Supplementary Information: Cost efficiency of institutional incentives for promoting cooperation in finite populations

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Abstract

In this Supplementary Information, we provide detailed calculations and proofs as well as illustrative figures for the analytical results in the main text of the paper: Cost efficiency of institutional incentives for promoting cooperation in finite populations.

1 Detailed computations and proofs: reward incentive

In this section we present detailed computations and prove Theorems 3.1-3.2 for the case of reward incentive.

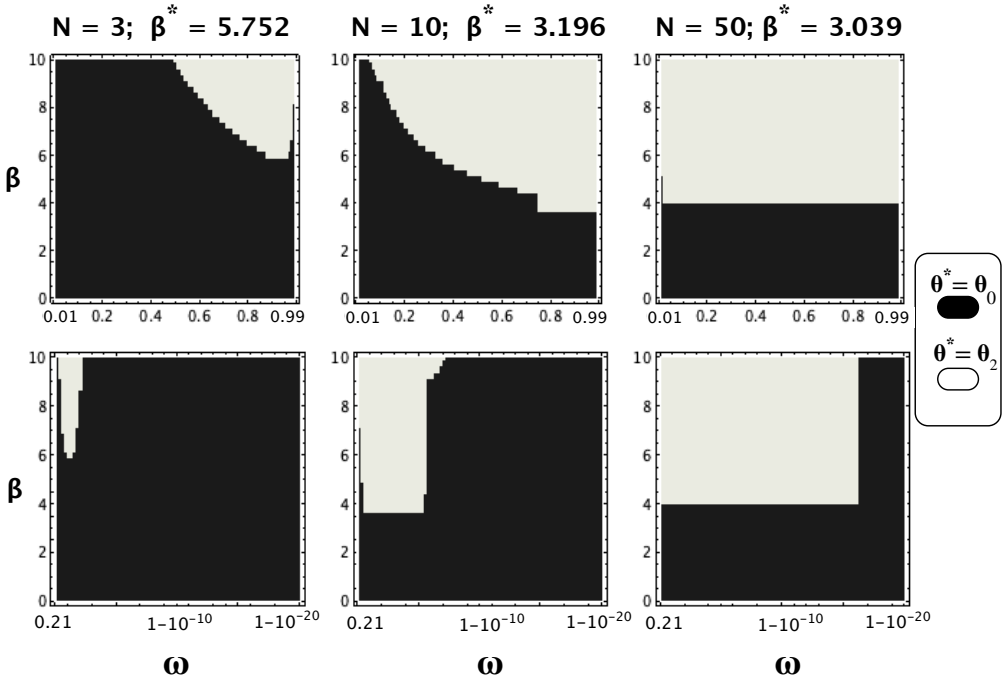

Figure 1: **Optimal value of the incentive cost $\theta^\star$, for varying the minimum required cooperation level ω and the intensity of selection β.** Left column: $N = 3$; Middle column: $N = 10$; Right column: $N = 50$. Top row shows results for a non-extreme value range of ω: $\omega \in [0.01, 0.99]$. Bottom row shows results in a log scale to examine values of ω extremely close to 1. Other parameters: Donation Game ($b = 1.8$, $c = 1$).

1.1 Computation of the fundamental matrix

The key in our analysis is that the fundamental matrix can be computed explicitly based on the following result.

Lemma 1.1. *(Inverse of a tridiagonal matrix [Huang and McColl, 1997]) Let T be a general Toeplitz tridiagonal matrix of the form*

$$T = \begin{pmatrix} 1 & -u & & & & & \\ -l & 1 & -u & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -l & 1 & -u & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -l & 1 & -u \\ & & & & & -l & 1 \end{pmatrix} \tag{1}$$

Then the inverse of T is given by

$$(T^{-1})_{ij} = \frac{(\lambda_+^i - \lambda_-^i)(\lambda_+^{n-j+1} - \lambda_-^{n-j+1})}{(\lambda_+ - \lambda_-)(\lambda_+^{n+1} - \lambda_-^{n+1})} u^{j-i} \qquad i < j, \tag{2}$$

$$(T^{-1})_{ij} = \frac{(\lambda_+^j - \lambda_-^j)(\lambda_+^{n-i+1} - \lambda_-^{n-i+1})}{(\lambda_+ - \lambda_-)(\lambda_+^{n+1} - \lambda_-^{n+1})} l^{j-i} \qquad i \geq j, \tag{3}$$

where

$$\lambda_+ = \frac{1 + \sqrt{1 - 4lu}}{2}, \quad \lambda_- = \frac{1 - \sqrt{1 - 4lu}}{2}. \tag{4}$$

The following lemma is a special case of Lemma 1.1 which will be used in the subsequent analysis.

