SUPPLEMENTARY MATERIAL

Co-evolution between positive reciprocity, punishment, and partner switching in repeated interactions

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SM-I Strategy set

In table S1 the move-wise strategies for each move of the stage game are listed, while table S2 lists the main classes of strategies.

In table S3 the full set of strategies is given. In the "Strategies" section of the main text the coding of the strategies is explained. Although the setup of our model allows for a great number of strategies, we have reduced the strategy space by removing phenotypically indistinguishable strategies (see also main text section "Removing phenotypically indistinguishable strategies"). For example, if the strategy specifies to always leave in move 2, regardless of the partner's action, it can never punish the partner, since the pair will be broken up and thus the actions specified for this move (punish or not punish) will never be played. Some strategies are therefore phenotypically indistinguishable in our model, and per set of phenotypically indistinguishable strategies only one strategy was used in the strategy space.

An X in a move-wise strategy in table S3 is a placeholder for a conditional action that is not played at any point during the game (C or D in move 1; P or N in move 3). Two strategies that are otherwise similar, but differing in this action would therefore never act differently (i.e., they are phenotypically indistinguishable). Only one of these two strategies is included in the strategy space. This can occur in two situations. First, if an individual leaves after the partner cooperates (or defects), then it cannot also punish or conditionally cooperate/defect in the following round since the pair is broken up, and thus an X is shown in place of the conditional action in both the move-wise strategy for move 1 and 3. Second, we assumed that a punishing act could not be followed by a conditional action in move 1 of the following round, and thus the action P in the move-wise strategy for move 3 is always combined with an X in the move-wise strategy for move 1.

SM-II Sensitivity analysis

SM-II.1 Parameter exploration in a well-mixed population

To test the robustness of our main result (the $\mathcal{S}_c$ class dominates for high T), we explored the parameter space more thoroughly than presented in the main text. The exploration was done as follows. The parameters B_h and D_p were set either to 2, 2.5, or 3, the parameters C_h and C_p were set either to 0.5, 1, or 1.5, and the cost of leaving (C_l) was set either to 0, 1, or 2. For each possible combination of these parameters we ran simulations with the number of rounds T ranging from 1 to 100.

In Fig. S1 the results for four combinations of parameters are shown. If the $B_\mathrm{h}/C_\mathrm{h}$ ratio is low ($B_\mathrm{h}/C_\mathrm{h} = 2/1.5$, panel a), we find that a higher number of rounds is required to reach high levels of cooperation compared to the baseline case (*cf.* main text Fig. 2a). Here, the $\mathcal{S}_c$ class is the dominant class of cooperative strategies. If the $B_\mathrm{h}/C_\mathrm{h}$ ratio is high ($B_\mathrm{h}/C_\mathrm{h} = 3/0.5$, panel b), only a few number of rounds is required for high levels of cooperation. The $\mathcal{S}_c$ dominates here for $T \geq 3$. If there is no cost of leaving ($C_\mathrm{l} = 0$, panel c), the $\mathcal{S}_c$ class is always the dominant cooperative class of strategies. If punishment is very effective in terms of payoff, i.e., the $D_\mathrm{p}/C_\mathrm{p}$ ratio is high ($D_\mathrm{p}/C_\mathrm{p} = 3/0.5$, panel d), the $\mathcal{P}_c$ class dominates for a larger range of T, compared to our baseline case (main text). However, for $T > 40$ the $\mathcal{S}_c$ class is again often found to be dominant.

In short, for any parameter combination we find that, all else being equal, the relative competitiveness of the $\mathcal{S}_c$ class increases with increasing number of rounds.

SM-II.1.1 Dynamic cost of leaving

In this section we investigate additional parameter values for a and k when using eq. 1 from the main text to calculate the cost of leaving. The results are plotted in Fig. S2. Again we find that, although the exact number of rounds where the $\mathcal{S}_c$ class becomes dominant depends both on a and k, the $\mathcal{S}_c$ class will always dominate for high T. This suggests that the $\mathcal{S}_c$ class can evolve irrespective of the underlying cost function.

