{l \in \mathcal{N}} W_{i \leftarrow l}^\circ(\mathbf{x}) = 1$; the focal agent cannot keep its own strategy.

- Similarly, agent j is selected as the focal agent with probability $1/N$ to update its strategy:

(i) The focal agent j mutates with probability u , becoming cooperation ($x_j \leftarrow 1$) with probability $1/2$, or defection ($x_j \leftarrow 0$) with probability $1/2$;

(ii) Agent j learns the strategy of a neighbor under the DB rule with probability $1 - u$. With probability $W_{j \leftarrow l}^\circ(\mathbf{x}) = p_{jl}$, agent j learns the strategy of agent l , $x_j \leftarrow x_l$.

- The focal agent is one of the remaining $N - 2$ agents other than i and j , with probability $1/N$. Since only the focal agent's strategy can update, both x_i and x_j remain unchanged.

Combining all the above possibilities of an elementary MCS, we can obtain the following recurrence relation under the MSS distribution:

$$\begin{aligned}
& \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
&= \frac{1}{N} \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(1 - 1/2)(x_j - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(0 - 1/2)(x_j - 1/2)] \right) \right. \\
&\quad \left. + (1 - u) \sum_{l \in \mathcal{N}} W_{i \leftarrow l}^\circ(\mathbf{x}) \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] \right\} \\
&\quad + \frac{1}{N} \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(1 - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(0 - 1/2)] \right) \right. \\
&\quad \left. + (1 - u) \sum_{l \in \mathcal{N}} W_{j \leftarrow l}^\circ(\mathbf{x}) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right\} \\
&\quad + (N - 2) \frac{1}{N} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
&= \frac{1}{N} \left\{ 0 + (1 - u) \sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] \right\} \\
&\quad + \frac{1}{N} \left\{ 0 + (1 - u) \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right\} \\
&\quad + (N - 2) \frac{1}{N} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]. \tag{S42}
\end{aligned}$$

Integrating $\mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]$ into the left-hand side and denoting $\underline{x}_i = x_i - 1/2$, we have

$$\mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] = \frac{1 - u}{2} \left(\sum_{l \in \mathcal{N}} p_{il} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{jl} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right), \tag{S43}$$

which is completely the same as the one under the PC rule (see Eq. (S20) for the result). Therefore, the subsequent steps are also the same and are not repeated here. We can ultimately use the defined variables τ_{ij} ,

$$\tau_{ij} = \frac{\frac{1}{2} - \mathbb{E}_{\text{RMC}}^\circ[x_i x_j]}{K/4}, \tag{S44}$$

to replace all $\mathbb{E}_{\text{RMC}}^\circ[x_i x_j]$.

Substituting all $\mathbb{E}_{\text{RMC}}^\circ[x_i x_j]$ into $\mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ (presented in Eq. (S18)) with computable τ_{ij} using Eq. (S44), and then substituting the result into Eq. (S17), where the positive factors $K/4$ and $1/(2N^2 \langle k \rangle)$ can be canceled out, we can organize and obtain the following condition for cooperation success:

$$\mathbb{E}_{\text{RMC}}^\circ[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0$$

$$\begin{aligned}
&\Leftrightarrow \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \left\{ \left(\frac{rc}{(k_i+1)^2} - c \right) \tau_{ij} + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i+1} + \frac{1}{k_l+1} \right) (-\tau_{il} + \tau_{jl}) \right. \\
&\quad + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) - \left. \left(\frac{rc}{(k_j+1)^2} - c \right) (-\tau_{ij}) \right. \\
&\quad \left. - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j+1} + \frac{1}{k_l+1} \right) (-\tau_{il} + \tau_{jl}) - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) \right\} > 0 \\
&\Leftrightarrow r > \frac{2 \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} (\Upsilon_{ij} + \Upsilon_{ji})}, \tag{S45}
\end{aligned}$$

where Υ_{ij} are also defined by Eq. (S32) (equivalent to Eq. (5) in the main text) and τ_{ij} can also be obtained by solving the system of Eqs. (S33) (or Eq. (4) in the main text).

According to Eq. (S82), we have $k_i p_{ij}^{(2)} = k_j p_{ji}^{(2)}$. Therefore, we can infer that $\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ji} = \sum_{i,j \in \mathcal{N}} k_j p_{ji}^{(2)} \Upsilon_{ji} = \sum_{j,i \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij}$, such that $\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} (\Upsilon_{ij} + \Upsilon_{ji}) = 2 \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij}$. Therefore, Eq. (S45) can be further simplified as

$$r > \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij}}, \tag{S46}$$

which gives the r^* value under the DB rule.

1.5 Beath-dirth (BD)

For the BD rule, the probability $e_{ij}(\mathbf{x})$ that agent i transmits its strategy to agent j can be calculated as follows. In each elementary MCS, agent i is selected as the focal agent with a probability $W_i(\mathbf{x})$ proportional to its fitness in the population,

$$W_i(\mathbf{x}) = \frac{F_i(\mathbf{x})}{\sum_{l \in \mathcal{N}} F_l(\mathbf{x})}, \tag{S47}$$

and transmits its strategy x_i to a random neighbor. That is,

$$e_{ij}(\mathbf{x}) = W_i(\mathbf{x}) \times p_{ij} = \frac{F_i(\mathbf{x})}{\sum_{l \in \mathcal{N}} F_l(\mathbf{x})} \times p_{ij}. \tag{S48}$$

Taking $\delta = 0$ in Eq. (S48), we have

$$e_{ij}^\circ(\mathbf{x}) = \frac{p_{ij}}{N}. \tag{S49}$$

Taking the derivative of Eq. (S48) with respect to δ at $\delta = 0$, we have

$$e'_{ij}(\mathbf{x}) = \frac{p_{ij}}{N} \left(f_i(\mathbf{x}) - \frac{1}{N} \sum_{l \in \mathcal{N}} f_l(\mathbf{x}) \right). \tag{S50}$$

Substituting Eq. (S49) into Eqs. (S5), we obtain

$$\sum_{j \in \mathcal{N}} e_{ji}^\circ(\mathbf{x}) v_i = \sum_{j \in \mathcal{N}} e_{ij}^\circ(\mathbf{x}) v_j \Leftrightarrow \sum_{j \in \mathcal{N}} \frac{p_{ji}}{N} v_i = \sum_{j \in \mathcal{N}} \frac{p_{ij}}{N} v_j, \tag{S51a}$$

$$\sum_{i \in \mathcal{N}} v_i = N. \tag{S51b}$$

The solution to Eqs. (S51) is $v_i = k_i^{-1} / \langle k^{-1} \rangle$ for $i \in \mathcal{N}$, where $k_i^{-1} = 1/k_i$, and $\langle k^{-1} \rangle = (\sum_{i \in \mathcal{N}} k_i^{-1}) / N$ represents the average of the reciprocals of the degree of all nodes.

Substituting $v_i = k_i^{-1} / \langle k^{-1} \rangle$ and Eq. (S50) into Eq. (S6), we can calculate $\hat{\Delta}'_{\text{sel}}(\mathbf{x})$ under the BD rule:

$$\hat{\Delta}'_{\text{sel}}(\mathbf{x}) = \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) (e'_{ij}(\mathbf{x}) v_j - e'_{ji}(\mathbf{x}) v_i)$$

$$\begin{aligned}
&= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) \left(\frac{p_{ij}}{N} \left(f_i(\mathbf{x}) - \frac{1}{N} \sum_{l \in \mathcal{N}} f_l(\mathbf{x}) \right) \frac{k_j^{-1}}{\langle k^{-1} \rangle} - \frac{p_{ji}}{N} \left(f_j(\mathbf{x}) - \frac{1}{N} \sum_{l \in \mathcal{N}} f_l(\mathbf{x}) \right) \frac{k_i^{-1}}{\langle k^{-1} \rangle} \right) \\
&= \frac{1}{2N} \sum_{i,j \in \mathcal{N}} (x_i - x_j) \left(\frac{k_{ij}}{N} \left(f_i(\mathbf{x}) - \frac{1}{N} \sum_{l \in \mathcal{N}} f_l(\mathbf{x}) \right) \frac{k_i^{-1} k_j^{-1}}{\langle k^{-1} \rangle} - \frac{k_{ji}}{N} \left(f_j(\mathbf{x}) - \frac{1}{N} \sum_{l \in \mathcal{N}} f_l(\mathbf{x}) \right) \frac{k_i^{-1} k_j^{-1}}{\langle k^{-1} \rangle} \right) \\
&= \frac{1}{2N^2 \langle k^{-1} \rangle} \sum_{i,j \in \mathcal{N}} (x_i - x_j) \frac{k_{ij}}{k_i k_j} (f_i(\mathbf{x}) - f_j(\mathbf{x})). \tag{S52}
\end{aligned}$$

Substituting Eq. (S52) into Eq. (S2), we obtain the condition for cooperation success under the BD rule:

$$\mathbb{E}_{\text{RMC}}^{\circ}[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0 \Leftrightarrow \frac{1}{2N^2 \langle k^{-1} \rangle} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0. \tag{S53}$$

We first calculate $\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ in Eq. (S53), which is the same as the one calculated under the PC rule (see Eq. (S18) for the same result). The remaining work is to calculate $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ for all $i, j \in \mathcal{N}$ under the BD rule.

Similarly, we begin with the MSS distribution and derive the recurrence relation by working through an elementary MCS. For the mutation mechanism under the BD rule, we specify that the event of a mutation is assigned to the focal agent rather than being transmitted to a random neighbor by the BD rule. This ensures the probability of the initial mutation on each node is $1/N$ in a fixation state, consistent with the PC and DB rules.

Therefore, under the BD rule, the possible events that happen within an elementary MCS can be classified into the following categories.

- Agent i is selected as the focal agent with probability $W_i^{\circ}(\mathbf{x}) = 1/N$ to propagate its strategy:
 - (i) The focal agent i mutates with probability u , becoming cooperation ($x_i \leftarrow 1$) with probability $1/2$, or defection ($x_i \leftarrow 0$) with probability $1/2$;
 - (ii) Agent i transmits the strategy to a random neighbor with probability $1 - u$. With probability $p_{i\ell}$, agent i transmits its strategy to agent ℓ ($\ell \in \mathcal{N}$), $x_{\ell} \leftarrow x_i$. If $\ell = j$, this influences the quantity $\mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)]$; otherwise the quantity keeps unchanged.
- Similarly, agent j is selected as the focal agent with probability $W_j^{\circ}(\mathbf{x}) = 1/N$ to propagate its strategy:
 - (i) The focal agent j mutates with probability u , becoming cooperation ($x_j \leftarrow 1$) with probability $1/2$, or defection ($x_j \leftarrow 0$) with probability $1/2$;
 - (ii) Agent j transmits the strategy to a random neighbor with probability $1 - u$. With probability $p_{j\ell}$, agent j transmits its strategy to agent ℓ ($\ell \in \mathcal{N}$), $x_{\ell} \leftarrow x_j$. Similarly, if $\ell = i$, this influences the quantity $\mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)]$; otherwise the quantity keeps unchanged.
- The focal agent, denoted by $l \in \mathcal{N} \setminus \{i, j\}$, is one of the remaining $N - 2$ agents other than i and j , with probability $W_l^{\circ}(\mathbf{x}) = 1/N$:
 - (i) The focal agent l mutates with probability u , which can only change x_l and has nothing to do with x_i or x_j ;
 - (ii) Agent l transmits the strategy to a random neighbor with probability $1 - u$. With probability $p_{l\ell}$, agent l transmits its strategy to agent ℓ ($\ell \in \mathcal{N}$), $x_{\ell} \leftarrow x_l$. If $\ell = i$ or $\ell = j$, this influences the quantity $\mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)]$; otherwise the quantity keeps unchanged.

Combining all the above possibilities of an elementary MCS, we obtain the following recurrence relation under the MSS distribution:

$$\begin{aligned}
&\mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)] \\
&= W_i^{\circ}(\mathbf{x}) \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^{\circ}[(1 - 1/2)(x_j - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^{\circ}[(0 - 1/2)(x_j - 1/2)] \right) \right. \\
&\quad \left. + (1 - u) \left(\sum_{\ell \in \mathcal{N} \setminus \{j\}} p_{i\ell} \mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_j - 1/2)] + p_{ij} \mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(x_i - 1/2)] \right) \right\} \\
&\quad + W_j^{\circ}(\mathbf{x}) \left\{ u \left(\frac{1}{2} \mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(1 - 1/2)] + \frac{1}{2} \mathbb{E}_{\text{MSS}}^{\circ}[(x_i - 1/2)(0 - 1/2)] \right) \right.
\end{aligned}$$

$$\begin{aligned}
& + (1-u) \left(\sum_{\ell \in \mathcal{N} \setminus \{i\}} p_{j\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + p_{ji} \mathbb{E}_{\text{MSS}}^\circ[(x_j - 1/2)(x_j - 1/2)] \right) \Big\} \\
& + \sum_{l \in \mathcal{N} \setminus \{i,j\}} W_l^\circ(\mathbf{x}) \left\{ u \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + (1-u) \left(\sum_{\ell \in \mathcal{N} \setminus \{i,j\}} p_{l\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right. \right. \\
& \left. \left. + p_{li} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + p_{lj} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right) \right\} \\
& = \frac{1}{N} \left\{ 0 + (1-u) \left(\sum_{\ell \in \mathcal{N} \setminus \{j\}} p_{i\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + p_{ij} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_i - 1/2)] \right) \right\} \\
& + \frac{1}{N} \left\{ 0 + (1-u) \left(\sum_{\ell \in \mathcal{N} \setminus \{i\}} p_{j\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + p_{ji} \mathbb{E}_{\text{MSS}}^\circ[(x_j - 1/2)(x_j - 1/2)] \right) \right\} \\
& + \frac{1}{N} \sum_{l \in \mathcal{N} \setminus \{i,j\}} \left\{ u \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + (1-u) \left(\sum_{\ell \in \mathcal{N} \setminus \{i,j\}} p_{l\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \right. \right. \\
& \left. \left. + p_{li} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + p_{lj} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right) \right\} \\
& = \frac{1-u}{N} \sum_{l \in \mathcal{N}} \left(p_{li} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + p_{lj} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right) \\
& + \frac{u}{N} \sum_{l \in \mathcal{N} \setminus \{i,j\}} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + \frac{1-u}{N} \sum_{l \in \mathcal{N}} \sum_{\ell \in \mathcal{N} \setminus \{i,j\}} p_{l\ell} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
& = \frac{1-u}{N} \sum_{l \in \mathcal{N}} \left(p_{li} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + p_{lj} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right) \\
& + \frac{u}{N} (N-2) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] + \frac{1-u}{N} \sum_{l \in \mathcal{N}} (1 - p_{li} - p_{lj}) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)] \\
& = \frac{1-u}{N} \sum_{l \in \mathcal{N}} \left(p_{li} \mathbb{E}_{\text{MSS}}^\circ[(x_l - 1/2)(x_j - 1/2)] + p_{lj} \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_l - 1/2)] \right) \\
& + \left(1 - \frac{2u}{N} - \frac{1-u}{N} \sum_{l \in \mathcal{N}} (p_{li} + p_{lj}) \right) \mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]. \tag{S54}
\end{aligned}$$

Integrating $\mathbb{E}_{\text{MSS}}^\circ[(x_i - 1/2)(x_j - 1/2)]$ into the left-hand side and denoting $\underline{x}_i = x_i - 1/2$, we obtain

$$\begin{aligned}
\mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] & = \frac{1-u}{2u + (1-u) \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{lj} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right) \\
\Leftrightarrow \left(\frac{2u}{(1-u) \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} + 1 \right) \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] & = \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{lj} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right). \tag{S55}
\end{aligned}$$

We define variables $\tilde{\phi}_{ij}(\mathbf{x})$,

$$\tilde{\phi}_{ij}(\mathbf{x}) = \underline{x}_i \underline{x}_j - \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \underline{x}_l \underline{x}_j + \sum_{l \in \mathcal{N}} p_{lj} \underline{x}_i \underline{x}_l \right), \tag{S56}$$

which satisfy the properties: $\tilde{\phi}_{ij}(\mathbf{C}) = \tilde{\phi}_{ij}(\mathbf{D}) = 0$. Therefore, $\tilde{\phi}_{ij}(\mathbf{x})$ can be used to relate the MSS and RMC distributions through Eq. (S11) as $u \rightarrow 0$.