Lemma 1.2. *Let W be the following Toeplitz tri-diagonal matrix of order $N-1$*

$$W = \begin{pmatrix} 1 & -a_1 & & & & & \\ -c_1 & 1 & -a_1 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & -c_1 & 1 & -a_1 & & \\ & & & \ddots & \ddots & \ddots & \\ & & & & -c_1 & 1 & -a_1 \\ & & & & & -c_1 & 1 \end{pmatrix}, \tag{5}$$

where

$$a_1 := (1+e^{-x})^{-1}, \quad c := (1+e^{x})^{-1}, \quad x = \beta(\theta - c - \frac{b}{N-1}).$$

Then

$$(W^{-1})_{1,j} = \frac{(e^{(N-1)x} - e^{(j-1)x})(1+e^x)}{e^{Nx}-1} = \frac{e^{(j-1)x}(1+e^x)(1+e^x+\ldots+e^{(N-j-1)x})}{1+e^x+\ldots+e^{(N-1)x}}$$
$$(W^{-1})_{N-1,j} = \frac{(e^{jx}-1)(1+e^x)}{e^{Nx}-1} = \frac{(1+e^x+\ldots+e^{(j-1)x})(1+e^x)}{1+e^x+\ldots+e^{(N-1)x}}.$$

Proof. Applying Lemma 1.1 for $u = a = (1+e^{-x})^{-1}, l = c = (1+e^x)^{-1},\ n = N-1$, we obtain

$$1 - 4lu = 1 - \frac{4}{(1+e^x)(1+e^{-x})} = \frac{e^x+e^{-x}-2}{e^x+e^{-x}+2} = \frac{e^{2x}-2e^x+1}{e^{2x}+2e^x+1} = \Big(\frac{e^x-1}{e^x+1}\Big)^2.$$

Hence

$$\lambda_\pm = \frac{1 \pm \sqrt{1-4lu}}{2} = \frac{1 \pm \left|\frac{e^x-1}{e^x+1}\right|}{2} = \frac{e^x+1 \pm |e^x-1|}{2(e^x+1)},$$

that is

$$\lambda_+ = \frac{e^x}{e^x+1}, \quad \lambda_- = \frac{1}{e^x+1} \quad \text{if} \quad x \geq 0,$$
$$\lambda_+ = \frac{1}{e^x+1}, \quad \lambda_- = \frac{e^x}{e^x+1} \quad \text{if} \quad x < 0.$$

According to Lemma 1.1 we have

$$(W^{-1})_{1j} = \frac{\lambda_+^{n-j+1} - \lambda_-^{n-j+1}}{\lambda_+^{n+1} - \lambda_-^{n+1}} u^{j-1} = \frac{\lambda_-^{n-j+1} - \lambda_+^{n-j+1}}{\lambda_-^{n+1} - \lambda_+^{n+1}} u^{j-1},$$
$$(W^{-1})_{N-1j} = \frac{\lambda_+^{j} - \lambda_-^{j}}{\lambda_+^{n+1} - \lambda_-^{n+1}} l^{j-1} = \frac{\lambda_-^{j} - \lambda_+^{j}}{\lambda_-^{n+1} - \lambda_+^{n+1}} l^{j-1},$$

Therefore, by swapping the role of λ_+ and λ_- in the case $x \geq 0$ and $x < 0$, we can assume without

affecting the computations that $\lambda_+ = e^x/(1+e^x)$ and $\lambda_- = 1/(1+e^x)$ and obtain