SM-II.1.2 Large T

To check to what extent the $\mathcal{S}_c$ class dominates for large T, we ran simulations with T up to 1000, while otherwise using our baseline set of parameters. We find that, although the $\mathcal{S}_c$ class is by far the most prevalent, other classes of cooperative strategies are maintained above frequencies higher than what would be expected from the mutation rate alone (Fig. S3). This results from the fact that the classes of cooperative strategies are nearly neutral in a population consisting of mainly those classes ($\mathcal{C}_c$, $\mathcal{R}_c$, $\mathcal{S}_c$, and $\mathcal{P}_c$), since these strategies will gain exactly the same payoff when paired with one another. Therefore, through genetic drift the different cooperative strategies may invade one another. However, uncooperative individuals will continue to enter the population via mutation. When paired with uncooperative individuals the cooperative strategies will respond differently, and thus gain different payoffs. Here, strategies of the $\mathcal{C}_c$ class will then be strongly selected against, but also strategies of the $\mathcal{R}_c$ and $\mathcal{P}_c$ class gain less payoff on average than those of the $\mathcal{S}_c$ class. Thus, through a mutation-selection-drift balance this polymorphism is maintained in the population.

SM-II.2 Parameter exploration in a group-structured population

In this section we present additional results for the group-structured case.

SM-II.2.1 Group-structure with small T

In this section, we tested if the $\mathcal{P}_c$ class is also relatively more favoured by selection in a structured population if T is small. For $T = 4$ in the well-mixed case the $\mathcal{R}_c$ class dominates the population (Fig. 2a). Using the same parameters as in the well-mixed case (except $T = 4, d = 250$, varying n), we find again that the $\mathcal{P}_c$ class is relatively more favoured by selection (Fig. S4a). Only in very large groups the $\mathcal{R}_c$ class outcompetes the $\mathcal{P}_c$ class ($n \geq 350$).

Interestingly, reducing D_p (the payoff reduction of being punished) did not affect the frequency of the $\mathcal{P}_c$ class, but instead negatively affected the frequency of the $\mathcal{R}_c$ class ($D_\mathrm{p} = 1.2$, Fig. S4b). This was due to $\mathcal{P}_c$ strategies having less impact on various defector strategies, which consequently increased in frequency, which in turn negatively affected the $\mathcal{R}_c$ class, but not the $\mathcal{P}_c$ class. However, when increasing the cost of punishment (C_p) the $\mathcal{P}_c$ class disappeared from the population and the $\mathcal{R}_c$ class dominated for all but the smallest groups ($C_\mathrm{p} = 2, n \geq 16$, Fig. S4c). This discrepancy with D_p is due to C_p affecting the payoff of the $\mathcal{P}_c$ class directly, while changing D_p affects recipients of punishment instead.

SM-II.2.2 Further parameter exploration

In this section we present results from a larger parameter space for the group-structured population.

First, we determined the minimum group size where the $\mathcal{S}_c$ class dominates in conditions where the $\mathcal{P}_c$ is not dominant. To achieve this we used the same parameters as in Fig. 3c from the main text with $z = 3$. Using these parameters we find that the $\mathcal{P}_c$ class no longer dominates, and instead the "rest" class and the $\mathcal{R}_c$ class dominate in small groups (Fig. S5a). The $\mathcal{S}_c$ class is now dominant in the population for $n \geq 20$ (compared to $n \geq 32$ for $z = 5$ in Fig. 3c in the main text). Thus, even in unfavourable conditions for the $\mathcal{P}_c$ class, the $\mathcal{S}_c$ class does not dominate in populations where interactions occur in small groups.

In Fig. S5b we use the same parameters as in panel a, but with $C_\mathrm{l} = 1, T = 7$ in order to determine if the $\mathcal{S}_c$ class can dominate in a group-structured population when T is low. However, we find here, similarly to our well-mixed population (Fig. 2a main text), that if T is low the $\mathcal{S}_c$ class is outcompeted by the $\mathcal{P}_c$ and $\mathcal{R}_c$ classes for group size smaller than 120, and by the $\mathcal{D}_c$ class in larger groups. This confirms that the $\mathcal{S}_c$ class needs a critical number of rounds in order to be favoured by selection over the other classes.

In Fig. S5c we use the same parameters as Fig. 4b from the main text, with $D_\mathrm{p} = 1$. This shows that, although reducing D_p initially affects only the frequency of the $\mathcal{S}_c$ and $\mathcal{R}_c$ classes (main text), if D_p is too low then the $\mathcal{P}_c$ disappears completely from the population and the $\mathcal{D}_c$ class is dominant for all group sizes.