We first calculate $\mathbb{E}_{\text{MSS}}^\circ[\tilde{\phi}_{ij}(\mathbf{x})]$. Writing down the expected value of Eq. (S56) and using Eq. (S55), we have

$$\mathbb{E}_{\text{MSS}}^\circ[\tilde{\phi}_{ij}(\mathbf{x})] = \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_j] - \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_l \underline{x}_j] + \sum_{l \in \mathcal{N}} p_{lj} \mathbb{E}_{\text{MSS}}^\circ[\underline{x}_i \underline{x}_l] \right)$$

$$\begin{aligned}
&= \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] - \left(\frac{2u}{(1-u) \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} + 1 \right) \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] \\
&= -\frac{2u}{(1-u) \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j].
\end{aligned} \tag{S57}$$

According to Eq. (S11), we can calculate $\mathbb{E}_{\text{RMC}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})]$ from $\mathbb{E}_{\text{MSS}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})]$,

$$\begin{aligned}
\mathbb{E}_{\text{RMC}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})] &= K \left. \frac{d\mathbb{E}_{\text{MSS}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})]}{du} \right|_{u=0} \\
&= K \left. \frac{d}{du} \right|_{u=0} \left(-\frac{2u}{(1-u) \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] \right) \\
&= K \left(-\frac{2}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \mathbb{E}_{\text{MSS}}^{\circ}[x_i x_j] \Big|_{u=0} + 0 \right) \\
&= -\frac{K}{2 \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})}.
\end{aligned} \tag{S58}$$

On the other hand, writing down the expected value of Eq. (S56) under the RMC distribution leads to another expression of $\mathbb{E}_{\text{RMC}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})]$:

$$\mathbb{E}_{\text{RMC}}^{\circ}[\tilde{\phi}_{ij}(\mathbf{x})] = \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \mathbb{E}_{\text{RMC}}^{\circ}[x_l x_j] + \sum_{l \in \mathcal{N}} p_{lj} \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] \right). \tag{S59}$$

Substituting the result of Eq. (S58) into Eq. (S59), we have

$$\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \mathbb{E}_{\text{RMC}}^{\circ}[x_l x_j] + \sum_{l \in \mathcal{N}} p_{lj} \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] \right) - \frac{K}{2 \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})}. \tag{S60}$$

We define variables $\tilde{\tau}_{ij}$ for $i, j \in \mathcal{N}$,

$$\tilde{\tau}_{ij} = \frac{\frac{1}{2} - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]}{K/2}. \tag{S61}$$

Obviously, $\tilde{\tau}_{ii} = 0$ when $i = j$, because $\mathbb{E}_{\text{RMC}}^{\circ}[x_i^2] = 1/2$. Also, $\tilde{\tau}_{ij} = \tilde{\tau}_{ji}$, because $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_i]$.

When $i \neq j$, we can solve for the values of $\tilde{\tau}_{ij}$ by the recurrence relation. According to Eq. (S27), we know that Eq. (S61) can be written as

$$\tilde{\tau}_{ij} = \frac{\frac{1}{2} - \left(\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] + \frac{1}{4} \right)}{K/2} = \frac{\frac{1}{2} - 2\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]}{K} \tag{S62}$$

or

$$\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] = \frac{\frac{1}{2} - K\tilde{\tau}_{ij}}{2}. \tag{S63}$$

Substituting Eq. (S63) into Eq. (S60), we obtain the recurrence relation of $\tilde{\tau}_{ij}$:

$$\begin{aligned}
\frac{\frac{1}{2} - K\tilde{\tau}_{ij}}{2} &= \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(\sum_{l \in \mathcal{N}} p_{li} \frac{\frac{1}{2} - K\tilde{\tau}_{jl}}{2} + \sum_{l \in \mathcal{N}} p_{lj} \frac{\frac{1}{2} - K\tilde{\tau}_{il}}{2} \right) - \frac{K}{2 \sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \\
\Leftrightarrow \tilde{\tau}_{ij} &= \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(1 + \sum_{l \in \mathcal{N}} p_{li} \tilde{\tau}_{jl} + \sum_{l \in \mathcal{N}} p_{lj} \tilde{\tau}_{il} \right).
\end{aligned} \tag{S64}$$

The recurrence relation Eq. (S64), together with $\tilde{\tau}_{ii} = 0$, form a system of linear equations, through which all $\tilde{\tau}_{ij}$ values ($i, j \in \mathcal{N}$) can be determined on a given network structure.

Substituting all $\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]$ into Eq. (S18) with computable $\tilde{\tau}_{ij}$ using Eq. (S61), and then substituting the result into the cooperation success condition Eq. (S53), where the positive factors $K/2$ and $1/(2N^2 \langle k^{-1} \rangle)$ can be canceled out, we arrive at the following condition for cooperation success:

$$\begin{aligned}
& \mathbb{E}_{\text{RMC}}^{\circ}[\hat{\Delta}'_{\text{sel}}(\mathbf{x})] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \left\{ \left(\frac{rc}{(k_i+1)^2} - c \right) \tilde{\tau}_{ij} + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i+1} + \frac{1}{k_l+1} \right) (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) \right. \\
& + \frac{rc}{k_i+1} \sum_{l \in \mathcal{N}_i} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_l} (-\tilde{\tau}_{i\ell} + \tilde{\tau}_{j\ell}) - \left(\frac{rc}{(k_j+1)^2} - c \right) (-\tilde{\tau}_{ij}) \\
& \left. - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j+1} + \frac{1}{k_l+1} \right) (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) - \frac{rc}{k_j+1} \sum_{l \in \mathcal{N}_j} \frac{1}{k_l+1} \sum_{\ell \in \mathcal{N}_l} (-\tilde{\tau}_{i\ell} + \tilde{\tau}_{j\ell}) \right\} > 0 \\
\Leftrightarrow & r > \frac{2 \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (\tilde{\Upsilon}_{ij} + \tilde{\Upsilon}_{ji})}, \tag{S65}
\end{aligned}$$

where $\tilde{\Upsilon}_{ij}$ are defined by

$$\tilde{\Upsilon}_{ij} = \frac{1}{k_i+1} \left(\frac{\tilde{\tau}_{ij} + k_i \sum_{l \in \mathcal{N}} p_{il} (\tilde{\tau}_{jl} - \tilde{\tau}_{il})}{k_i+1} + k_i \sum_{l \in \mathcal{N}} p_{il} \frac{(\tilde{\tau}_{jl} - \tilde{\tau}_{il}) + k_l \sum_{\ell \in \mathcal{N}} p_{l\ell} (\tilde{\tau}_{j\ell} - \tilde{\tau}_{i\ell})}{k_l+1} \right). \tag{S66}$$

And according to the previous discussion, $\tilde{\tau}_{ij}$ can be solved by the following system of linear equations:

$$\begin{cases} \tilde{\tau}_{ij} = \frac{1}{\sum_{l \in \mathcal{N}} (p_{li} + p_{lj})} \left(1 + \sum_{l \in \mathcal{N}} (p_{li} \tilde{\tau}_{jl} + p_{lj} \tilde{\tau}_{il}) \right), & \text{if } j \neq i, \\ \tilde{\tau}_{ij} = 0, & \text{if } j = i. \end{cases} \tag{S67}$$

In applications, we can use the following equivalent form, which is more intuitive for calculation:

$$\begin{cases} \tilde{\tau}_{ij} = \frac{1}{\sum_{l \in \mathcal{N}_i} k_l^{-1} + \sum_{l \in \mathcal{N}_j} k_l^{-1}} \left(1 + \sum_{l \in \mathcal{N}_i} k_l^{-1} \tilde{\tau}_{jl} + \sum_{l \in \mathcal{N}_j} k_l^{-1} \tilde{\tau}_{il} \right), & \text{if } j \neq i, \\ \tilde{\tau}_{ij} = 0, & \text{if } j = i. \end{cases} \tag{S68}$$

Finally, $\sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) \tilde{\Upsilon}_{ji} = \sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) \tilde{\Upsilon}_{ij}$. Therefore, $\sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) (\tilde{\Upsilon}_{ij} + \tilde{\Upsilon}_{ji}) = 2 \sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) \tilde{\Upsilon}_{ij}$. As a result, Eq. (S65) can be further simplified as

$$r > \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\Upsilon}_{ij}}. \tag{S69}$$

The right-hand side is the r^* value under the BD rule. Furthermore, let $\tilde{\tau}^{(1)} = \sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) \tilde{\tau}_{ij}$, $\tilde{\Upsilon}^{(1)} = \sum_{i,j \in \mathcal{N}} k_{ij}/(k_i k_j) \tilde{\Upsilon}_{ij}$, then the r^* value under the BD rule can also be expressed in shorthand as

$$r^* = \frac{\tilde{\tau}^{(1)}}{\tilde{\Upsilon}^{(1)}}. \tag{S70}$$

1.6 Variation of the model: Accumulated payoff

In the previous deduction, we assume that an agent i 's actual payoff is averaged over the $1 + k_i$ games organized by itself and its neighbors, ensuring the consistency of payoff scales across different numbers of neighbors. Another approach is to take the accumulated payoff from these games. On homogeneous graphs, there is no difference between these two approaches in the weak selection limit, but on heterogeneous graphs, agents with more neighbors tend to have higher & lower payoffs because they participate in more games. From a physical perspective, the accumulated payoff is also a more intuitive model detail in real-world systems. We are thus interested in examining the conditions for cooperation success when using accumulated payoffs.

1.6.1 Modified payoff calculation

We do not normalize agent i 's actual payoff by dividing $1 + k_i$ but take the accumulated payoff directly. Similar to Eq. (S1), the calculation of agent i 's actual payoff $f_i(\mathbf{x})$ follows Eq. (S71).

$$\begin{aligned}
f_i(\mathbf{x}) &= \sum_{l \in \mathcal{G}_i} \left(\frac{r \sum_{\ell \in \mathcal{G}_l} x_{\ell} c}{G_l} - x_i c \right) \\
&= \left(\frac{r(x_i + \sum_{l \in \mathcal{N}_i} x_l) c}{k_i + 1} - x_i c \right) + \sum_{l \in \mathcal{N}_i} \left(\frac{r(x_l + \sum_{\ell \in \mathcal{N}_l} x_{\ell}) c}{k_l + 1} - x_i c \right) \\
&= \left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) x_i + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) x_l + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} x_{\ell}.
\end{aligned} \tag{S71}$$

The dynamics of strategy evolution remain the same under neutral drift. Only the quantity $\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ is influenced by the modified payoff calculation $f_i(\mathbf{x})$ ($f_j(\mathbf{x})$) and is recalculated as follows.

$$\begin{aligned}
&\mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] \\
&= \mathbb{E}_{\text{RMC}}^{\circ} \left[\left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) (x_i^2 - x_i x_j) + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (x_i x_l - x_j x_l) \right. \\
&\quad + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (x_i x_{\ell} - x_j x_{\ell}) - \left(\frac{rc}{k_j + 1} - (k_j + 1)c \right) (x_i x_j - x_j^2) \\
&\quad \left. - rc \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (x_i x_l - x_j x_l) - rc \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (x_i x_{\ell} - x_j x_{\ell}) \right] \\
&= \left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i^2] - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]) + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_l]) \\
&\quad + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_{\ell}] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_{\ell}]) - \left(\frac{rc}{k_j + 1} - (k_j + 1)c \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j^2]) \\
&\quad - rc \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_l] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_l]) - rc \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (\mathbb{E}_{\text{RMC}}^{\circ}[x_i x_{\ell}] - \mathbb{E}_{\text{RMC}}^{\circ}[x_j x_{\ell}]).
\end{aligned} \tag{S72}$$

1.6.2 Pairwise comparison

The cooperation condition under the PC rule is still Eq. (S17), because the condition was obtained under neutral drift and thus remains independent of the later introduced marginal effect of games. Using the result of Eq. (S72) and $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]) / (K/4)$ as defined by Eq. (S26), we calculate

$$\begin{aligned}
&\frac{1}{4N^2 \langle k \rangle} \sum_{i, j \in \mathcal{N}} k_i p_{ij} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
&\Leftrightarrow \sum_{i, j \in \mathcal{N}} k_i p_{ij} \left\{ \left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) \tau_{ij} + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (-\tau_{il} + \tau_{jl}) \right. \\
&\quad + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) - \left(\frac{rc}{k_j + 1} - (k_j + 1)c \right) (-\tau_{ij}) \\
&\quad \left. - rc \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (-\tau_{il} + \tau_{jl}) - rc \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) \right\} > 0 \\
&\Leftrightarrow r > \frac{\sum_{i, j \in \mathcal{N}} k_i p_{ij} (k_i + k_j + 2) \tau_{ij}}{\sum_{i, j \in \mathcal{N}} k_i p_{ij} [(k_i + 1) \Upsilon_{ij} + (k_j + 1) \Upsilon_{ji}]}.
\end{aligned} \tag{S73}$$

Further simplifying Eq. (S73) (using Eq. (S83)) leads to

$$r > \frac{\sum_{i, j \in \mathcal{N}} k_i (k_i + 1) p_{ij} \tau_{ij}}{\sum_{i, j \in \mathcal{N}} k_i (k_i + 1) p_{ij} \Upsilon_{ij}}. \tag{S74}$$

The right-hand side is the r^* value for cooperation success when using accumulated payoffs under the PC rule. The τ_{ij} values are still obtained by solving Eqs. (S33) on the given network structure, and the Υ_{ij} values are still obtained by Eq. (S32).

1.6.3 Death-birth

The cooperation condition under the DB rule is Eq. (S41). Using the result of Eq. (S72) and $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]) / (K/4)$ as defined by Eq. (S44), we calculate

$$\begin{aligned}
& \frac{1}{2N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \left\{ \left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) \tau_{ij} + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (-\tau_{il} + \tau_{jl}) \right. \\
& + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) - \left(\frac{rc}{k_j + 1} - (k_j + 1)c \right) (-\tau_{ij}) \\
& \left. - rc \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (-\tau_{il} + \tau_{jl}) - rc \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tau_{i\ell} + \tau_{j\ell}) \right\} > 0 \\
\Leftrightarrow & r > \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} (k_i + k_j + 2) \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} [(k_i + 1) \Upsilon_{ij} + (k_j + 1) \Upsilon_{ji}]} . \tag{S75}
\end{aligned}$$

Further simplifying Eq. (S75) leads to

$$r > \frac{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij}^{(2)} \Upsilon_{ij}} . \tag{S76}$$

The right-hand side is the r^* value for cooperation success when using accumulated payoffs under the DB rule. The τ_{ij} values are still obtained by solving Eqs. (S33) on the given network structure, and the Υ_{ij} values are still obtained by Eq. (S32).

1.6.4 Birth-death

The cooperation condition under the BD rule is Eq. (S53). Using the result of Eq. (S72) and $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^{\circ}[x_i x_j]) / (K/2)$ as defined by Eq. (S61), we calculate

$$\begin{aligned}
& \frac{1}{2N^2 \langle k^{-1} \rangle} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \mathbb{E}_{\text{RMC}}^{\circ}[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \left\{ \left(\frac{rc}{k_i + 1} - (k_i + 1)c \right) \tilde{\tau}_{ij} + rc \sum_{l \in \mathcal{N}_i} \left(\frac{1}{k_i + 1} + \frac{1}{k_l + 1} \right) (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) \right. \\
& + rc \sum_{l \in \mathcal{N}_i} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tilde{\tau}_{i\ell} + \tilde{\tau}_{j\ell}) - \left(\frac{rc}{k_j + 1} - (k_j + 1)c \right) (-\tilde{\tau}_{ij}) \\
& \left. - rc \sum_{l \in \mathcal{N}_j} \left(\frac{1}{k_j + 1} + \frac{1}{k_l + 1} \right) (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) - rc \sum_{l \in \mathcal{N}_j} \frac{1}{k_l + 1} \sum_{\ell \in \mathcal{N}_l} (-\tilde{\tau}_{i\ell} + \tilde{\tau}_{j\ell}) \right\} > 0 \\
\Leftrightarrow & r > \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + k_j + 2) \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} [(k_i + 1) \tilde{\Upsilon}_{ij} + (k_j + 1) \tilde{\Upsilon}_{ji}]} . \tag{S77}
\end{aligned}$$

Further simplifying Eq. (S75) leads to

$$r > \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\Upsilon}_{ij}} . \tag{S78}$$

The right-hand side is the r^* value for cooperation success when using accumulated payoffs under the BD rule. The $\tilde{\tau}_{ij}$ values are obtained by solving Eqs. (S67) on the given network structure, and the $\tilde{\Upsilon}_{ij}$ values are obtained by Eq. (S66).

Supplementary Note 2: Applications to specific network structures

With the cooperation conditions obtained in [Supplementary Note 1](#), we can calculate the critical synergy factor for cooperation success in spatial PGGs on any given network structure. Here, we present the calculation process for five examples: regular graphs, star graphs, hub-to-hub star graphs, m -hub star graphs, and fans.

2.1 Regular graphs

The theoretical results of spatial PGG on regular graphs have been previously obtained⁴⁰, and our framework on any network structure can reproduce these results when applied to regular networks. On a regular graph, all nodes have the same number of neighbors, $k_i \equiv k$ for $i \in \mathcal{N}$, so $p_{ij} = p_{ji} \equiv 1/k$ for $i, j \in \mathcal{N}$, $i \neq j$.

The calculation for regular graphs is, in fact, the least intuitive compared to other heterogeneous networks when using this framework. We cannot directly solve the system of linear equations for τ_{ij} but instead need to construct intermediate quantities and special recurrence relations for regular graphs¹⁰.