$$\begin{aligned}
(W^{-1})_{1j} &= \frac{\left(\frac{\lambda_+}{\lambda_-}\right)^{n-j+1} - 1}{\left(\frac{\lambda_+}{\lambda_-}\right)^{n+1} - 1} \cdot \frac{\lambda_-^{n-j+1}}{\lambda_-^{n+1}} \cdot u^{j-1} \\
&= \frac{e^{(n-j+1)x} - 1}{e^{(n+1)x} - 1} \cdot \frac{(1+e^x)^{-(n-j+1)}}{(1+e^x)^{-(n+1)}} \cdot (1+e^{-x})^{1-j} \\
&= \frac{e^{(n-j+1)x} - 1}{e^{(n+1)x} - 1} \cdot (1+e^x)^j \cdot (1+e^{-x})^{1-j} \\
&= \frac{e^{(n-j+1)x} - 1}{e^{(n+1)x} - 1} \cdot e^{jx}(1+e^{-x})^j \cdot (1+e^{-x})^{1-j} \\
&= \frac{e^{(n-j+1)x} - 1}{e^{(n+1)x} - 1} \cdot e^{jx}(1+e^{-x}) \\
&= \frac{e^{(n+1)x} - e^{jx}}{e^{(n+1)x} - 1} \cdot (1+e^{-x}) \\
&= \frac{e^{nx} - e^{(j-1)x}}{e^{(n+1)x} - 1} \cdot (1+e^x) \\
&= \frac{e^{(N-1)x} - e^{(j-1)x}}{e^{Nx} - 1} \cdot (1+e^x).
\end{aligned}$$

Similar computations yield

$$(W^{-1})_{N-1,j} = \frac{(e^{jx}-1)(1+e^x)}{e^{Nx}-1}.$$

This completes the proof of the lemma. □

1.2 The total cost function and its derivative

Using results from the previous section, in this section we will compute the total cost of interference and its derivative.

Lemma 1.3. *Recalling that $x = \beta(\theta - c - \frac{b}{N-1}) := \beta(\theta - a)$ (where $a := c + b/(N-1) = -\delta$), the total cost of interference for the institutional reward is given by*

$$E_r(\theta) = \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\left[\left(1+e^x+\ldots+e^{(N-2)x}\right)\sum_{j=1}^{N-1}\frac{1}{j} + e^{(N-1)x}\sum_{j=1}^{N-1}\frac{e^{-jx}}{j}\right]. \tag{6}$$

It derivative is given by

$$E_r'(\theta) = \frac{1}{g(x)^2}\left[f(x)g(x) - (x+\beta a)(f(x)g'(x) - f'(x)g(x))\right].$$

When $(f(x)g'(x) - f'(x)g(x)) > 0$ we write $E_r'(\theta)$ as

$$E_r'(\theta) = \frac{1}{g(x)^2}(f(x)g'(x) - f'(x)g(x))\Big(F(u) - \beta a\Big), \tag{7}$$

where $u = e^x$, and F is given in (11).

Proof. Let $V := \{v_{ij}\}_{i,j=1}^{N-1} = I - U$, we have

$$\begin{aligned}
v_{i,i\pm j} &= 0 \qquad \text{for all } j \geq 2, \\
v_{i,i\pm 1} &= -\frac{N-i}{N}\frac{i}{N}\left(1+e^{\mp\beta[\delta+\theta]}\right)^{-1}, \\
v_{i,i} &= u_{i,i+1} + u_{i,i-1} = \frac{N-i}{N}\frac{i}{N},
\end{aligned} \tag{8}$$

Let $a_1 := \big(1+e^{-\beta(\theta+\delta)}\big)^{-1}$ and $c_1 := \big(1+e^{\beta(\theta+\delta)}\big)^{-1}$. The fundamental matrix $\mathbb{N} = (I-U)^{-1} = V^{-1}$ (see Section 2.2 in the main text) can be expressed as

$$\mathbb{N}^{-1} = W^{-1}\mathrm{diag}\Big\{\frac{N^2}{(N-1)}, \frac{N^2}{2(N-2)}, \ldots, \frac{N^2}{(N-1)}\Big\},$$

where W is the Toeplitz tri-diagonal matrix given in (5). Therefore, from Lemma 1.2 the expected total cost of interference for institutional reward given in Section 2.2 can be expressed as