In Fig. S5d we use the same parameters as in Fig. 4c from the main text, but with $T = 7$. In the well-mixed population we have found that a higher number of rounds generally favours the $\mathcal{P}_c$ class over the $\mathcal{R}_c$ class. Similarly, in Fig. 4c (main text) we find the $\mathcal{R}_c$ class dominates if punishment is costly to the punisher ($C_\mathrm{p} = 2$). However, if the number of rounds is increased, then we find that the $\mathcal{P}_c$ is dominant for group size $n \leq 60$. This confirms that also in the a group-structured population, all else being equal, a higher number of rounds increases the relative competitiveness of the $\mathcal{P}_c$ class over the $\mathcal{R}_c$ class.

SM-III Co-evolution of the $\mathcal{P}_c$ class and response to punishment

In this section we show that the response to punishment by altering behaviour ($x_4 = \mathrm{A}$) co-evolves with the $\mathcal{P}_c$ class. To demonstrate this we used the same data as our baseline case (main text Fig. 2a), but pooled the time average frequency of all strategies into three groups, based on their response to punishment (ignore, alter, or leave) (Fig. S6). The frequency of each group is plotted together with the frequency of the $\mathcal{P}_c$ class. The results show that if $\mathcal{P}_c$ strategies are frequent, then strategies that alter behaviour after punishment ($x_4 = \mathrm{A}$) are also selected for.

Table S 1: The sets of move-wise strategies for each move of the stage game. The coding of strategies is explained in the "Strategies" section.

Move 1:	$\{\mathrm{CCC}, \mathrm{CCD}, \mathrm{CDC}, \mathrm{CDD}, \mathrm{DCC}, \mathrm{DCD}, \mathrm{DDC}, \mathrm{DDD}\}$
Move 2:	$\{\mathrm{LL}, \mathrm{SS}, \mathrm{LS}, \mathrm{SL}\}$
Move 3:	$\{\mathrm{PP}, \mathrm{NN}, \mathrm{PN}, \mathrm{NP}\}$
Move 4:	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$

Table S 2: Main classes of strategies.

Name	Move 1	Move 2	Move 3	Move 4
Always cooperate $\mathcal{C}_c$	CCC	SS	NN	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$
Positive reciprocity $\mathcal{R}_c$	CCD	SS	NN	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$
Partner switching $\mathcal{S}_c$	CCC	SL	NN	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$
Punishment $\mathcal{P}_c$	CCC	SS	NP	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$
Always defect $\mathcal{D}_c$	DDD	SS	NN	$\{\mathrm{I}, \mathrm{A}, \mathrm{L}\}$

Table S 3: Full set of strategies used in all simulations. The coding is explained in the main text.