We first define

$$\tau_i = 1 + \sum_{j \in \mathcal{N}} p_{ij} \tau_{ij}, \quad (\text{S79})$$

with which we calculate the recurrence relation of $\tau^{(n)}$ defined in the main text:

$$\begin{aligned} \tau^{(n)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \tau_{ij} \\ &= \sum_{\substack{i,j \in \mathcal{N} \\ i \neq j}} k_i p_{ij}^{(n)} \left(1 + \frac{1}{2} \sum_{l \in \mathcal{N}} p_{il} \tau_{jl} + \frac{1}{2} \sum_{l \in \mathcal{N}} p_{jl} \tau_{il} \right) \\ &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \left(1 + \frac{1}{2} \sum_{l \in \mathcal{N}} p_{il} \tau_{jl} + \frac{1}{2} \sum_{l \in \mathcal{N}} p_{jl} \tau_{il} \right) - \sum_{i \in \mathcal{N}} k_i p_{ii}^{(n)} \left(1 + \sum_{l \in \mathcal{N}} p_{il} \tau_{il} \right) \\ &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} + \frac{1}{2} \sum_{i,j,l \in \mathcal{N}} k_j p_{ji}^{(n)} p_{il} \tau_{jl} + \frac{1}{2} \sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(n)} p_{jl} \tau_{il} - \sum_{i \in \mathcal{N}} k_i p_{ii}^{(n)} \tau_i \\ &= N \langle k \rangle + \frac{1}{2} \sum_{j,l \in \mathcal{N}} k_j p_{jl}^{(n+1)} \tau_{jl} + \frac{1}{2} \sum_{i,l \in \mathcal{N}} k_i p_{il}^{(n+1)} \tau_{il} - \sum_{i \in \mathcal{N}} k_i p_{ii}^{(n)} \tau_i \\ &= N \langle k \rangle + \tau^{(n+1)} - \sum_{i \in \mathcal{N}} k_i p_{ii}^{(n)} \tau_i. \end{aligned} \quad (\text{S80})$$

Therefore, we have the following recurrence relation:

$$\tau^{(n+1)} = \tau^{(n)} + \sum_{i \in \mathcal{N}} k_i p_{ii}^{(n)} \tau_i - N \langle k \rangle. \quad (\text{S81})$$

The fourth line in Eq. (S80) used the following fact:

$$k_i p_{ij}^{(n)} = \sum_{\ell_1 \in \mathcal{N}} k_{i\ell_1} p_{\ell_1 j}^{(n-1)} = \sum_{\ell_1, \ell_2, \dots, \ell_{n-1} \in \mathcal{N}} k_{i\ell_1} \frac{k_{\ell_1 \ell_2} \cdots k_{\ell_{n-1} j}}{k_{\ell_1} \cdots k_{\ell_{n-1}}} = \sum_{\ell_1, \ell_2, \dots, \ell_{n-1} \in \mathcal{N}} k_{j\ell_{n-1}} \frac{k_{\ell_{n-1} \ell_{n-2}} \cdots k_{\ell_1 i}}{k_{\ell_{n-1}} \cdots k_{\ell_1}} = k_j p_{ji}^{(n)}. \quad (\text{S82})$$

With the help of the recurrence relation Eq. (S81), we can start from $\tau^{(0)}$ and obtain all $\tau^{(n)}$ values step by step. For $i = j$, we have $\tau_{ij} = 0$. Moreover, one stays in the original position if not walking, so $p_{ij}^{(0)} = 1$ if $i = j$ and $p_{ij}^{(0)} = 0$ if $i \neq j$. Therefore, $\tau^{(0)} = \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(0)} \tau_{ij} = 0$. Substituting these to Eq. (S81), we have the following results:

$$\tau^{(0)} = 0, \quad (\text{S83a})$$

$$\tau^{(1)} = \sum_{i \in \mathcal{N}} k_i \tau_i - N \langle k \rangle, \quad (\text{S83b})$$

$$\tau^{(2)} = \sum_{i \in \mathcal{N}} k_i \tau_i (1 + p_{ii}^{(1)}) - 2N \langle k \rangle, \quad (\text{S83c})$$

$$\tau^{(3)} = \sum_{i \in \mathcal{N}} k_i \tau_i (1 + p_{ii}^{(1)} + p_{ii}^{(2)}) - 3N \langle k \rangle, \quad (\text{S83d})$$

$$\tau^{(4)} = \sum_{i \in \mathcal{N}} k_i \tau_i (1 + p_{ii}^{(1)} + p_{ii}^{(2)} + p_{ii}^{(3)}) - 4N \langle k \rangle. \quad (\text{S83e})$$

As declared by Ref. ¹⁰, there is a relation: $\lim_{n \rightarrow \infty} p_{ii}^{(n)} = k_i / (N \langle k \rangle)$. Then, taking $n \rightarrow \infty$ in the recurrence relation Eq. (S81), we have

$$\tau^{(\infty)} = \tau^{(\infty)} + \sum_{i \in \mathcal{N}} k_i p_{ii}^{(\infty)} \tau_i - N \langle k \rangle \Leftrightarrow \sum_{i \in \mathcal{N}} k_i^2 \tau_i = N^2 \langle k \rangle^2. \quad (\text{S84})$$

Supposing all nodes on the regular graph are transitive, we denote $p_{ii}^{(n)} \equiv p^{(n)}$ in shorthand. Obviously, $p^{(1)} = 0$, because we assumed no self-loops on the network, and one cannot leave and return to the same node within a single step; $p^{(2)} = 1/k$, since for each possible first step, the probability of returning to the original node in the second step is $1/k$. The average degree of the network is $\langle k \rangle = k$, so we have $\sum_{i \in \mathcal{N}} k_i \tau_i \equiv N^2 k$ according to Eq. (S84). To summarize, Eqs. (S83) can be calculated as

$$\tau^{(0)} = 0, \quad (\text{S85a})$$

$$\tau^{(1)} = \sum_{i \in \mathcal{N}} k_i \tau_i - Nk = (N-1)Nk, \quad (\text{S85b})$$

$$\tau^{(2)} = \sum_{i \in \mathcal{N}} k_i \tau_i - 2Nk = (N-2)Nk, \quad (\text{S85c})$$

$$\tau^{(3)} = \sum_{i \in \mathcal{N}} k_i \tau_i \left(1 + \frac{1}{k}\right) - 3Nk = \left[N \left(1 + \frac{1}{k}\right) - 3\right] Nk, \quad (\text{S85d})$$

$$\tau^{(4)} = \sum_{i \in \mathcal{N}} k_i \tau_i \left(1 + \frac{1}{k} + p^{(3)}\right) - 4Nk = \left[N \left(1 + \frac{1}{k} + p^{(3)}\right) - 4\right] Nk. \quad (\text{S85e})$$

Since $k_i \equiv k$ on a regular graph, Υ_{ij} in Eq. (S32) can be simplified as

$$\Upsilon_{ij} = \frac{1}{(k+1)^2} \left(\tau_{ij} + 2k \sum_{l \in \mathcal{N}} p_{il} (\tau_{jl} - \tau_{il}) + k^2 \sum_{l \in \mathcal{N}} p_{il}^{(2)} (\tau_{jl} - \tau_{il}) \right). \quad (\text{S86})$$

Now, we can calculate the critical synergy factor for cooperation success in spatial PGGs. The general approach is to calculate the numerator $\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \tau_{ij}$ and denominator $\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(n)} \Upsilon_{ij}$ separately, expressing them by $\tau^{(0)}$, $\tau^{(1)}$, $\tau^{(2)}$, etc., and applying the results of Eqs. (S85).

For the PC rule, the numerator of r^* is

$$\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij} = \tau^{(1)}, \quad (\text{S87})$$

and by Eq. (S86), the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij} &= \frac{1}{(k+1)^2} \left(\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij} + 2k \sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il} \tau_{jl} - 2k \sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il} \tau_{il} \right. \\ &\quad \left. + k^2 \sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il}^{(2)} \tau_{jl} - k^2 \sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il}^{(2)} \tau_{il} \right) \\ &= \frac{1}{(k+1)^2} \left(\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij} + 2k \sum_{j,l \in \mathcal{N}} k_j p_{jl}^{(2)} \tau_{jl} - 2k \sum_{i,l \in \mathcal{N}} k_i p_{il} \tau_{il} \right. \\ &\quad \left. + k^2 \sum_{j,l \in \mathcal{N}} k_j p_{jl}^{(3)} \tau_{jl} - k^2 \sum_{i,l \in \mathcal{N}} k_i p_{il}^{(2)} \tau_{il} \right) \\ &= \frac{\tau^{(1)} + 2k(\tau^{(2)} - \tau^{(1)}) + k^2(\tau^{(3)} - \tau^{(2)})}{(k+1)^2}. \end{aligned} \quad (\text{S88})$$

Assembling Eq. (S87) and Eq. (S88) and inserting the results of Eqs. (S85), we have

$$r^* = \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij}}$$

$$\begin{aligned}
&= \frac{(k+1)^2 \tau^{(1)}}{\tau^{(1)} + 2k(\tau^{(2)} - \tau^{(1)}) + k^2(\tau^{(3)} - \tau^{(2)})} \\
&= \frac{(N-1)G}{N-G} \xrightarrow{N \rightarrow \infty} G,
\end{aligned} \tag{S89}$$

which is the critical synergy factor for cooperation success in spatial PGGs on regular graphs under the PC rule, consistent with the previous research^{31,40}. Eq. (S89) has replaced the number of neighbors k by the group size $G = k + 1$ for intuitive understanding in PGGs.

For the DB rule, the calculation is similar. The numerator of r^* is

$$\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij} = \tau^{(2)}, \tag{S90}$$

and by Eq. (S86), the denominator is

$$\begin{aligned}
\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij} &= \frac{1}{(k+1)^2} \left(\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij} + 2k \sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il} \tau_{jl} - 2k \sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il} \tau_{il} \right. \\
&\quad \left. + k^2 \sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il}^{(2)} \tau_{jl} - k^2 \sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il}^{(2)} \tau_{il} \right) \\
&= \frac{1}{(k+1)^2} \left(\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij} + 2k \sum_{j,l \in \mathcal{N}} k_j p_{jl}^{(3)} \tau_{jl} - 2k \sum_{i,l \in \mathcal{N}} k_i p_{il} \tau_{il} \right. \\
&\quad \left. + k^2 \sum_{j,l \in \mathcal{N}} k_j p_{jl}^{(4)} \tau_{jl} - k^2 \sum_{i,l \in \mathcal{N}} k_i p_{il}^{(2)} \tau_{il} \right) \\
&= \frac{\tau^{(2)} + 2k(\tau^{(3)} - \tau^{(1)}) + k^2(\tau^{(4)} - \tau^{(2)})}{(k+1)^2}.
\end{aligned} \tag{S91}$$

Assembling Eq. (S90) and Eq. (S91) and inserting the results of Eq. (S85), we have

$$\begin{aligned}
r^* &= \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij}} \\
&= \frac{(k+1)^2 \tau^{(2)}}{\tau^{(2)} + 2k(\tau^{(3)} - \tau^{(1)}) + k^2(\tau^{(4)} - \tau^{(2)})} \\
&= \frac{(N-2)G^2}{N(G-1)^2 p^{(3)} + N(G+2) - 2G^2} \\
&= \frac{(N-2)G^2}{N(G-2)\mathcal{C} + N(G+2) - 2G^2} \xrightarrow{N \rightarrow \infty} \frac{G^2}{(G-2)\mathcal{C} + G + 2}.
\end{aligned} \tag{S92}$$

This is the critical synergy factor for cooperation success in spatial PGGs on regular graphs under the DB rule, consistent with the previous research^{31,33,40}. Eq. (S92) has replaced the three-step random walk probability $p^{(3)}$ by clustering coefficient $\mathcal{C} = k^2 p^{(3)} / (k-1)$, which is an intuitive and commonly used concept in network science.

For the BD rule, the recurrence relation Eq. (S68) reduces to the following form on a regular graph:

$$\begin{cases} \tilde{\tau}_{ij} = \frac{1}{2} \left(1 + \sum_{l \in \mathcal{N}_i} \tilde{\tau}_{jl} + \sum_{l \in \mathcal{N}_j} \tilde{\tau}_{il} \right), & \text{if } j \neq i, \\ \tilde{\tau}_{ij} = 0, & \text{if } j = i. \end{cases} \tag{S93}$$

For the critical synergy factor, $\tilde{\tau}_{ij}$ in the numerator and denominator are homogeneous (see Eq. (S69) and Eq. (S66)). Therefore, the critical synergy factor is invariant by replacing $\tilde{\tau}_{ij} \leftarrow \tilde{\tau}_{ij}^*/2$, which makes Eq. (S93) the same recurrence relation for $\tilde{\tau}_{ij}^*$ as the one for τ_{ij} under the PC and DB rules. The solution for $\tilde{\tau}_{ij}^*$ is thus equal to τ_{ij} . On the other hand, we have $k_{ij}/(k_i k_j) = k_i p_{ij}/k^2$ on regular graphs, where k^2 can be canceled simultaneously in the numerator and denominator of the critical synergy factor, making it (Eq. (S69)) the same as the one for the PC rule (Eq. (S34)).

Therefore, on regular graphs, the condition for cooperation success in spatial PGGs under the BD rule is equal to the one under the PC rule (i.e., Eq. (S89)).

- Accumulated payoff

On regular graphs, $k_i \equiv k$ for $i \in \mathcal{N}$. Therefore, $k_i + 1$ can be canceled simultaneously in the numerator and denominator in Eq. (S74), Eq. (S76), and Eq. (S78). As a consequence, the critical synergy factors for accumulated payoff are equal to the ones for averaged payoff under the three update rules (Eq. (S34), Eq. (S46), and Eq. (S69)). For the results under the PC and BD rules, please refer to Eq. (S89), and for the result under the DB rule, please refer to Eq. (S92).

2.2 Star graph

For heterogeneous network structures, we can calculate the critical synergy factor by solving the recurrence relation and assembling the resultant τ_{ij} values.

On a star graph, there is one hub (H) and n leaves (L). The hub node has $k_H = n$ neighbors, and each leaf node has $k_L = 1$ neighbor. The values are equal among τ_{ij} of the same type, and for the star graph, there are only two non-zero τ_{ij} types: τ_{HL} , the relation between the hub and a leaf, and $\tau_{LL'}$, the relation between a leaf and another leaf. According to Eq. (4) in the main text, we have the system of linear equations:

$$\begin{cases} \tau_{HL} = 1 + \frac{n-1}{2n} \tau_{LL'}, \\ \tau_{LL'} = 1 + \frac{1}{2} \tau_{HL} + \frac{1}{2} \tau_{HL}. \end{cases} \quad (\text{S94})$$

The solution is

$$\begin{cases} \tau_{HL} = \frac{3n-1}{n+1}, \\ \tau_{LL'} = \frac{4n}{n+1}. \end{cases} \quad (\text{S95})$$

Unlike τ_{ij} , the values of Υ_{ij} are asymmetric with respect to i and j . Therefore, we need to calculate three Υ_{ij} types: Υ_{HL} , Υ_{LH} , and $\Upsilon_{LL'}$. Inserting the τ_{ij} values of Eq. (S95) into Eq. (5) in the main text, we obtain the required Υ_{ij} values:

$$\begin{aligned} \Upsilon_{HL} &= \frac{1}{k_H + 1} \left(\frac{\tau_{HL} + \sum_{l \in \mathcal{N}_H} (\tau_{Ll} - \tau_{Hl})}{k_L + 1} + \sum_{l \in \mathcal{N}_H} \frac{(\tau_{Ll} - \tau_{Hl}) + \sum_{\ell \in \mathcal{N}_l} (\tau_{L\ell} - \tau_{H\ell})}{k_l + 1} \right) \\ &= \frac{1}{k_H + 1} \left\{ \frac{\tau_{HL} + [(n-1)\tau_{LL'} - n\tau_{HL}]}{k_H + 1} \right. \\ &\quad \left. + \left[\frac{(\tau_{LL} - \tau_{HL}) + (\tau_{HL} - \tau_{HH})}{k_L + 1} + (n-1) \frac{(\tau_{LL'} - \tau_{HL}) + (\tau_{HL} - \tau_{HH})}{k_L + 1} \right] \right\} \\ &= \frac{(n-1)[(n+3)\tau_{LL'} - 2\tau_{HL}]}{2(n+1)^2} \\ &= \frac{2n^2 - n - 1}{(n+1)^2}, \end{aligned} \quad (\text{S96a})$$

$$\begin{aligned} \Upsilon_{LH} &= \frac{1}{k_L + 1} \left(\frac{\tau_{HL} + (\tau_{HH} - \tau_{HL})}{k_L + 1} + \frac{(\tau_{HH} - \tau_{HL}) + [(\tau_{HL} - \tau_{LL}) + (n-1)(\tau_{HL} - \tau_{LL'})]}{k_H + 1} \right) \\ &= \frac{(n-1)(\tau_{HL} - \tau_{LL'})}{2(n+1)} \\ &= -\frac{n-1}{2(n+1)}, \end{aligned} \quad (\text{S96b})$$

$$\begin{aligned} \Upsilon_{LL'} &= \frac{1}{k_L + 1} \left(\frac{\tau_{LL'} + \sum_{l \in \mathcal{N}_L} (\tau_{L'l} - \tau_{Ll})}{k_L + 1} + \sum_{l \in \mathcal{N}_L} \frac{(\tau_{L'l} - \tau_{Ll}) + \sum_{\ell \in \mathcal{N}_l} (\tau_{L'\ell} - \tau_{L\ell})}{k_l + 1} \right) \\ &= \frac{1}{k_L + 1} \left(\frac{\tau_{LL'} + (\tau_{L'H} - \tau_{LH})}{k_L + 1} \right. \\ &\quad \left. + \frac{(\tau_{L'H} - \tau_{LH}) + [(\tau_{L'L} - \tau_{LL}) + (\tau_{L'L'} - \tau_{LL'}) + (n-2)(\tau_{L'L''} - \tau_{LL'})]}{k_H + 1} \right) \end{aligned}$$

$$= \frac{n}{n+1}. \quad (\text{S96c})$$

Some informal variations of the symbols during the calculation are for intuitive understanding. For example, L' refers to “another leaf” and thus $\tau_{L'L'} = \tau_{LL}$, $\tau_{L'L'} = \tau_{LL}$.