Strategy	Move 1	Move 2	Move 3	Move 4	Strategy	Move 1	Move 2	Move 3	Move 4
1	CCC	SS	NN	I	47	DCC	SS	NN	I
2	CCC	SS	NN	A	48	DCC	SS	NN	A
3	CCC	SS	NN	L	49	DCC	SS	NN	L
4	CCD	SS	NN	I	50	DCD	SS	NN	I
5	CCD	SS	NN	A	51	DCD	SS	NN	A
6	CCD	SS	NN	L	52	DCD	SS	NN	L
7	CCX	SL	NX	I	53	DCX	SL	NX	I
8	CCX	SL	NX	A	54	DCX	SL	NX	A
9	CCX	SL	NX	L	55	DCX	SL	NX	L
10	CCX	SS	NP	I	56	DCX	SS	NP	I
11	CCX	SS	NP	A	57	DCX	SS	NP	A
12	CCX	SS	NP	L	58	DCX	SS	NP	L
13	CDC	SS	NN	I	59	DDC	SS	NN	I
14	CDC	SS	NN	A	60	DDC	SS	NN	A
15	CDC	SS	NN	L	61	DDC	SS	NN	L
16	CDD	SS	NN	I	62	DDD	SS	NN	I
17	CDD	SS	NN	A	63	DDD	SS	NN	A
18	CDD	SS	NN	L	64	DDD	SS	NN	L
19	CDX	SL	NX	I	65	DDX	SL	NX	I
20	CDX	SL	NX	A	66	DDX	SL	NX	A
21	CDX	SL	NX	L	67	DDX	SL	NX	L
22	CDX	SS	NP	I	68	DDX	SS	NP	I
23	CDX	SS	NP	A	69	DDX	SS	NP	A
24	CDX	SS	NP	L	70	DDX	SS	NP	L
25	CXC	LS	XN	I	71	DXC	LS	XN	I
26	CXC	LS	XN	A	72	DXC	LS	XN	A
27	CXC	LS	XN	L	73	DXC	LS	XN	L
28	CXD	LS	XN	I	74	DXD	LS	XN	I
29	CXD	LS	XN	A	75	DXD	LS	XN	A
30	CXD	LS	XN	L	76	DXD	LS	XN	L
31	CXX	LL	XX	I	77	DXX	LL	XX	I
32	CXX	LS	XP	I	78	DXX	LS	XP	I
33	CXX	LS	XP	A	79	DXX	LS	XP	A
34	CXX	LS	XP	L	80	DXX	LS	XP	L
35	CXC	SS	PN	I	81	DXC	SS	PN	I
36	CXC	SS	PN	A	82	DXC	SS	PN	A
37	CXC	SS	PN	L	83	DXC	SS	PN	L
38	CXD	SS	PN	I	84	DXD	SS	PN	I
39	CXD	SS	PN	A	85	DXD	SS	PN	A
40	CXD	SS	PN	L	86	DXD	SS	PN	L
41	CXX	SL	PX	I	87	DXX	SL	PX	I
42	CXX	SL	PX	A	88	DXX	SL	PX	A
43	CXX	SL	PX	L	89	DXX	SL	PX	L
44	CXX	SS	PP	I	90	DXX	SS	PP	I
45	CXX	SS	PP	A	91	DXX	SS	PP	A
46	CXX	SS	PP	L	92	DXX	SS	PP	L

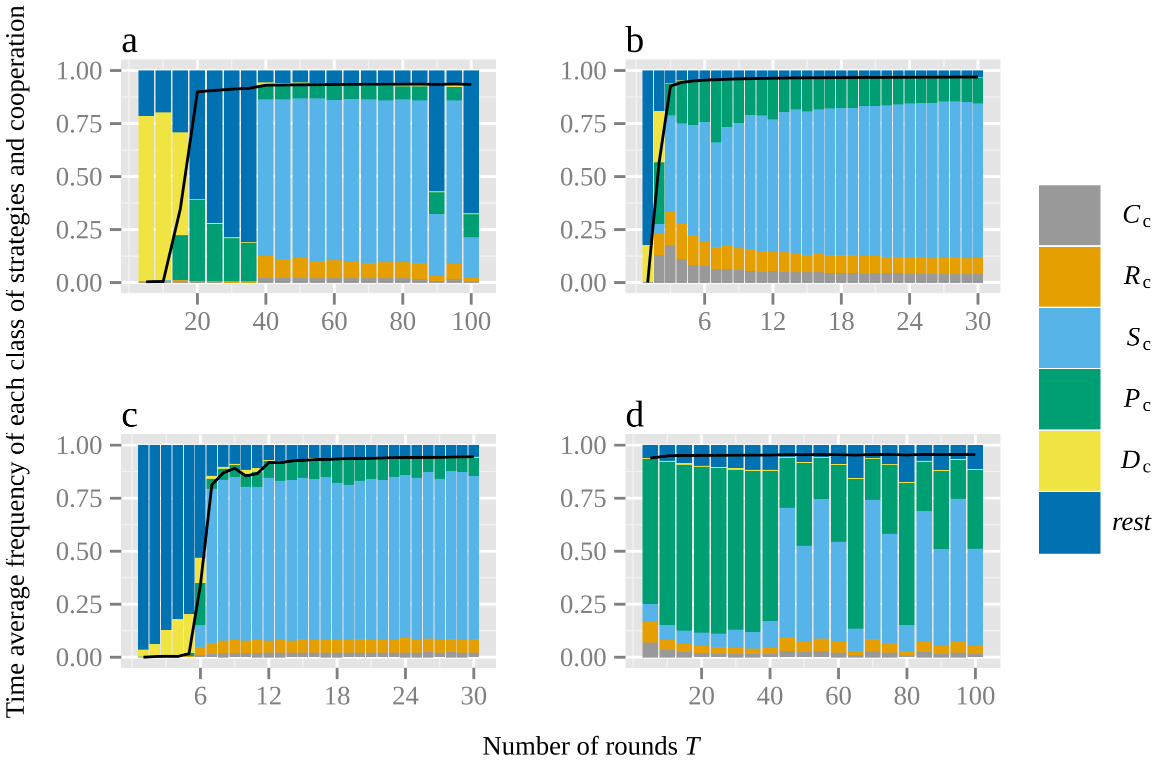

Figure S 1: Time average frequency (over 10^6 generations) of the frequency of cooperation (black line) and the six classes of strategies ($\mathcal{R}_c$, $\mathcal{S}_c$, $\mathcal{P}_c$, $\mathcal{C}_c$, $\mathcal{D}_c$, and "*rest*") plotted as a function of the number of rounds T of the repeated game. Parameter values: $B_{\rm h} = 2, C_{\rm h} = 1, D_{\rm p} = 2, C_{\rm p} = 1, C_{\rm l} = 1, z = T, \mu = 0.01, d = 1, n = 10000$. Panel specific parameters: $C_{\rm h} = 1.5$ (panel a), $B_{\rm h} = 3, C_{\rm h} = 0.5$ (panel b), $C_{\rm l} = 0$ (panel c), $D_{\rm p} = 3, C_{\rm p} = 0.5$ (panel d).

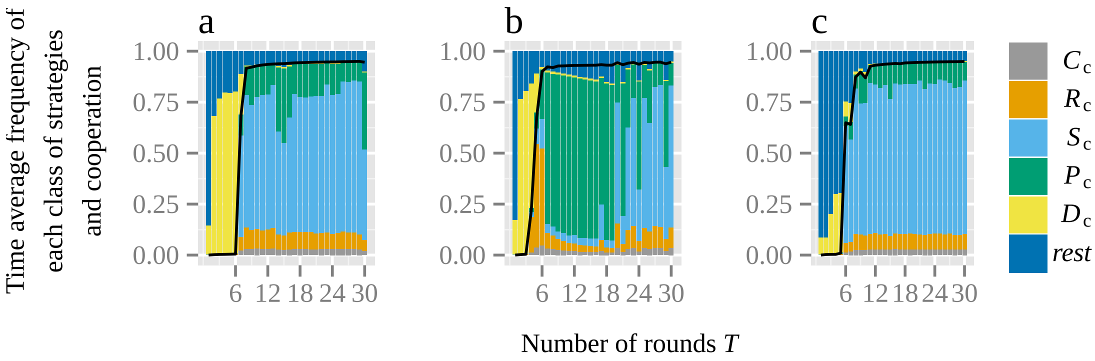

Figure S 2: Time average frequency (over 10^6 generations) of the frequency of cooperation (black line) and the six classes of strategies ($\mathcal{R}_c$, $\mathcal{S}_c$, $\mathcal{P}_c$, $\mathcal{C}_c$, $\mathcal{D}_c$, and "*rest*") plotted as a function of the number of rounds T of the repeated game. Parameter values: $B_{\rm h} = 2, C_{\rm h} = 1, D_{\rm p} = 2, C_{\rm p} = 1, z = T, \mu = 0.01, d = 1, n = 10000$, using eq. 1 to calculate the cost of switching. Panel specific parameters: $a = 50, k = 0.8$ (panel a), $a = 100, k = 0.8$ (panel b), $a = 100, k = 1$ (panel c).

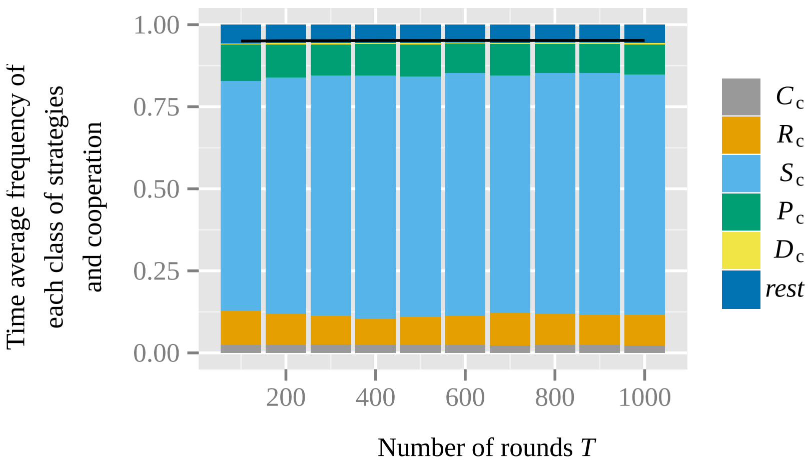

Figure S 3: Same as the baseline case (Fig. 2a, main text) but with a high number of rounds T.