Then, we can apply these τ_{ij} and Υ_{ij} values to calculate the critical synergy factor on the star graph. For the PC rule, the numerator is

$$\begin{aligned} \tau^{(1)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij} \\ &= k_H(p_{HH}\tau_{HH} + np_{HL}\tau_{HL}) + nk_L(p_{LH}\tau_{LH} + p_{LL}\tau_{LL} + (n-1)p_{LL'}\tau_{LL'}) \\ &= 2n\tau_{HL} \\ &= \frac{2n(3n-1)}{n+1}, \end{aligned} \quad (\text{S97})$$

where the p_{ij} values are obtained by the network structure directly. For example, $p_{HH} = p_{LL} = 0$ (no self-loops), $p_{LL'} = 0$ (no edges between leaves), $p_{HL} = 1/k_H = 1/n$, $p_{LH} = 1/k_L = 1$. Similarly, the denominator is

$$\begin{aligned} \Upsilon^{(1)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij} \Upsilon_{ij} \\ &= k_H(p_{HH}\Upsilon_{HH} + np_{HL}\Upsilon_{HL}) + nk_L(p_{LH}\Upsilon_{LH} + p_{LL}\Upsilon_{LL} + (n-1)p_{LL'}\Upsilon_{LL'}) \\ &= n(\Upsilon_{HL} + \Upsilon_{LH}) \\ &= \frac{n(3n^2 - 2n - 1)}{2(n+1)^2}. \end{aligned} \quad (\text{S98})$$

Therefore, the critical synergy factor on star graphs under the PC rule is

$$r^* = \frac{\tau^{(1)}}{\Upsilon^{(1)}} = \frac{4(3n-1)(n+1)}{3n^2 - 2n - 1} \xrightarrow{n \rightarrow \infty} 4. \quad (\text{S99})$$

For the DB rule, the numerator is

$$\begin{aligned} \tau^{(2)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij} \\ &= k_H(p_{HH}^{(2)}\tau_{HH} + np_{HL}^{(2)}\tau_{HL}) + nk_L(p_{LH}^{(2)}\tau_{LH} + p_{LL}^{(2)}\tau_{LL} + (n-1)p_{LL'}^{(2)}\tau_{LL'}) \\ &= (n-1)\tau_{LL'} \\ &= \frac{4n(n-1)}{n+1}, \end{aligned} \quad (\text{S100})$$

where the $p_{ij}^{(2)}$ values are also directly obtained by the network structure: $p_{HH}^{(2)} = 1$ (the first step must walk to one of the leaves and second step must walk to the hub), $p_{LL}^{(2)} = 1/n$, $p_{LL'}^{(2)} = 1/n$, $p_{HL}^{(2)} = 0$, $p_{LH}^{(2)} = 0$. Similarly, the denominator is

$$\begin{aligned} \Upsilon^{(2)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij} \\ &= k_H(p_{HH}^{(2)}\Upsilon_{HH} + np_{HL}^{(2)}\Upsilon_{HL}) + nk_L(p_{LH}^{(2)}\Upsilon_{LH} + p_{LL}^{(2)}\Upsilon_{LL} + (n-1)p_{LL'}^{(2)}\Upsilon_{LL'}) \\ &= (n-1)\Upsilon_{LL'} \\ &= \frac{n(n-1)}{n+1}. \end{aligned} \quad (\text{S101})$$

Therefore, the critical synergy factor on star graphs under the DB rule is

$$r^* = \frac{\tau^{(2)}}{\Upsilon^{(2)}} \equiv 4. \quad (\text{S102})$$

For the BD rule, we list the system of linear equations according to Eq. (S68):

$$\begin{cases} \tilde{\tau}_{HL} = \frac{n}{n^2+1} + \frac{n(n-1)}{n^2+1} \tilde{\tau}_{LL'}, \\ \tilde{\tau}_{LL'} = \frac{n}{2} + \tilde{\tau}_{HL}. \end{cases} \quad (\text{S103})$$

The solution is

$$\begin{cases} \tilde{\tau}_{HL} = \frac{n(n^2 - n + 2)}{2(n+1)}, \\ \tilde{\tau}_{LL'} = \frac{n(n^2 + 3)}{2(n+1)}. \end{cases} \quad (\text{S104})$$

Inserting these $\tilde{\tau}_{ij}$ values into Eq. (S66), we obtain the required $\tilde{\Upsilon}_{ij}$ values:

$$\tilde{\Upsilon}_{HL} = \frac{(n-1)[(n+3)\tilde{\tau}_{LL'} - 2\tilde{\tau}_{HL}]}{2(n+1)^2} = \frac{n(n^3 - n^2 + 5n - 5)}{4(n+1)^2}, \quad (\text{S105a})$$

$$\tilde{\Upsilon}_{LH} = \frac{(n-1)(\tilde{\tau}_{HL} - \tilde{\tau}_{LL'})}{2(n+1)} = \frac{n(n-1)}{4(n+1)}. \quad (\text{S105b})$$

Then, we apply these $\tilde{\tau}_{ij}$ and $\tilde{\Upsilon}_{ij}$ values to calculate the critical synergy factor on the star graph under the BD rule. The numerator is

$$\tilde{\tau}^{(1)} = \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij} = 2\tilde{\tau}_{HL} = \frac{n(n^2 - n + 2)}{n+1}, \quad (\text{S106})$$

and the denominator is

$$\tilde{\Upsilon}^{(1)} = \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\Upsilon}_{ij} = \tilde{\Upsilon}_{HL} + \tilde{\Upsilon}_{LH} = \frac{n(n^3 - 2n^2 + 5n - 4)}{4(n+1)^2}. \quad (\text{S107})$$

Therefore, the critical synergy factor on star graphs under the BD rule is

$$r^* = \frac{\tilde{\tau}^{(1)}}{\tilde{\Upsilon}^{(1)}} = \frac{4n^3 + 4n + 8}{n^3 - 2n^2 + 5n - 4} \xrightarrow{n \rightarrow \infty} 4. \quad (\text{S108})$$

- Accumulated payoff

When using accumulated payoffs, the values of τ_{ij} , Υ_{ij} , $\tilde{\tau}_{ij}$, and $\tilde{\Upsilon}_{ij}$ keep unchanged, but the formulas of the critical synergy factors are different.

For the PC rule, we follow Eq. (S74). The numerator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i + 1)p_{ij}\tau_{ij} = (n+3)\tau_{HL} = \frac{(3n-1)(n+3)}{n+1}, \quad (\text{S109})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i + 1)p_{ij}\Upsilon_{ij} = (n+1)\Upsilon_{HL} + 2\Upsilon_{LH} = \frac{2n(n-1)}{n+1}. \quad (\text{S110})$$

The critical synergy factor on star graphs under the PC rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{(3n-1)(n+3)}{2n(n-1)} \xrightarrow{n \rightarrow \infty} \frac{3}{2}. \quad (\text{S111})$$

For the DB rule, we follow Eq. (S76). The numerator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i + 1)p_{ij}^{(2)}\tau_{ij} = 2(n-1)\tau_{LL'} = \frac{8n(n-1)}{n+1}, \quad (\text{S112})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i + 1)p_{ij}^{(2)}\Upsilon_{ij} = 2(n-1)\Upsilon_{LL'} = \frac{2n(n-1)}{n+1} \quad (\text{S113})$$

The critical synergy factor on star graphs under the DB rule when using accumulated payoff is

$$r_{\text{accu}}^* \equiv 4. \quad (\text{S114})$$

For the BD rule, we follow Eq. (S78). The numerator is

$$\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\tau}_{ij} = (n+3) \tilde{\tau}_{HL} = \frac{n(n+3)(n^2 - n + 2)}{2(n+1)}, \quad (\text{S115})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{Y}_{ij} = (n+1) \tilde{Y}_{HL} + 2 \tilde{Y}_{LH} = \frac{n(n^3 - n^2 + 3n - 3)}{4(n+1)}. \quad (\text{S116})$$

The critical synergy factor on star graphs under the BD rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{2(n+3)(n^2 - n + 2)}{n^3 - n^2 + 3n - 3} \xrightarrow{n \rightarrow \infty} 2. \quad (\text{S117})$$

2.3 Hub-to-hub star

On a hub-to-hub star graph, there are two hubs (H), each has n leaves (L). A hub node has $k_H = n + 1$ neighbors (n leaves and the other hub), and each leaf node has $k_L = 1$ neighbor. There are five non-zero τ_{ij} types: $\tau_{HH'}$, the relation between the two hubs; $\tau_{LL'}$, the relation between two leaves of the same hub; $\tau_{LL''}$, the relation between a leaf of one hub and another leaf of the other hub; τ_{HL} , the relation between a hub and one of its leaves; $\tau_{HL'}$, the relation between a hub and a leaf of the other hub. According to Eq. (4) in the main text, we have the system of linear equations:

$$\begin{cases} \tau_{HH'} = 1 + \frac{n}{n+1} \tau_{HL'}, \\ \tau_{HL} = 1 + \frac{1}{2(n+1)} \tau_{HL'} + \frac{n-1}{2(n+1)} \tau_{LL'}, \\ \tau_{HL'} = 1 + \frac{1}{2(n+1)} \tau_{HL} + \frac{n}{2(n+1)} \tau_{LL''} + \frac{1}{2} \tau_{HH'}, \\ \tau_{LL'} = 1 + \tau_{HL}, \\ \tau_{LL''} = 1 + \tau_{HL'}. \end{cases} \quad (\text{S118})$$

The solution is

$$\begin{cases} \tau_{HH'} = \frac{4n^3 + 20n^2 + 17n + 5}{(2n+5)(n+1)}, \\ \tau_{HL} = \frac{5(2n+1)}{2n+5}, \\ \tau_{HL'} = \frac{2(2n^2 + 9n + 5)}{2n+5}, \\ \tau_{LL'} = \frac{2(6n+5)}{2n+5}, \\ \tau_{LL''} = \frac{4n^2 + 20n + 15}{2n+5}. \end{cases} \quad (\text{S119})$$

Inserting these τ_{ij} values into Eq. (5) in the main text, we obtain the required Y_{ij} values:

$$\begin{aligned} Y_{HH'} &= \frac{n}{2(n+2)} (\tau_{HH'} - \tau_{HL} + \tau_{HL'}) \\ &= \frac{n(4n^3 + 16n^2 + 15n + 5)}{2n^3 + 11n^2 + 19n + 10}, \end{aligned} \quad (\text{S120a})$$

$$\begin{aligned}\Upsilon_{HL} &= -\frac{2}{(n+2)^2}\tau_{HH'} - \frac{n-2}{(n+2)^2}\tau_{HL} - \frac{n-2}{(n+2)^2}\tau_{HL'} + \frac{n^2+3n-4}{2(n+2)^2}\tau_{LL'} + \frac{2}{(n+2)^2}\tau_{LL''} \\ &= \frac{n(6n^3+21n^2+30n+23)}{(n+2)^2(2n^2+7n+5)},\end{aligned}\quad (\text{S120b})$$

$$\begin{aligned}\Upsilon_{LH} &= \frac{1}{2(n+2)}\tau_{HH'} + \frac{n-1}{2(n+2)}\tau_{HL} - \frac{1}{2(n+2)}\tau_{HL'} - \frac{n-1}{2(n+2)}\tau_{LL'} \\ &= -\frac{n(2n^2+7n+9)}{4n^3+22n^2+38n+20},\end{aligned}\quad (\text{S120c})$$

$$\begin{aligned}\Upsilon_{HL'} &= -\frac{2}{(n+2)^2}\tau_{HH'} - \frac{n^2+4n-4}{2(n+2)^2}\tau_{HL} + \frac{n^2+4}{2(n+2)^2}\tau_{HL'} + \frac{n-1}{(n+2)^2}\tau_{LL'} + \frac{n^2+4n}{2(n+2)^2}\tau_{LL''} \\ &= \frac{4n^5+26n^4+64n^3+84n^2+60n+10}{(n+2)^2(2n^2+7n+5)},\end{aligned}\quad (\text{S120d})$$

$$\begin{aligned}\Upsilon_{LH'} &= \frac{n+4}{4(n+2)}\tau_{HH'} - \frac{n+4}{4(n+2)}\tau_{HL} + \frac{3n}{4(n+2)}\tau_{HL'} - \frac{n-1}{2(n+2)}\tau_{LL'} \\ &= \frac{8n^4+34n^3+53n^2+31n+10}{2(2n^3+11n^2+19n+10)},\end{aligned}\quad (\text{S120e})$$

$$\begin{aligned}\Upsilon_{LL'} &= \frac{\tau_{LL'}}{4} \\ &= \frac{6n+5}{2(2n+5)}.\end{aligned}\quad (\text{S120f})$$

Then, we apply these τ_{ij} and Υ_{ij} values to calculate the critical synergy factor on the hub-to-hub star graph. For the PC rule, the numerator is

$$\begin{aligned}\tau^{(1)} &= 2\tau_{HH'} + 4n\tau_{HL} \\ &= \frac{2(24n^3+50n^2+27n+5)}{2n^2+7n+5},\end{aligned}\quad (\text{S121})$$

and the denominator is

$$\begin{aligned}\Upsilon^{(1)} &= 2\Upsilon_{HH'} + 2n\Upsilon_{HL} + 2n\Upsilon_{LH} \\ &= \frac{n(18n^4+79n^3+131n^2+98n+20)}{(n+2)^2(2n^2+7n+5)}.\end{aligned}\quad (\text{S122})$$

Therefore, the critical synergy factor on hub-to-hub star graphs under the PC rule is

$$r^* = \frac{\tau^{(1)}}{\Upsilon^{(1)}} = \frac{2(n+2)^2(24n^3+50n^2+27n+5)}{n(18n^4+79n^3+131n^2+98n+20)} \xrightarrow{n \rightarrow \infty} \frac{8}{3}.\quad (\text{S123})$$

For the DB rule, the numerator is

$$\begin{aligned}\tau^{(2)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij} \\ &= \frac{2n}{n+1}\tau_{HL} + \frac{2n(n-1)}{n+1}\tau_{LL'} + \frac{2n}{n+1}\tau_{HL'} \\ &= \frac{4n(10n^2+17n+5)}{2n^2+7n+5},\end{aligned}\quad (\text{S124})$$

and the denominator is

$$\begin{aligned}\Upsilon^{(2)} &= \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \Upsilon_{ij} \\ &= \frac{2n}{n+1}\Upsilon_{HL'} + \frac{2n(n-1)}{n+1}\Upsilon_{LL'} + \frac{2n}{n+1}\Upsilon_{L'H}\end{aligned}$$

$$= \frac{n(22n^5 + 131n^4 + 287n^3 + 296n^2 + 148n + 20)}{(2n+5)(n^2+3n+2)^2}. \quad (\text{S125})$$

Therefore, the critical synergy factor on hub-to-hub star graphs under the DB rule is

$$r^* = \frac{4(n+2)^2(10n^3 + 27n^2 + 22n + 5)}{22n^5 + 131n^4 + 287n^3 + 296n^2 + 148n + 20} \xrightarrow{n \rightarrow \infty} \frac{20}{11}. \quad (\text{S126})$$

For the BD rule, we list the system of linear equations according to Eq. (S68):

$$\begin{cases} \tilde{\tau}_{HH'} = \frac{n+1}{2(n^2+n+1)}(1+2n\tilde{\tau}_{HL'}), \\ \tilde{\tau}_{HL} = \frac{n+1}{n^2+n+2} \left(1 + \frac{1}{n+1}\tilde{\tau}_{HL'} + (n-1)\tilde{\tau}_{LL'} \right), \\ \tilde{\tau}_{HL'} = \frac{n+1}{n^2+n+2} \left(1 + \frac{1}{n+1}\tilde{\tau}_{HH'} + \frac{1}{n+1}\tilde{\tau}_{HL} + n\tilde{\tau}_{LL''} \right), \\ \tilde{\tau}_{LL'} = \frac{n+1}{2} + \tilde{\tau}_{HL}, \\ \tilde{\tau}_{LL''} = \frac{n+1}{2} + \tilde{\tau}_{HL'}. \end{cases} \quad (\text{S127})$$

The solution is

$$\begin{cases} \tilde{\tau}_{HH'} = \frac{(n+1)(n^5 + 6n^4 + 10n^3 + 12n^2 + 9n + 5)}{2(n^3 + 3n^2 + 4n + 5)}, \\ \tilde{\tau}_{HL} = \frac{2n^5 + 5n^4 + 10n^3 + 11n^2 + 9n + 5}{2(n^3 + 3n^2 + 4n + 5)}, \\ \tilde{\tau}_{HL'} = \frac{n^6 + 7n^5 + 17n^4 + 28n^3 + 30n^2 + 23n + 10}{2(n^3 + 3n^2 + 4n + 5)}, \\ \tilde{\tau}_{LL'} = \frac{n^5 + 3n^4 + 7n^3 + 9n^2 + 9n + 5}{n^3 + 3n^2 + 4n + 5}, \\ \tilde{\tau}_{LL''} = \frac{n^6 + 7n^5 + 18n^4 + 32n^3 + 37n^2 + 32n + 15}{2(n^3 + 3n^2 + 4n + 5)}. \end{cases} \quad (\text{S128})$$

Inserting these $\tilde{\tau}_{ij}$ values into Eq. (S66), we obtain the required $\tilde{\Upsilon}_{ij}$ values:

$$\begin{aligned} \tilde{\Upsilon}_{HH'} &= \frac{n}{2(n+2)}(\tilde{\tau}_{HH'} - \tilde{\tau}_{HL} + \tilde{\tau}_{HL'}) \\ &= \frac{n(n^6 + 6n^5 + 14n^4 + 20n^3 + 20n^2 + 14n + 5)}{2(n^4 + 5n^3 + 10n^2 + 13n + 10)}, \end{aligned} \quad (\text{S129a})$$

$$\begin{aligned} \tilde{\Upsilon}_{HL} &= -\frac{2}{(n+2)^2}\tilde{\tau}_{HH'} - \frac{n-2}{(n+2)^2}\tilde{\tau}_{HL} - \frac{n-2}{(n+2)^2}\tilde{\tau}_{HL'} + \frac{n^2+3n-4}{2(n+2)^2}\tilde{\tau}_{LL'} + \frac{2}{(n+2)^2}\tilde{\tau}_{LL''} \\ &= \frac{n(n^6 + 4n^5 + 12n^4 + 24n^3 + 36n^2 + 36n + 15)}{2(n+2)^2(n^3 + 3n^2 + 4n + 5)}, \end{aligned} \quad (\text{S129b})$$

$$\begin{aligned} \tilde{\Upsilon}_{LH} &= \frac{1}{2(n+2)}\tilde{\tau}_{HH'} + \frac{n-1}{2(n+2)}\tilde{\tau}_{HL} - \frac{1}{2(n+2)}\tilde{\tau}_{HL'} - \frac{n-1}{2(n+2)}\tilde{\tau}_{LL'} \\ &= -\frac{n(n^4 + 4n^3 + 9n^2 + 11n + 5)}{4(n^4 + 5n^3 + 10n^2 + 13n + 10)}. \end{aligned} \quad (\text{S129c})$$

Then, we apply these $\tilde{\tau}_{ij}$ and $\tilde{\Upsilon}_{ij}$ values to calculate the critical synergy factor on the hub-to-hub star graph under the BD rule. The numerator is

$$\tilde{\tau}^{(1)} = \frac{2}{(n+1)^2}\tilde{\tau}_{HH'} + \frac{4n}{n+1}\tilde{\tau}_{HL} = \frac{4n^6 + 11n^5 + 26n^4 + 32n^3 + 30n^2 + 19n + 5}{n^4 + 4n^3 + 7n^2 + 9n + 5}, \quad (\text{S130})$$

and the denominator is

$$\tilde{\Upsilon}^{(1)} = \frac{2}{(n+1)^2} \tilde{\Upsilon}_{HH'} + \frac{2n}{n+1} \tilde{\Upsilon}_{HL} + \frac{2n}{n+1} \tilde{\Upsilon}_{LH} = \frac{n(2n^7 + 9n^6 + 32n^5 + 69n^4 + 101n^3 + 107n^2 + 66n + 20)}{2(n+2)^2(n^4 + 4n^3 + 7n^2 + 9n + 5)}. \quad (\text{S131})$$

Therefore, the critical synergy factor on hub-to-hub star graphs under the BD rule is

$$r^* = \frac{\tilde{\tau}^{(1)}}{\tilde{\Upsilon}^{(1)}} = \frac{2(n+2)^2(4n^6 + 11n^5 + 26n^4 + 32n^3 + 30n^2 + 19n + 5)}{n(2n^7 + 9n^6 + 32n^5 + 69n^4 + 101n^3 + 107n^2 + 66n + 20)} \xrightarrow{n \rightarrow \infty} 4. \quad (\text{S132})$$

- Accumulated payoff

When using accumulated payoffs, we follow Eq. (S74) for the PC rule. The numerator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\tau_{ij} &= 2(n+2)\tau_{HH'} + 2n(n+4)\tau_{HL} \\ &= \frac{2(14n^4 + 83n^3 + 122n^2 + 59n + 10)}{2n^2 + 7n + 5}, \end{aligned} \quad (\text{S133})$$

and the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\Upsilon_{ij} &= 2(n+2)\Upsilon_{HH'} + 2n(n+2)\Upsilon_{HL} + 4n\Upsilon_{LH} \\ &= \frac{2n(10n^4 + 43n^3 + 70n^2 + 49n + 10)}{2n^3 + 11n^2 + 19n + 10}. \end{aligned} \quad (\text{S134})$$

The critical synergy factor on hub-to-hub star graphs under the PC rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{14n^5 + 111n^4 + 288n^3 + 303n^2 + 128n + 20}{n(10n^4 + 43n^3 + 70n^2 + 49n + 10)} \xrightarrow{n \rightarrow \infty} \frac{7}{5}. \quad (\text{S135})$$

For the DB rule, we follow Eq. (S76). The numerator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\tau_{ij} &= \frac{2n(n+4)}{n+1}\tau_{HL'} + \frac{4n(n-1)}{n+1}\tau_{LL'} \\ &= \frac{4n(2n^3 + 29n^2 + 39n + 10)}{2n^2 + 7n + 5}, \end{aligned} \quad (\text{S136})$$

and the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\Upsilon_{ij} &= \frac{2n(n+2)}{n+1}\Upsilon_{HL'} + \frac{4n}{n+1}\Upsilon_{LH'} + \frac{4n(n-1)}{n+1}\Upsilon_{LL'} \\ &= \frac{2n(4n^5 + 40n^4 + 115n^3 + 141n^2 + 74n + 10)}{(n+1)^2(2n^2 + 9n + 10)}. \end{aligned} \quad (\text{S137})$$

The critical synergy factor on hub-to-hub star graphs under the DB rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{4n^5 + 70n^4 + 260n^3 + 370n^2 + 216n + 40}{4n^5 + 40n^4 + 115n^3 + 141n^2 + 74n + 10} \xrightarrow{n \rightarrow \infty} 1. \quad (\text{S138})$$

Eq. (S138) is the result of the super structure for cooperation presented in the main text.

For the BD rule, we follow Eq. (S78). The numerator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i+1)\tilde{\tau}_{ij} &= \frac{2(n+2)}{(n+1)^2} \tilde{\tau}_{HH'} + \frac{2n(n+4)}{n+1} \tilde{\tau}_{HL} \\ &= \frac{2n^7 + 14n^6 + 38n^5 + 73n^4 + 85n^3 + 74n^2 + 43n + 10}{n^4 + 4n^3 + 7n^2 + 9n + 5}, \end{aligned} \quad (\text{S139})$$

and the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{Y}_{ij} &= \frac{2(n+2)}{(n+1)^2} \tilde{Y}_{HH'} + \frac{2n(n+2)}{n+1} \tilde{Y}_{HL} + \frac{4n}{n+1} \tilde{Y}_{LH} \\ &= \frac{n(n^7 + 5n^6 + 18n^5 + 39n^4 + 56n^3 + 56n^2 + 33n + 10)}{n^5 + 6n^4 + 15n^3 + 23n^2 + 23n + 10}. \end{aligned} \quad (\text{S140})$$

The critical synergy factor on hub-to-hub star graphs under the BD rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{2n^8 + 18n^7 + 66n^6 + 149n^5 + 231n^4 + 244n^3 + 191n^2 + 96n + 20}{n(n^7 + 5n^6 + 18n^5 + 39n^4 + 56n^3 + 56n^2 + 33n + 10)} \xrightarrow{n \rightarrow \infty} 2. \quad (\text{S141})$$

2.4 m -hub star

On an m -hub star graph, there are m hubs (H), each has n leaves (L). A hub node has $k_H = n + m - 1$ neighbors (n leaves and the remaining $m - 1$ hubs), and each leaf node has $k_L = 1$ neighbor. There are five non-zero τ_{ij} types: $\tau_{HH'}$, the relation between one hub and another hub; $\tau_{LL'}$, the relation between two leaves of the same hub; $\tau_{LL''}$, the relation between two leaves of different hubs; τ_{HL} , the relation between a hub and one of its leaves; $\tau_{HL'}$, the relation between a hub and a leaf of another hub. The m -hub star reduces to a hub-to-hub star when $m = 2$. According to Eq. (4) in the main text, we have the system of linear equations:

$$\begin{cases} \tau_{HH'} = 1 + \frac{m-2}{n+m-1} \tau_{HH'} + \frac{n}{n+m-1} \tau_{HL'}, \\ \tau_{HL} = 1 + \frac{m-1}{2(n+m-1)} \tau_{HL'} + \frac{n-1}{2(n+m-1)} \tau_{LL'}, \\ \tau_{HL'} = 1 + \frac{1}{2(n+m-1)} \tau_{HL} + \frac{m-2}{2(n+m-1)} \tau_{HL'} + \frac{n}{2(n+m-1)} \tau_{LL''} + \frac{1}{2} \tau_{HH'}, \\ \tau_{LL'} = 1 + \tau_{HL}, \\ \tau_{LL''} = 1 + \tau_{HL'}. \end{cases} \quad (\text{S142})$$

The solution is

$$\begin{cases} \tau_{HH'} = \frac{2m^3 + 9m^2n - 4m^2 + 12mn^2 - 10mn + 3m + 4n^3 - 4n^2 + n - 1}{2m^2 + 4mn - 2m + 2n^2 - n + 1}, \\ \tau_{HL} = \frac{m^3 + 4m^2n + m^2 + 4mn^2 + 2mn - 4m + 2n^2 - 5n + 1}{2m^2 + 4mn - 2m + 2n^2 - n + 1}, \\ \tau_{HL'} = \frac{2m^3 + 9m^2n - m^2 + 12mn^2 - 4mn + 4n^3 - 2n^2 - 2}{2m^2 + 4mn - 2m + 2n^2 - n + 1}, \\ \tau_{LL'} = \frac{m^3 + 4m^2n + 3m^2 + 4mn^2 + 6mn - 6m + 4n^2 - 6n + 2}{2m^2 + 4mn - 2m + 2n^2 - n + 1}, \\ \tau_{LL''} = \frac{2m^3 + 9m^2n + m^2 + 12mn^2 - 2m + 4n^3 - n - 1}{2m^2 + 4mn - 2m + 2n^2 - n + 1}. \end{cases} \quad (\text{S143})$$

Inserting these τ_{ij} values into Eq. (5) in the main text, we obtain the required Υ_{ij} values:

$$\begin{aligned} \Upsilon_{HH'} &= \frac{n}{2(n+m)} (\tau_{HL'} - \tau_{HL} + \tau_{HH'}) \\ &= \frac{n(3m^3 + 14m^2n - 6m^2 + 20mn^2 - 16mn + 7m + 8n^3 - 8n^2 + 6n - 4)}{2(2m^3 + 6m^2n - 2m^2 + 6mn^2 - 3mn + m + 2n^3 - n^2 + n)}, \\ \Upsilon_{HL} &= -\frac{m(m-1)}{(m+n)^2} \tau_{HH'} + \frac{m-n}{(m+n)^2} \tau_{HL} + \frac{(m-n)(m-1)}{(m+n)^2} \tau_{HL'} \\ &\quad + \frac{(n-1)(m+n+2)}{2(m+n)^2} \tau_{LL'} + \frac{n(m-1)}{(m+n)^2} \tau_{LL''} \end{aligned} \quad (\text{S144a})$$

$$\begin{aligned}
&= \left\{ m^4 n + 7m^4 + 5m^3 n^2 + 22m^3 n - 15m^3 + 8m^2 n^3 + 21m^2 n^2 - 37m^2 n - 4m^2 \right. \\
&\quad \left. + 4mn^4 + 10mn^3 - 32mn^2 - 4mn + 14m + 4n^4 - 10n^3 + 10n - 4 \right\} / \left\{ 2(m+n)^2 \right. \\
&\quad \left. \times (2m^2 + 4mn - 2m + 2n^2 - n + 1) \right\}, \tag{S144b}
\end{aligned}$$

$$\begin{aligned}
\Upsilon_{LH} &= \frac{m-1}{2(m+n)} \tau_{HH'} + \frac{n-1}{2(m+n)} \tau_{HL} - \frac{m-1}{2(m+n)} \tau_{HL'} - \frac{n-1}{2(m+n)} \tau_{LL'} \\
&= \frac{-3m^3 - 8m^2 n + 8m^2 - 6mn^2 + 13mn - 4m - 2n^3 + 5n^2 - 3n}{2(2m^3 + 6m^2 n - 2m^2 + 6mn^2 - 3mn + m + 2n^3 - n^2 + n)}, \tag{S144c}
\end{aligned}$$

$$\begin{aligned}
\Upsilon_{HL'} &= -\frac{m(m-1)}{(m+n)^2} \tau_{HH'} + \frac{2m-2n-mn-n^2}{2(m+n)^2} \tau_{HL} + \frac{2m^2-mn-2m+n^2+2n}{2(m+n)^2} \tau_{HL'} \\
&\quad + \frac{n-1}{(m+n)^2} \tau_{LL'} + \frac{3mn-2n+n^2}{2(m+n)^2} \tau_{LL''} \\
&= \left\{ 3m^4 n + 8m^4 + 17m^3 n^2 + 23m^3 n - 12m^3 + 34m^2 n^3 + 13m^2 n^2 - 20m^2 n - 10m^2 \right. \\
&\quad \left. + 28mn^4 - 6mn^3 - 4mn^2 - 22mn + 16m + 8n^5 - 4n^4 + 4n^3 - 12n^2 + 12n - 4 \right\} \\
&\quad / \left\{ 2(m+n)^2 (2m^2 + 4mn - 2m + 2n^2 - n + 1) \right\}, \tag{S144d}
\end{aligned}$$

$$\begin{aligned}
\Upsilon_{LH'} &= \frac{3m+n-2}{4(m+n)} \tau_{HH'} - \frac{m+n+2}{4(m+n)} \tau_{HL} + \frac{3n-m+2}{4(m+n)} \tau_{HL'} - \frac{n-1}{2(m+n)} \tau_{LL'} \\
&= \left\{ 3m^4 + 19m^3 n - 12m^3 + 44m^2 n^2 - 42m^2 n + 23m^2 + 44mn^3 - 48mn^2 + 47mn \right. \\
&\quad \left. - 12m + 16n^4 - 20n^3 + 26n^2 - 16n \right\} / \left\{ 4(2m^3 + 6m^2 n - 2m^2 + 6mn^2 - 3mn \right. \\
&\quad \left. + m + 2n^3 - n^2 + n) \right\}, \tag{S144e}
\end{aligned}$$

$$\begin{aligned}
\Upsilon_{LL'} &= \frac{\tau_{LL'}}{4} \\
&= \frac{m^3 + 4m^2 n + 3m^2 + 4mn^2 + 6mn - 6m + 4n^2 - 6n + 2}{4(2m^2 + 4mn - 2m + 2n^2 - n + 1)}. \tag{S144f}
\end{aligned}$$

Then, we apply these τ_{ij} and Υ_{ij} values to calculate the critical synergy factor on the m -hub star graph. For the PC rule, the numerator is

$$\begin{aligned}
\tau^{(1)} &= m(m-1)\tau_{HH'} + 2mn\tau_{HL} \\
&= \left\{ m(2m^4 + 11m^3 n - 6m^3 + 20m^2 n^2 - 17m^2 n + 7m^2 + 12mn^3 - 12mn^2 + 3mn \right. \\
&\quad \left. - 4m - 6n^2 + n + 1) \right\} / \left\{ 2m^2 + 4mn - 2m + 2n^2 - n + 1 \right\} \tag{S145}
\end{aligned}$$

and the denominator is

$$\begin{aligned}
\Upsilon^{(1)} &= m(m-1)\Upsilon_{HH'} + mn\Upsilon_{HL} + mn\Upsilon_{LH} \\
&= \left\{ mn(3m^5 + 18m^4 n - 5m^4 + 39m^3 n^2 - 28m^3 n + 6m^3 + 36m^2 n^3 - 51m^2 n^2 \right. \\
&\quad \left. + 19m^2 n - 19m^2 + 12mn^4 - 34mn^3 + 16mn^2 - 28mn + 18m - 6n^4 + 3n^3 - 9n^2 \right. \\
&\quad \left. + 14n - 4) \right\} / \left\{ 2(m+n)^2 (2m^2 + 4mn - 2m + 2n^2 - n + 1) \right\} \tag{S146}
\end{aligned}$$