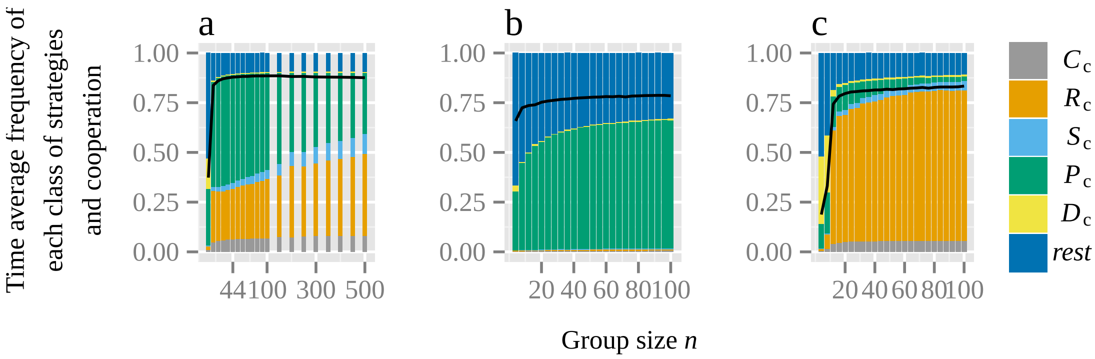

Figure S 4: Time average frequency (over 10^6 generations) of the frequency of cooperation (black line) and the six classes of strategies ($\mathcal{R}_c$, $\mathcal{S}_c$, $\mathcal{P}_c$, $\mathcal{C}_c$, $\mathcal{D}_c$, and "*rest*") plotted as a function of group size n. Parameter values: $B_\text{h} = 2, C_\text{h} = 1, C_\text{l} = 1, T = 4, z = T, \mu = 0.01, d = 250$. Panel specific parameters: $D_\text{p} = 2, C_\text{p} = 1$ (panel a), $D_\text{p} = 1.2, C_\text{p} = 1$ (panel b), $D_\text{p} = 2, C_\text{p} = 2$ (panel c)