Therefore, the critical synergy factor on m -hub star graphs under the PC rule is

$$r^* = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} \frac{4m}{2m-1} \xrightarrow{m=2} \frac{8}{3} \xrightarrow{m \rightarrow \infty} 2, \tag{S147}$$

where

$$\text{nume} = 2(m+n)^2 (2m^4 + 11m^3 n - 6m^3 + 20m^2 n^2 - 17m^2 n + 7m^2 + 12mn^3)$$

$$\begin{aligned}
& -12mn^2 + 3mn - 4m - 6n^2 + n + 1), \\
\text{deno} = & n(3m^5 + 18m^4n - 5m^4 + 39m^3n^2 - 28m^3n + 6m^3 + 36m^2n^3 - 51m^2n^2 + 19m^2n \\
& - 19m^2 + 12mn^4 - 34mn^3 + 16mn^2 - 28mn + 18m - 6n^4 + 3n^3 - 9n^2 + 14n - 4).
\end{aligned} \tag{S148}$$

For the DB rule, the numerator is

$$\begin{aligned}
\tau^{(2)} = & \frac{m(m-1)(m-2)}{n+m-1} \tau_{HH'} + \frac{2mn(m-1)}{n+m-1} \tau_{HL'} + \frac{mn(n-1)}{n+m-1} \tau_{LL'} \\
= & \left\{ m(2m^4 + 11m^3n - 8m^3 + 20m^2n^2 - 25m^2n + 11m^2 + 12mn^3 - 22mn^2 + 12mn \right. \\
& \left. - 7m - 4n^3 - 2n^2 - 2n + 2) \right\} / \left\{ 2m^2 + 4mn - 2m + 2n^2 - n + 1 \right\}
\end{aligned} \tag{S149}$$

and the denominator is

$$\begin{aligned}
\Upsilon^{(2)} = & \frac{m(m-1)(m-2)}{n+m-1} \Upsilon_{HH'} + \frac{mn(m-1)}{n+m-1} \Upsilon_{HL'} + \frac{mn(m-1)}{n+m-1} \Upsilon_{LH'} + \frac{mn(n-1)}{n+m-1} \Upsilon_{LL'} \\
= & \left\{ mn(9m^6 + 63m^5n - 30m^5 + 171m^4n^2 - 185m^4n + 54m^4 + 225m^3n^3 - 414m^3n^2 \right. \\
& + 246m^3n - 99m^3 + 144m^2n^4 - 413m^2n^3 + 384m^2n^2 - 256m^2n + 114m^2 + 36mn^5 \\
& - 182mn^4 + 242mn^3 - 215mn^2 + 168mn - 56m - 28n^5 + 50n^4 - 58n^3 + 62n^2 \\
& \left. - 40n + 8) \right\} / \left\{ 4(m+n)^2(2m^3 + 6m^2n - 4m^2 + 6mn^2 - 7mn + 3m + 2n^3 - 3n^2 \right. \\
& \left. + 2n - 1) \right\}
\end{aligned} \tag{S150}$$

Therefore, the critical synergy factor on m -hub star graphs under the DB rule is

$$r^* = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} \frac{12m-4}{9m-7} \xrightarrow{m=2} \frac{20}{11} \xrightarrow{m \rightarrow \infty} \frac{4}{3}, \tag{S151}$$

where

$$\begin{aligned}
\text{nume} = & 4(m+n)^2(2m^3 + 6m^2n - 4m^2 + 6mn^2 - 7mn + 3m + 2n^3 - 3n^2 + 2n - 1) \\
& \times (2m^4 + 11m^3n - 8m^3 + 20m^2n^2 - 25m^2n + 11m^2 + 12mn^3 - 22mn^2 + 12mn \\
& - 7m - 4n^3 - 2n^2 - 2n + 2), \\
\text{deno} = & n(2m^2 + 4mn - 2m + 2n^2 - n + 1)(9m^6 + 63m^5n - 30m^5 + 171m^4n^2 - 185m^4n \\
& + 54m^4 + 225m^3n^3 - 414m^3n^2 + 246m^3n - 99m^3 + 144m^2n^4 - 413m^2n^3 + 384m^2n^2 \\
& - 256m^2n + 114m^2 + 36mn^5 - 182mn^4 + 242mn^3 - 215mn^2 + 168mn - 56m - 28n^5 \\
& + 50n^4 - 58n^3 + 62n^2 - 40n + 8).
\end{aligned} \tag{S152}$$

For the BD rule, we list the system of linear equations according to Eq. (S68):

$$\left\{ \begin{aligned}
\tilde{\tau}_{HH'} &= \frac{n+m-1}{2(n^2-n+mn+m-1)} \left(1 + \frac{2(m-2)}{n+m-1} \tilde{\tau}_{HH'} + 2n\tilde{\tau}_{HL'} \right), \\
\tilde{\tau}_{HL} &= \frac{n+m-1}{n^2-n+mn+m} \left(1 + \frac{m-1}{n+m-1} \tilde{\tau}_{HL'} + (n-1)\tilde{\tau}_{LL'} \right), \\
\tilde{\tau}_{HL'} &= \frac{n+m-1}{n^2-n+mn+m} \left(1 + \frac{1}{n+m-1} \tilde{\tau}_{HL} + \frac{m-2}{n+m-1} \tilde{\tau}_{HL'} + n\tilde{\tau}_{LL'} + \frac{1}{n+m-1} \tilde{\tau}_{HH'} \right), \\
\tilde{\tau}_{LL'} &= \frac{n+m-1}{2} + \tilde{\tau}_{HL}, \\
\tilde{\tau}_{LL''} &= \frac{n+m-1}{2} + \tilde{\tau}_{HL},
\end{aligned} \right. \tag{S153}$$

which can be solved, but the solution for $\tilde{\tau}_{ij}$ is too long and thus not presented here. Inserting these $\tilde{\tau}_{ij}$ values into Eq. (S66), we can obtain the required \tilde{Y}_{ij} values. Finally, we can apply these $\tilde{\tau}_{ij}$ and \tilde{Y}_{ij} values to calculate the critical synergy factor on the m -hub star graph under the BD rule. The numerator is

$$\tilde{\tau}^{(1)} = \frac{m(m-1)}{(n+m-1)^2} \tilde{\tau}_{HH'} + \frac{2mn}{n+m-1} \tilde{\tau}_{HL}, \quad (\text{S154})$$

and the denominator is

$$\tilde{Y}^{(1)} = \frac{m(m-1)}{(n+m-1)^2} \tilde{Y}_{HH'} + \frac{mn}{n+m-1} \tilde{Y}_{HL} + \frac{mn}{n+m-1} \tilde{Y}_{LH}. \quad (\text{S155})$$

Therefore, the critical synergy factor on m -hub star graphs under the BD rule is

$$r^* = \frac{\tilde{\tau}^{(1)}}{\tilde{Y}^{(1)}} = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} 4, \quad (\text{S156})$$

where

$$\begin{aligned} \text{nume} &= 2(m+n)^2(2m^4n^3 + 2m^4n^2 + 6m^3n^4 - m^3n^3 - 2m^3n^2 + 3m^3n + 6m^2n^5 - 8m^2n^4 + m^2n^3 \\ &\quad + 6m^2n^2 - 3m^2n + 3m^2 + 2mn^6 - 5mn^5 + 10mn^3 - 12mn^2 + 7mn - 4m - 3n^5 + 10n^4 \\ &\quad - 16n^3 + 14n^2 - 7n + 1), \\ \text{deno} &= n(m^5n^3 + 4m^5n^2 + 2m^5n + 4m^4n^4 + 10m^4n^3 - 7m^4n^2 + 2m^4n + 2m^4 + 6m^3n^5 + 6m^3n^4 \\ &\quad - 23m^3n^3 + 24m^3n^2 - 7m^3n + 5m^3 + 4m^2n^6 - 2m^2n^5 - 20m^2n^4 + 40m^2n^3 - 35m^2n^2 \\ &\quad + 17m^2n - 17m^2 + mn^7 - 2mn^6 - 9mn^5 + 28mn^4 - 41mn^3 + 23mn^2 - 20mn + 6m \\ &\quad - 3n^6 + 10n^5 - 19n^4 + 15n^3 - 7n^2 - 2n + 4). \end{aligned} \quad (\text{S157})$$

- Accumulated payoff

When using accumulated payoffs, we follow Eq. (S74) for the PC rule. The numerator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\tau_{ij} = m(m+n)(m-1)\tau_{HH'} + mn(m+n+2)\tau_{HL}, \quad (\text{S158})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\Upsilon_{ij} = m(m+n)(m-1)\Upsilon_{HH'} + mn(m+n)\Upsilon_{HL} + 2mn\Upsilon_{LH}. \quad (\text{S159})$$

The critical synergy factor on m -hub star graphs under the PC rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} \frac{4m-1}{3m-1} \xrightarrow{m \rightarrow \infty} \frac{4}{3}, \quad (\text{S160})$$

where

$$\begin{aligned} \text{nume} &= 2(2m^3 + 6m^2n - 2m^2 + 6mn^2 - 3mn + m + 2n^3 - n^2 + n)(2m^5 + 12m^4n - 6m^4 \\ &\quad + 26m^3n^2 - 22m^3n + 7m^3 + 24m^2n^3 - 24m^2n^2 + 16m^2n - 4m^2 + 8mn^4 - 8mn^3 \\ &\quad + 10mn^2 - 12mn + m - 2n^4 + 3n^3 - 10n^2 + 3n), \\ \text{deno} &= n(2m^2 + 4mn - 2m + 2n^2 - n + 1)(3m^5 + 18m^4n - 2m^4 + 39m^3n^2 - 17m^3n - 8m^3 \\ &\quad + 36m^2n^3 - 37m^2n^2 - 18m^2n + m^2 + 12mn^4 - 26mn^3 - 14mn^2 + 5mn + 10m \\ &\quad - 4n^4 - 6n^3 + 4n^2 + 8n - 4). \end{aligned} \quad (\text{S161})$$

For the DB rule, we follow Eq. (S76). The numerator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\tau_{ij} = \frac{m(m+n)(m-1)(m-2)}{m+n-1}\tau_{HH'} + \frac{mn(m-1)(m+n+2)}{m+n-1}\tau_{HL} + \frac{2mn(n-1)}{m+n-1}\tau_{LL'}, \quad (\text{S162})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\Upsilon_{ij} = \frac{m(m+n)(m-1)(m-2)}{m+n-1}\Upsilon_{HH'} + \frac{mn(m+n)(m-1)}{m+n-1}\Upsilon_{HL'} + \frac{2mn(n-1)}{m+n-1}\Upsilon_{LH'} + \frac{2mn(n-1)}{m+n-1}\Upsilon_{LL'}. \quad (\text{S163})$$

The critical synergy factor on m -hub star graphs under the DB rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} 1, \quad (\text{S164})$$

where

$$\begin{aligned} \text{nume} &= 2(2m^4 + 8m^3n - 4m^3 + 12m^2n^2 - 11m^2n + 3m^2 + 8mn^3 - 10mn^2 + 5mn - m + 2n^4 \\ &\quad - 3n^3 + 2n^2 - n)(2m^5 + 11m^4n - 8m^4 + 21m^3n^2 - 27m^3n + 11m^3 + 16m^2n^3 - 25m^2n^2 \\ &\quad + 23m^2n - 7m^2 + 4mn^4 - 6mn^3 + 14mn^2 - 17mn + 2m - 4n^4 + 6n^3 - 18n^2 + 2n), \\ \text{deno} &= n(2m^2 + 4mn - 2m + 2n^2 - n + 1)(3m^6 + 20m^5n - 4m^5 + 51m^4n^2 - 33m^4n - 5m^4 \\ &\quad + 62m^3n^3 - 81m^3n^2 + 7m^3n - 3m^3 + 36m^2n^4 - 80m^2n^3 + 38m^2n^2 - 15m^2n + 23m^2 \\ &\quad + 8mn^5 - 36mn^4 + 32mn^3 - 22mn^2 + 23mn - 18m - 8n^5 + 8n^4 - 10n^3 + 6n^2 - 6n + 4). \end{aligned} \quad (\text{S165})$$

For the BD rule, we follow Eq. (S78). The numerator is

$$\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\tau}_{ij} = \frac{m(m+n)(m-1)}{(n+m-1)^2} \tilde{\tau}_{HH'} + \frac{mn(m+n+2)}{n+m-1} \tilde{\tau}_{HL}, \quad (\text{S166})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\Upsilon}_{ij} = \frac{m(m+n)(m-1)}{(n+m-1)^2} \tilde{\Upsilon}_{HH'} + \frac{mn(m+n)}{n+m-1} \tilde{\Upsilon}_{HL} + \frac{2mn}{n+m-1} \tilde{\Upsilon}_{LH}. \quad (\text{S167})$$

The critical synergy factor on m -hub star graphs under the BD rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{\text{nume}}{\text{deno}} \xrightarrow{n \rightarrow \infty} 2, \quad (\text{S168})$$

where

$$\begin{aligned} \text{nume} &= 2(m^4n + 4m^3n^2 - 2m^3n + 3m^3 + 6m^2n^3 - 6m^2n^2 + 9m^2n - 4m^2 + 4mn^4 - 6mn^3 + 9mn^2 \\ &\quad - 7mn + m + n^5 - 2n^4 + 3n^3 - 3n^2 + n)(m^5n^3 + 2m^5n^2 + 4m^4n^4 + 6m^4n^3 - 4m^4n^2 \\ &\quad + 3m^4n + 6m^3n^5 + 6m^3n^4 - 15m^3n^3 + 15m^3n^2 - 4m^3n + 3m^3 + 4m^2n^6 + 2m^2n^5 - 20m^2n^4 \\ &\quad + 29m^2n^3 - 17m^2n^2 + 10m^2n - 4m^2 + mn^7 - 11mn^5 + 21mn^4 - 16mn^3 + 6mn^2 - 4mn \\ &\quad + m - 2n^6 + 4n^5 - n^4 - 7n^3 + 10n^2 - 5n), \\ \text{deno} &= n(m^3n + 3m^2n^2 - 2m^2n + 3m^2 + 3mn^3 - 4mn^2 + 6mn - 4m + n^4 - 2n^3 + 3n^2 - 3n + 1) \\ &\quad \times (m^5n^3 + 4m^5n^2 + 4m^5n + 4m^4n^4 + 10m^4n^3 + m^4n^2 - 9m^4n + 4m^4 + 6m^3n^5 + 6m^3n^4 \\ &\quad - 10m^3n^3 - 11m^3n^2 + 22m^3n - 5m^3 + 4m^2n^6 - 2m^2n^5 - 9m^2n^4 - 3m^2n^3 + 27m^2n^2 \\ &\quad - 28m^2n - m^2 + mn^7 - 2mn^6 - 4mn^5 + 3mn^4 + 9mn^3 - 31mn^2 + 13mn - 2m - 2n^6 \\ &\quad + 4n^5 - 4n^4 - 6n^3 + 10n^2 - 8n + 4). \end{aligned} \quad (\text{S169})$$

2.5 Ceiling fan

On a ceiling fan graph, there is one hub (H) and n leaves (L), each leaf consists of two connected nodes. The hub node has $k_H = 2n$ neighbors, and each leaf node has $k_L = 2$ neighbors (the hub and the other leaf node). There are three non-zero τ_{ij} types: τ_{HL} , the relation between the hub and a leaf node; $\tau_{LL'}$, the relation between the two leaf nodes of the same leaf; $\tau_{LL''}$,

the relation between two leaf nodes of two different leaves. According to Eq. (4) in the main text, we have the system of linear equations:

$$\begin{cases} \tau_{HL} = 1 + \frac{1}{4n}(\tau_{LL'} + (2n-2)\tau_{LL''}) + \frac{1}{4}\tau_{HL}, \\ \tau_{LL'} = 1 + \frac{1}{4}\tau_{HL} + \frac{1}{4}\tau_{HL}, \\ \tau_{LL''} = 1 + \frac{1}{4}(\tau_{HL} + \tau_{LL''}) + \frac{1}{4}(\tau_{HL} + \tau_{LL''}). \end{cases} \quad (\text{S170})$$

The solution is

$$\begin{cases} \tau_{HL} = \frac{2(8n-3)}{2n+3}, \\ \tau_{LL'} = \frac{10n}{2n+3}, \\ \tau_{LL''} = \frac{20n}{2n+3}. \end{cases} \quad (\text{S171})$$

Inserting these τ_{ij} values into Eq. (5) in the main text, we calculate the required Υ_{ij} values:

$$\begin{aligned} \Upsilon_{HL} &= -\frac{4n^2+8n-3}{3(2n+1)^2}\tau_{HL} + \frac{4n+5}{3(2n+1)^2}\tau_{LL'} + \frac{8n^2+2n-10}{3(2n+1)^2}\tau_{LL''} \\ &= \frac{2(16n^3-4n^2-9n-3)}{(2n+1)^2(2n+3)}, \end{aligned} \quad (\text{S172a})$$

$$\begin{aligned} \Upsilon_{LH} &= \frac{10n-1}{9(2n+1)}\tau_{HL} - \frac{4n+5}{9(2n+1)}\tau_{LL'} - \frac{2n-2}{3(2n+1)}\tau_{LL''} \\ &= -\frac{2(n-1)}{3(4n^2+8n+3)}, \end{aligned} \quad (\text{S172b})$$

$$\Upsilon_{LL'} = 0, \quad (\text{S172c})$$

$$\Upsilon_{LL''} = -\frac{2}{9}\tau_{LL'} + \frac{4}{9}\tau_{LL''} = \frac{20n}{6n+9}. \quad (\text{S172d})$$

Then, we apply these τ_{ij} and Υ_{ij} values to calculate the critical synergy factor on the ceiling fan graph. For the PC rule, the numerator is

$$\tau^{(1)} = 4n\tau_{HL} + 2n\tau_{LL'} = \frac{12n(7n-2)}{2n+3}, \quad (\text{S173})$$

and the denominator is

$$\Upsilon^{(1)} = 2n\Upsilon_{HL} + 2n\Upsilon_{LH} + 2n\Upsilon_{LL'} = \frac{8n(24n^3-7n^2-13n-4)}{3(2n+1)^2(2n+3)}. \quad (\text{S174})$$

Therefore, the critical synergy factor on ceiling fan graphs under the PC rule is

$$r^* = \frac{9(2n+1)^2(7n-2)}{2(24n^3-7n^2-13n-4)} \xrightarrow{n \rightarrow \infty} \frac{21}{4}. \quad (\text{S175})$$

For the DB rule, the numerator is

$$\tau^{(2)} = 2n\tau_{HL} + \tau_{LL'} + (2n-2)\tau_{LL''} = \frac{6n(12n-7)}{2n+3}, \quad (\text{S176})$$

and the denominator is

$$\Upsilon^{(2)} = n\Upsilon_{HL} + n\Upsilon_{LH} + \Upsilon_{LL'} + (2n-2)\Upsilon_{LL''} = \frac{4n(64n^3-7n^2-43n-14)}{3(2n+1)^2(2n+3)}. \quad (\text{S177})$$

Therefore, the critical synergy factor on ceiling fan graphs under the DB rule is

$$r^* = \frac{9(2n+1)^2(12n-7)}{2(64n^3-7n^2-43n-14)} \xrightarrow{n \rightarrow \infty} \frac{27}{8}. \quad (\text{S178})$$

For the BD rule, we list the system of linear equations according to Eq. (S68):

$$\begin{cases} \tilde{\tau}_{HL} = \frac{2n}{2n^2+n+1} \left(1 + \frac{1}{2} \tilde{\tau}_{LL'} + (n-1) \tilde{\tau}_{LL''} + \frac{1}{2} \tilde{\tau}_{HL} \right), \\ \tilde{\tau}_{LL'} = \frac{n}{n+1} \left(1 + \frac{1}{n} \tilde{\tau}_{HL} \right), \\ \tilde{\tau}_{LL''} = \frac{n}{n+1} \left(1 + \frac{1}{n} \tilde{\tau}_{HL} + \tilde{\tau}_{LL''} \right). \end{cases} \quad (\text{S179})$$

The solution is

$$\begin{cases} \tilde{\tau}_{HL} = \frac{2n^4+n^2+2n}{2n^2+2n+1}, \\ \tilde{\tau}_{LL'} = \frac{n(2n^2+3)}{2n^2+2n+1}, \\ \tilde{\tau}_{LL''} = \frac{n(2n^2+3)(n+1)}{2n^2+2n+1}. \end{cases} \quad (\text{S180})$$

Inserting these $\tilde{\tau}_{ij}$ values into Eq. (S66), we obtain the required \tilde{Y}_{ij} values:

$$\begin{aligned} \tilde{Y}_{HL} &= -\frac{4n^2+8n-3}{3(2n+1)^2} \tilde{\tau}_{HL} + \frac{4n+5}{3(2n+1)^2} \tilde{\tau}_{LL'} + \frac{8n^2+2n-10}{3(2n+1)^2} \tilde{\tau}_{LL''} \\ &= \frac{n(8n^5+4n^4+18n^3+4n^2-25n-9)}{3(2n+1)^2(2n^2+2n+1)}, \end{aligned} \quad (\text{S181a})$$

$$\begin{aligned} \tilde{Y}_{LH} &= \frac{10n-1}{9(2n+1)} \tilde{\tau}_{HL} - \frac{4n+5}{9(2n+1)} \tilde{\tau}_{LL'} - \frac{2n-2}{3(2n+1)} \tilde{\tau}_{LL''} \\ &= \frac{n(8n^4-10n^3-6n^2+7n+1)}{9(4n^3+6n^2+4n+1)}, \end{aligned} \quad (\text{S181b})$$

$$\tilde{Y}_{LL'} = 0. \quad (\text{S181c})$$

Then, we apply these $\tilde{\tau}_{ij}$ and \tilde{Y}_{ij} values to calculate the critical synergy factor on the ceiling fan graph under the BD rule. The numerator is

$$\tilde{\tau}^{(1)} = \tilde{\tau}_{HL} + \frac{n}{2} \tilde{\tau}_{LL'} = \frac{n(6n^3+5n+4)}{2(2n^2+2n+1)}, \quad (\text{S182})$$

and the denominator is

$$\tilde{Y}^{(1)} = \frac{1}{2} \tilde{Y}_{HL} + \frac{1}{2} \tilde{Y}_{LH} + \frac{n}{2} \tilde{Y}_{LL'} = \frac{n(20n^5+16n^3+10n^2-33n-13)}{9(2n+1)^2(2n^2+2n+1)}. \quad (\text{S183})$$

Therefore, the critical synergy factor on ceiling fan graphs under the BD rule is

$$r^* = \frac{\tilde{\tau}^{(1)}}{\tilde{Y}^{(1)}} = \frac{9(2n+1)^2(6n^3+5n+4)}{2(20n^5+16n^3+10n^2-33n-13)} \xrightarrow{n \rightarrow \infty} \frac{27}{5}. \quad (\text{S184})$$

- Accumulated payoff

When using accumulated payoffs, we follow Eq. (S74) for the PC rule. The numerator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\tau_{ij} = 4n(n+2)\tau_{HL} + 6n\tau_{LL'} = \frac{4n(16n^2+41n-12)}{2n+3}, \quad (\text{S185})$$

and the denominator is

$$\sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}\Upsilon_{ij} = 2n(2n+1)\Upsilon_{HL} + 6n\Upsilon_{LH} + 6n\Upsilon_{LL'} = \frac{8n(4n^2 - 3n - 1)}{2n+3}. \quad (\text{S186})$$

The critical synergy factor on ceiling fan graphs under the PC rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{16n^2 + 41n - 12}{2(4n^2 - 3n - 1)} \xrightarrow{n \rightarrow \infty} 2. \quad (\text{S187})$$

For the DB rule, we follow Eq. (S76). The numerator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\tau_{ij} &= 2n(n+2)\tau_{HL} + 3\tau_{LL'} + 6(n-1)\tau_{LL''} \\ &= \frac{2n(16n^2 + 86n - 57)}{2n+3}, \end{aligned} \quad (\text{S188})$$

and the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} k_i(k_i+1)p_{ij}^{(2)}\Upsilon_{ij} &= n(2n+1)\Upsilon_{HL} + 3n\Upsilon_{LH} + 3\Upsilon_{LL'} + 6(n-1)\Upsilon_{LL''} \\ &= \frac{4n(4n^2 + 7n - 11)}{2n+3}. \end{aligned} \quad (\text{S189})$$

The critical synergy factor on ceiling fan graphs under the DB rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{16n^2 + 86n - 57}{2(4n^2 + 7n - 11)} \xrightarrow{n \rightarrow \infty} 2. \quad (\text{S190})$$

For the BD rule, we follow Eq. (S78). The numerator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i+1)\tilde{\tau}_{ij} &= (n+2)\tilde{\tau}_{HL} + \frac{3n}{2}\tilde{\tau}_{LL'} \\ &= \frac{n(4n^4 + 14n^3 + 2n^2 + 17n + 8)}{2(2n^2 + 2n + 1)}, \end{aligned} \quad (\text{S191})$$

and the denominator is

$$\begin{aligned} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i+1)\tilde{\Upsilon}_{ij} &= \frac{2n+1}{2}\tilde{\Upsilon}_{HL} + \frac{3}{2}\tilde{\Upsilon}_{LH} + \frac{3n}{2}\tilde{\Upsilon}_{LL'} \\ &= \frac{n(2n^4 + 2n^3 + n^2 - n - 4)}{3(2n^2 + 2n + 1)}. \end{aligned} \quad (\text{S192})$$

The critical synergy factor on ceiling fan graphs under the BD rule when using accumulated payoff is

$$r_{\text{accu}}^* = \frac{3(4n^4 + 14n^3 + 2n^2 + 17n + 8)}{2(2n^4 + 2n^3 + n^2 - n - 4)} \xrightarrow{n \rightarrow \infty} 3. \quad (\text{S193})$$

By analogy, the critical synergy factor for spatial PGGs on any other network structures can be calculated using the same method in the future.

Supplementary Note 3: Some extensions to the donation game (DG)

Here, we give the details of deducing cooperation conditions in pairwise donation games (DGs). These results can be derived through the techniques in previous literature¹⁰. Unfortunately, while the previous literature indicated the methods to obtain these results, they did not publish them. In particular, only the results under the DB and BD updates using averaged payoff can be found in previous literature¹⁰. To compare our spatial PGGs with pairwise DGs across different model details, we have to deduce the unpublished results of pairwise DGs and present them in our work.

The actual payoff of agent i is averaged over k_i DGs played with all neighbors $l \in \mathcal{N}_i$. In each DG, a cooperator pays c and the other player receives b ($b > c$), while a defector pays nothing and the other player receives nothing. Namely, the actual payoff $f_i(\mathbf{x})$ of agent i is expressed as follows.

$$f_i(\mathbf{x}) = \frac{1}{k_i} \sum_{l \in \mathcal{N}_i} (-x_i c + x_l b) = -x_i c + \frac{1}{k_i} \sum_{l \in \mathcal{N}_i} x_l b. \quad (\text{S194})$$

The dynamics of strategy evolution under neutral drift remain the same. Only the quantity $\mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ is influenced by the payoff calculation in pairwise DGs. Applying the payoff in Eq. (S194), we have

$$\begin{aligned} & \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] \\ &= \mathbb{E}_{\text{RMC}}^\circ \left[- (x_i^2 - x_i x_j) c + \frac{1}{k_i} \sum_{l \in \mathcal{N}_i} (x_i x_l - x_j x_l) b + (x_i x_j - x_j^2) c - \frac{1}{k_j} \sum_{l \in \mathcal{N}_j} (x_i x_l - x_j x_l) b \right] \\ &= -c (\mathbb{E}_{\text{RMC}}^\circ[x_i^2] - 2\mathbb{E}_{\text{RMC}}^\circ[x_i x_j] + \mathbb{E}_{\text{RMC}}^\circ[x_j^2]) + \frac{b}{k_i} \sum_{l \in \mathcal{N}_i} (\mathbb{E}_{\text{RMC}}^\circ[x_i x_l] - \mathbb{E}_{\text{RMC}}^\circ[x_j x_l]) \\ & \quad - \frac{b}{k_j} \sum_{l \in \mathcal{N}_j} (\mathbb{E}_{\text{RMC}}^\circ[x_i x_l] - \mathbb{E}_{\text{RMC}}^\circ[x_j x_l]). \end{aligned} \quad (\text{S195})$$

3.1 Pairwise comparison

The cooperation condition under the PC rule is Eq. (S17). Using the result of Eq. (S195) and applying $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^\circ[x_i x_j]) / (K/4)$ defined by Eq. (S26), we calculate the cooperation condition under the PC rule as

$$\begin{aligned} & \frac{1}{4N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij} \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\ & \Leftrightarrow \sum_{i,j \in \mathcal{N}} k_i p_{ij} \left\{ -2c\tau_{ij} + \frac{b}{k_i} \sum_{l \in \mathcal{N}_i} (-\tau_{il} + \tau_{jl}) - \frac{b}{k_j} \sum_{l \in \mathcal{N}_j} (-\tau_{il} + \tau_{jl}) \right\} > 0 \\ & \Leftrightarrow \frac{b}{c} > \frac{2 \sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij} (p_{il} - p_{jl})(\tau_{jl} - \tau_{il})}. \end{aligned} \quad (\text{S196})$$

Further simplifying Eq. (S196) (using Eq. (S83)) leads to

$$\frac{b}{c} > \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il} (\tau_{jl} - \tau_{il})} = \frac{\tau^{(1)}}{\tau^{(2)} - \tau^{(1)}}. \quad (\text{S197})$$

The right-hand side is the $(b/c)^*$ value for cooperation success in pairwise DGs under the PC rule. The τ_{ij} values should be obtained by solving Eqs. (S33) on a given network structure.

3.2 Death-birth

The critical $(b/c)^*$ value under the DB update has been first obtained in Ref.¹⁰. Trivially, in our calculation, the cooperation condition under the DB rule is Eq. (S41). Using the result of Eq. (S195) and applying $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^\circ[x_i x_j]) / (K/4)$ defined by Eq. (S44), we calculate Eq. (S41) as

$$\begin{aligned} & \frac{1}{2N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\ & \Leftrightarrow \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \left\{ -2c\tau_{ij} + \frac{b}{k_i} \sum_{l \in \mathcal{N}_i} (-\tau_{il} + \tau_{jl}) - \frac{b}{k_j} \sum_{l \in \mathcal{N}_j} (-\tau_{il} + \tau_{jl}) \right\} > 0 \\ & \Leftrightarrow \frac{b}{c} > \frac{2 \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} (p_{il} - p_{jl})(\tau_{jl} - \tau_{il})}. \end{aligned} \quad (\text{S198})$$

Further simplifying Eq. (S196) leads to

$$\frac{b}{c} > \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il} (\tau_{jl} - \tau_{il})} = \frac{\tau^{(2)}}{\tau^{(3)} - \tau^{(1)}}. \quad (\text{S199})$$

The right-hand side is the $(b/c)^*$ value for cooperation success in pairwise DGs under the DB rule, which is consistent with “ $t_2/(t_3 - t_1)$ ” in the main text of Ref.¹⁰. The τ_{ij} values should be obtained by solving Eqs. (S33) on a given network structure.

3.3 Birth-death

The critical $(b/c)^*$ value under the BD update has also been mentioned in Ref.¹⁰. We examine their results here. The cooperation condition under the BD rule is Eq. (S53). Using the result of Eq. (S195) and applying $\tau_{ij} = (1/2 - \mathbb{E}_{\text{RMC}}^\circ[x_i x_j]) / (K/2)$ as defined by Eq. (S61), we calculate Eq. (S53) follows.

$$\begin{aligned}
& \frac{1}{2N^2 \langle k^{-1} \rangle} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \left\{ -2c\tilde{\tau}_{ij} + \frac{b}{k_i} \sum_{l \in \mathcal{N}_i} (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) - \frac{b}{k_j} \sum_{l \in \mathcal{N}_j} (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) \right\} > 0 \\
\Leftrightarrow & \frac{b}{c} > \frac{2 \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (p_{il} - p_{jl})(\tilde{\tau}_{jl} - \tilde{\tau}_{il})} = \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} \frac{k_{ij} k_{il}}{k_i^2 k_j} (\tilde{\tau}_{jl} - \tilde{\tau}_{il})}. \tag{S200}
\end{aligned}$$

The right-hand side is the $(b/c)^*$ value for cooperation success in pairwise DGs under the BD rule. The $\tilde{\tau}_{ij}$ values should be obtained by solving Eqs. (S67) on a given network structure.