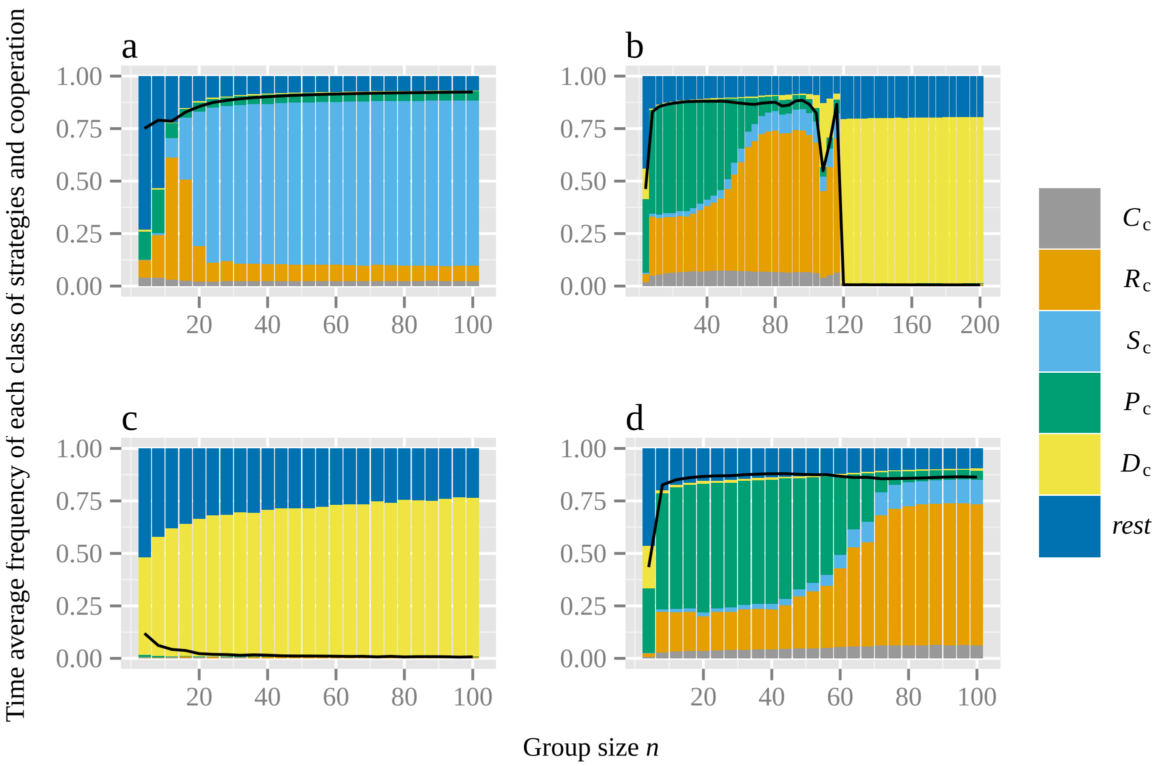

Figure S 5: Time average frequency (over 10^6 generations) of the frequency of cooperation (black line) and the six classes of strategies ($\mathcal{R}_c$, $\mathcal{S}_c$, $\mathcal{P}_c$, $\mathcal{C}_c$, $\mathcal{D}_c$, and "*rest*") plotted as a function of group size n. Parameter values: $B_\mathrm{h} = 2, C_\mathrm{h} = 1, \mu = 0.01, d = 250$. Panel specific parameters: $D_\mathrm{p} = 2, C_\mathrm{p} = 1, C_\mathrm{l} = 0, T = 30, z = 3$ (panel a), $D_\mathrm{p} = 2, C_\mathrm{p} = 1, C_\mathrm{l} = 1, T = 7, z = 3$ (panel b), $D_\mathrm{p} = 1, C_\mathrm{p} = 1, C_\mathrm{l} = 1, T = 4, z = T$ (panel c), $D_\mathrm{p} = 2, C_\mathrm{p} = 2, C_\mathrm{l} = 1, T = 7, z = T$ (panel d).

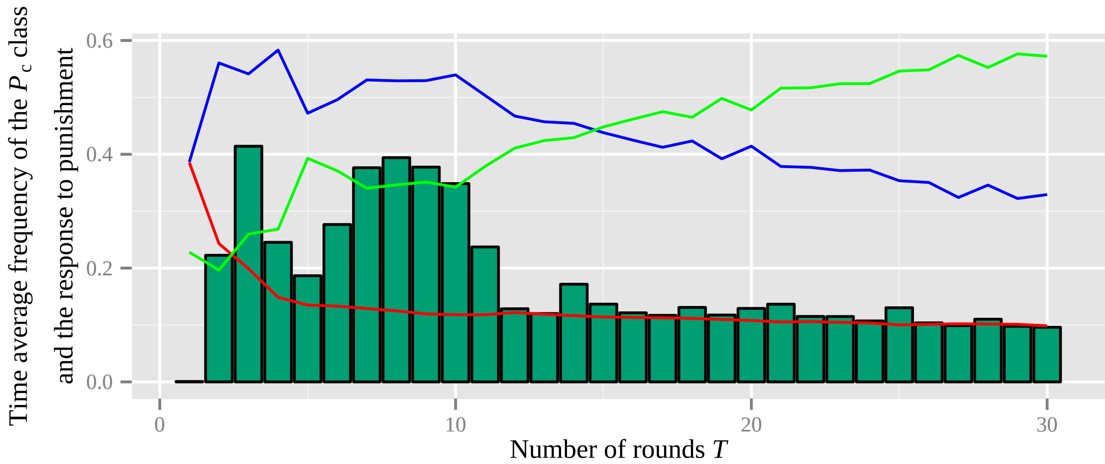

Figure S 6: Same as the baseline case (Fig. 2a, main text), but only showing the frequency of the $\mathcal{P}_c$ class (bars), together with three sets of strategies based on the response to punishment (x_4). The red line is the frequency of all strategies for which $x_4 = \text{I}$, the blue line for which $x_4 = \text{A}$, and the green line for which $x_4 = \text{L}$.