3.4 Variation of the model: Accumulated payoff

When using accumulated payoffs, the actual payoff of agent i is accumulated through the k_i DGs played with neighbors. The actual payoff $f_i(\mathbf{x})$ of agent i is

$$f_i(\mathbf{x}) = \sum_{l \in \mathcal{N}_i} (-x_i c + x_l b) = -k_i x_i c + \sum_{l \in \mathcal{N}_i} x_l b. \tag{S201}$$

The dynamics of strategy evolution under neutral drift remain the same, no matter the payoff calculation is averaged, accumulated or other. Only the quantity $\mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))]$ is influenced. Applying the accumulated payoff calculation in Eq. (S201), we have

$$\begin{aligned}
& \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] \\
= & \mathbb{E}_{\text{RMC}}^\circ \left[-k_i(x_i^2 - x_i x_j)c + \sum_{l \in \mathcal{N}_i} (x_i x_l - x_j x_l)b + k_j(x_i x_j - x_j^2)c - \sum_{l \in \mathcal{N}_j} (x_i x_l - x_j x_l)b \right] \\
= & -c \left(k_i \mathbb{E}_{\text{RMC}}^\circ[x_i^2] - (k_i + k_j) \mathbb{E}_{\text{RMC}}^\circ[x_i x_j] + k_j \mathbb{E}_{\text{RMC}}^\circ[x_j^2] \right) + b \sum_{l \in \mathcal{N}_i} (\mathbb{E}_{\text{RMC}}^\circ[x_i x_l] - \mathbb{E}_{\text{RMC}}^\circ[x_j x_l]) \\
& - b \sum_{l \in \mathcal{N}_j} (\mathbb{E}_{\text{RMC}}^\circ[x_i x_l] - \mathbb{E}_{\text{RMC}}^\circ[x_j x_l]). \tag{S202}
\end{aligned}$$

3.4.1 Pairwise comparison

The cooperation condition under the PC rule is still Eq. (S17). Using the result of Eq. (S195) and Eq. (S26), we calculate

$$\begin{aligned}
& \frac{1}{4N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij} \mathbb{E}_{\text{RMC}}^\circ[(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} k_i p_{ij} \left\{ -(k_i + k_j)c\tau_{ij} + b \sum_{l \in \mathcal{N}_i} (-\tau_{il} + \tau_{jl}) - b \sum_{l \in \mathcal{N}_j} (-\tau_{il} + \tau_{jl}) \right\} > 0 \\
\Leftrightarrow & \frac{b}{c} > \frac{\sum_{i,j \in \mathcal{N}} k_i (k_i + k_j) p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij} (k_{il} - k_{jl})(\tau_{jl} - \tau_{il})} = \frac{\sum_{i,j \in \mathcal{N}} k_i^2 p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i^2 p_{ij} p_{il} (\tau_{jl} - \tau_{il})}. \tag{S203}
\end{aligned}$$

The right-hand side is the $(b/c)_{\text{accu}}^*$ value in pairwise DGs using accumulated payoffs under the PC rule. The τ_{ij} values should be obtained by solving Eqs. (S33) on a given network structure.

3.4.2 Death-birth

The cooperation condition under the DB rule is still Eq. (S41). Using the result of Eq. (S195) and Eq. (S44), we calculate

$$\begin{aligned}
& \frac{1}{2N^2 \langle k \rangle} \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \mathbb{E}_{\text{RMC}}^\circ [(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \left\{ -(k_i + k_j)c\tau_{ij} + b \sum_{l \in \mathcal{N}_i} (-\tau_{il} + \tau_{jl}) - b \sum_{l \in \mathcal{N}_j} (-\tau_{il} + \tau_{jl}) \right\} > 0 \\
\Leftrightarrow & \frac{b}{c} > \frac{2 \sum_{i,j \in \mathcal{N}} k_i (k_i + k_j) p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} (k_{il} - k_{jl})(\tau_{jl} - \tau_{il})} = \frac{\sum_{i,j \in \mathcal{N}} k_i^2 p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i^2 p_{ij}^{(2)} p_{il} (\tau_{jl} - \tau_{il})}. \tag{S204}
\end{aligned}$$

The right-hand side is the $(b/c)_{\text{accu}}^*$ value in pairwise DGs using accumulated payoffs under the DB rule. The τ_{ij} values should be obtained by solving Eqs. (S33) on a given network structure.

3.4.3 Birth-death

The cooperation condition under the BD rule is still Eq. (S53). Using the result of Eq. (S195) and Eq. (S61), we calculate

$$\begin{aligned}
& \frac{1}{2N^2 \langle k^{-1} \rangle} \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \mathbb{E}_{\text{RMC}}^\circ [(x_i - x_j)(f_i(\mathbf{x}) - f_j(\mathbf{x}))] > 0 \\
\Leftrightarrow & \sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \left\{ -(k_i + k_j)c\tilde{\tau}_{ij} + b \sum_{l \in \mathcal{N}_i} (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) - b \sum_{l \in \mathcal{N}_j} (-\tilde{\tau}_{il} + \tilde{\tau}_{jl}) \right\} > 0 \\
\Leftrightarrow & \frac{b}{c} > \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + k_j) \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_{il} - k_{jl})(\tilde{\tau}_{jl} - \tilde{\tau}_{il})} = \frac{\sum_{i,j \in \mathcal{N}} p_{ij} \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} p_{ji} p_{il} (\tilde{\tau}_{jl} - \tilde{\tau}_{il})}. \tag{S205}
\end{aligned}$$

The right-hand side is the $(b/c)_{\text{accu}}^*$ value in pairwise DGs using accumulated payoffs under the BD rule. The $\tilde{\tau}_{ij}$ values should be obtained by solving Eqs. (S67) on a given network structure.

The steps to calculate the cooperation conditions of both PGGs and DGs across all model details (PC, DB, and BD updates & averaged and accumulated payoffs) are summarized in Fig. S1.

	PC	DB	BD	
STEP 1	Input network structure: $k_{ij} \in \{0,1\}$ ($k_{ji} = k_{ij}$) for all nodes $i, j \in \mathcal{N}$. If $k_{ij} = 1$, then $j \in \mathcal{N}_i$. If $k_{ij} = 0$, then $j \notin \mathcal{N}_i$. Calculate necessary quantities: $k_i = \sum_{j \in \mathcal{N}} k_{ij}$, $G_i = k_i + 1$, $p_{ij} = \frac{k_{ij}}{k_i}$, $p_{ij}^{(2)} = \sum_{l \in \mathcal{N}} p_{il} p_{lj}$.			
STEP 2	$\begin{cases} \tau_{ij} = 1 + \frac{1}{2k_i} \sum_{l \in \mathcal{N}_i} \tau_{jl} + \frac{1}{2k_j} \sum_{l \in \mathcal{N}_j} \tau_{il}, & j \neq i \\ \tau_{ij} = 0, & j = i \end{cases}$		$\begin{cases} \tilde{\tau}_{ij} = \frac{1}{\sum_{l \in \mathcal{N}_i} k_l^{-1} + \sum_{l \in \mathcal{N}_j} k_l^{-1}} \left(1 + \sum_{l \in \mathcal{N}_i} k_l^{-1} \tilde{\tau}_{jl} + \sum_{l \in \mathcal{N}_j} k_l^{-1} \tilde{\tau}_{il} \right), & j \neq i \\ \tilde{\tau}_{ij} = 0, & j = i \end{cases}$	
STEP 3	$Y_{ij} = \frac{1}{G_i} \left(\frac{\tau_{ij} + \sum_{l \in \mathcal{N}_i} (\tau_{jl} - \tau_{il})}{G_i} + \sum_{l \in \mathcal{N}_i} \frac{(\tau_{jl} - \tau_{il}) + \sum_{\ell \in \mathcal{N}_i} (\tau_{\ell l} - \tau_{i\ell})}{G_l} \right)$		\tilde{Y}_{ij} : the same as Y_{ij} , but just use $\tilde{\tau}_{ij}$ instead of τ_{ij}	
	PGG	$r^* = \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij} Y_{ij}}$	$r^* = \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} Y_{ij}}$	$r^* = \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{Y}_{ij}}$
	PGG	$r_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij} Y_{ij}}$	$r_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j \in \mathcal{N}} k_i (k_i + 1) p_{ij}^{(2)} Y_{ij}}$	$r_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{\tau}_{ij}}{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} (k_i + 1) \tilde{Y}_{ij}}$
	DG	$\left(\frac{b}{c}\right)^* = \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij} p_{il} (\tau_{jl} - \tau_{il})}$	$\left(\frac{b}{c}\right)^* = \frac{\sum_{i,j \in \mathcal{N}} k_i p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i p_{ij}^{(2)} p_{il} (\tau_{jl} - \tau_{il})}$	$\left(\frac{b}{c}\right)^* = \frac{\sum_{i,j \in \mathcal{N}} \frac{k_{ij}}{k_i k_j} \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} \frac{k_{ij} k_{il}}{k_i^2 k_j} (\tilde{\tau}_{jl} - \tilde{\tau}_{il})}$
DG	$\left(\frac{b}{c}\right)_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} k_i^2 p_{ij} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i^2 p_{ij} p_{il} (\tau_{jl} - \tau_{il})}$	$\left(\frac{b}{c}\right)_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} k_i^2 p_{ij}^{(2)} \tau_{ij}}{\sum_{i,j,l \in \mathcal{N}} k_i^2 p_{ij}^{(2)} p_{il} (\tau_{jl} - \tau_{il})}$	$\left(\frac{b}{c}\right)_{\text{accu}}^* = \frac{\sum_{i,j \in \mathcal{N}} p_{ij} \tilde{\tau}_{ij}}{\sum_{i,j,l \in \mathcal{N}} p_{il} p_{il} (\tilde{\tau}_{jl} - \tilde{\tau}_{il})}$	

Figure S1. Steps to calculate the theoretical conditions for cooperation success in both PGGs and DGs, including PC, DB, and BD update rules and averaged & accumulated payoff calculations. Step 1: Input network structure $k_{ij} \in \{0, 1\}$ between all nodes and calculate necessary quantities. **Step 2:** Solve for the linear equations to obtain τ_{ij} (for PC and DB updates) or $\tilde{\tau}_{ij}$ (for BD update). Note that $\tau_{ij} = \tau_{ji}$, $\tilde{\tau}_{ij} = \tilde{\tau}_{ji}$. **Step 3:** Insert the obtained values into the formulas for cooperation conditions. Note that usually $Y_{ij} \neq Y_{ji}$, $\tilde{Y}_{ij} \neq \tilde{Y}_{ji}$. r^* is the critical synergy factor using averaged payoff and r_{accu}^* is using accumulated payoff, and similar to $(b/c)^*$ and $(b/c)_{\text{accu}}^*$.

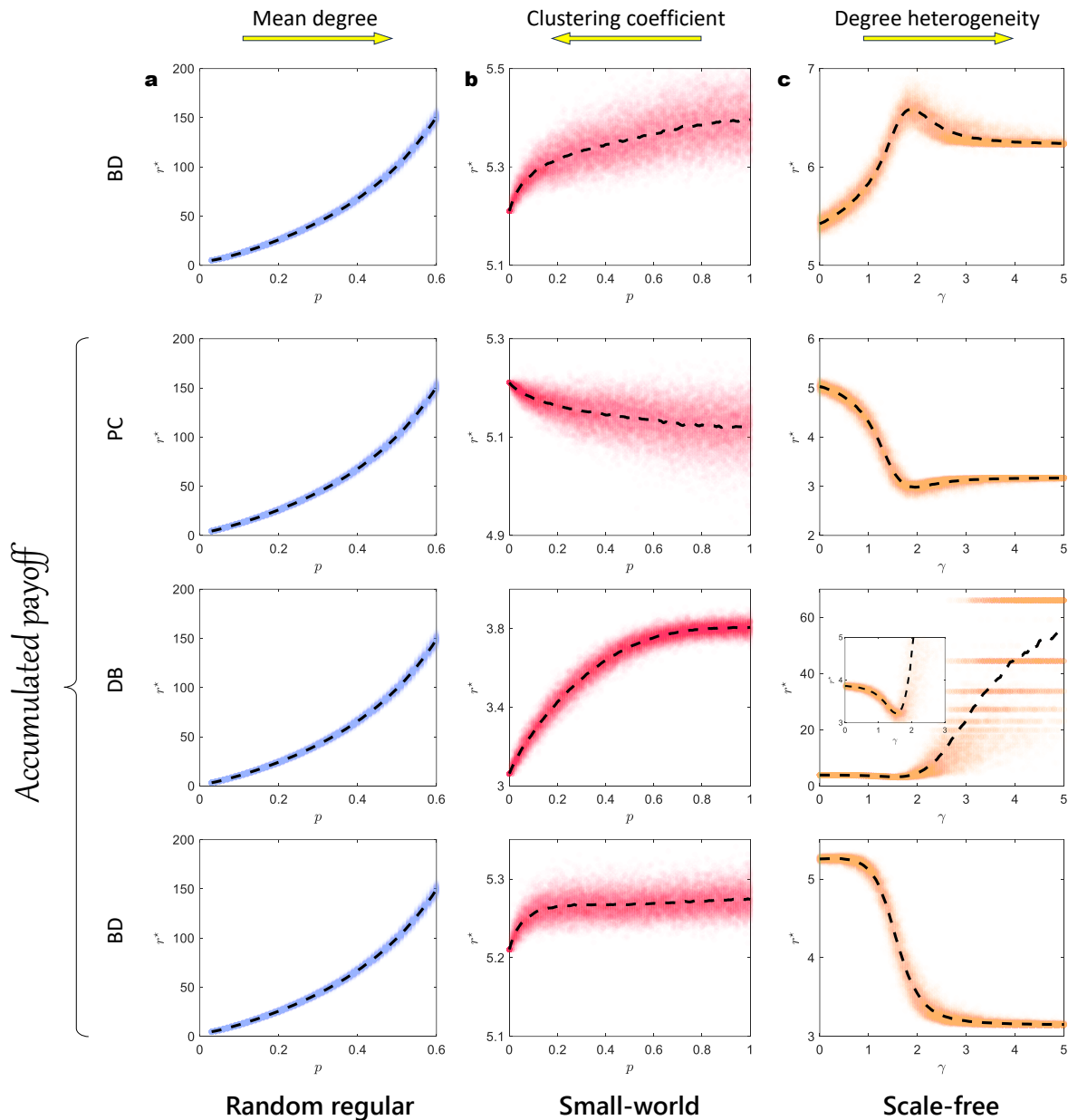


Figure S2. Supplementary results across more model details (BD update and accumulated payoff) for effects of local structures on cooperation in spatial PGGs. a, ER networks. The increasing average degree consistently inhibits cooperation. **b, SW networks.** The increasing clustering coefficient promotes cooperation, but the PC rule using accumulated payoffs presents the opposite effect. **c, BA networks.** The increasing degree heterogeneity initially promotes but ultimately inhibits cooperation under the PC and DB rules. However, this does not hold under the BD rule. The parameters are the same as the ones in Fig. 3 in the main text.

$N = 3$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 1/2	0	*
	DB 1/2	0	*
	BD 1/2	0	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 0	0	100%
	BD 0	0	100%

$N = 4$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 5/6	0	*
	DB 5/6	0	*
	BD 5/6	0	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 1/6	0	5/6
	BD 0	0	100%

$N = 5$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 90.48%	4.76%	*
	DB 90.48%	4.76%	*
	BD 90.48%	4.76%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 23.81%	4.76%	71.43%
	BD 0	0	100%

$N = 6$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 94.64%	4.46%	*
	DB 95.54%	3.57%	*
	BD 96.43%	2.68%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 31.25%	6.25%	62.50%
	BD 0	0	100%

$N = 7$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 97.30%	2.58%	*
	DB 98.12%	1.76%	*
	BD 97.89%	1.99%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 32.94%	13.13%	53.93%
	BD 0	0	100%

$N = 8$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 98.81%	1.18%	*
	DB 99.27%	0.72%	*
	BD 99.21%	0.78%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 31.58%	17.25%	51.17%
	BD 0	0	100%

Figure S3. Supplementary results for spatial PGGs on all networks of different sizes $3 \leq N \leq 8$. The categories of networks classified by their critical synergy factors are presented. The symbol * means that the only structure that does not support cooperation is the fully connected network. The results are obtained using averaged payoffs.

Accumulated payoff

$N = 3$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 1/2	0	*
	DB 1/2	0	*
	BD 1/2	0	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 0	0	100%
	BD 0	0	100%

$N = 4$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 5/6	0	*
	DB 5/6	0	*
	BD 5/6	0	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 1/6	0	5/6
	BD 0	0	100%

$N = 5$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 90.48%	4.76%	*
	DB 90.48%	4.76%	*
	BD 90.48%	4.76%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 23.81%	4.76%	71.43%
	BD 0	0	100%

$N = 6$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 96.43%	2.68%	*
	DB 95.54%	3.57%	*
	BD 96.43%	2.68%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0	100%
	DB 29.46%	7.14%	63.40%
	BD 0	0	100%

$N = 7$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 97.77%	2.11%	*
	DB 98.36%	1.52%	*
	BD 98.94%	0.94%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0	0.12%	99.88%
	DB 29.66%	11.96%	58.38%
	BD 0	0	100%

$N = 8$	$0 < r^* \leq 30$	$r^* > 30$	$r^* < 0$ or $r^* \rightarrow \infty$
PGG	PC 99.25%	0.74%	*
	DB 99.40%	0.59%	*
	BD 99.66%	0.33%	*
	$0 < (b/c)^* \leq 30$	$(b/c)^* > 30$	$(b/c)^* < 0$ or $(b/c)^* \rightarrow \infty$
DG	PC 0.01%	0.03%	99.96%
	DB 27.57%	17.04%	55.39%
	BD 0	0	100%

Figure S4. Supplementary results to Fig. S3 for spatial PGGs on all networks of different sizes $3 \leq N \leq 8$. The results are obtained using accumulated payoffs.

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