$$\begin{aligned}
E_r(\theta) &= \frac{\theta}{2}\sum_{i=1}^{N-1}(n_{1i}+n_{N-1,i})i \\
&= \frac{1}{2}\sum_{j=1}^{N-1}\frac{N^2}{(N-j)j}\Big((W^{-1})_{1j}+(W^{-1})_{N-1,j}\Big)j\theta \\
&= \frac{N^2\theta(1+e^x)}{2(e^{Nx}-1)}\sum_{j=1}^{N-1}\frac{e^{(N-1)x}-e^{(j-1)x}+e^{jx}-1}{N-j} \\
&= \frac{N^2\theta(1+e^x)}{2(e^{Nx}-1)}\Big[\big(e^{(N-1)x}-1\big)\sum_{j=1}^{N-1}\frac{1}{j}+(e^x-1)\sum_{j=1}^{N-1}\frac{e^{(j-1)x}}{N-j}\Big] \\
&= \frac{N^2\theta(1+e^x)}{2(e^{Nx}-1)}\Big[\big(e^{(N-1)x}-1\big)\sum_{j=1}^{N-1}\frac{1}{j}+(e^x-1)e^{(N-1)x}\sum_{j=1}^{N-1}\frac{e^{-jx}}{j}\Big] \\
&= \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\Big[\big(1+e^x+\ldots+e^{(N-2)x}\big)\sum_{j=1}^{N-1}\frac{1}{j}+e^{(N-1)x}\sum_{j=1}^{N-1}\frac{e^{-jx}}{j}\Big] \\
&:= \frac{N^2\theta}{2}\frac{f(x)}{g(x)},
\end{aligned}$$

where (recalling the definition of the harmonic number H_N in Section 3 in the main text)

$$\begin{aligned}
f(x) &= (1+e^x)\Big[(1+e^x+\ldots+e^{(N-2)x})H_N+e^{(N-1)x}\sum_{j=1}^{N-1}e^{-jx}/j\Big], \\
g(x) &= 1+e^x+\ldots+e^{(N-1)x},
\end{aligned}$$

Since $x=\beta(\theta-a)$, we have

$$\begin{aligned}
\frac{d}{d\theta}E_r(\theta) = \beta\frac{d}{dx}E_r(\theta) &= \frac{\beta N^2}{2}\left\{\frac{1}{\beta}\frac{f(x)}{g(x)}+\theta\Big(\frac{f'(x)}{g(x)}-\frac{f(x)g'(x)}{g(x)^2}\Big)\right\} \\
&= \frac{N^2}{2}\left\{\left[\frac{f(x)}{g(x)}+(x+\beta a)\Big(\frac{f'(x)}{g(x)}-\frac{f(x)g'(x)}{g(x)^2}\Big)\right]\right\} \\
&= \frac{N^2}{2}\frac{1}{g(x)^2}\Big[f(x)g(x)-(x+\beta a)(f(x)g'(x)-f'(x)g(x))\Big]. \qquad (9)
\end{aligned}$$

Let $u := e^x$. From the formula of f and g, it is more convenient to express the right-hand side of

(9) in terms of u. We have

$$f(x) = (1+e^x)\Big[(1+e^x+\ldots+e^{(N-2)x})H_N + e^{(N-1)x}\sum_{j=1}^{N-1} e^{-jx}/j\Big] = (1+u)\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j,$$

$$\begin{aligned} f'(x) &= u\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j + (1+u)\Big(H_N\sum_{j=0}^{N-2} je^{jx} + \sum_{j=0}^{N-2}\frac{j}{N-1-j}e^{jx}\Big) \\ &= \sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j(j(1+u)+u), \end{aligned}$$

$$g(x) = 1+e^x+\ldots+e^{(N-1)x} = \sum_{j=0}^{N-1} u^j,$$

$$g'(x) = \sum_{j=1}^{N-1} je^{jx} = \sum_{j=1}^{N-1} ju^j.$$

Therefore

$$\begin{aligned} &f(x)g'(x) - f'(x)g(x) \\ &\quad = (1+u)\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1} ju^j\Big) \\ &\quad - \Big(\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j(j(1+u)+u)\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) \\ &\quad = (1+u)u\Bigg[\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1} ju^{j-1}\Big) - \Big(\sum_{j=1}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)ju^{j-1}\Big)\Big(\sum_{j=0}^{N-1} u^j\Big)\Bigg] \\ &\qquad - u\Big(\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) \\ &\quad := uP(u), \end{aligned}$$

where

$$\begin{aligned} P(u) := (1+u)&\Bigg[\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1} ju^{j-1}\Big) - \Big(\sum_{j=1}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)ju^{j-1}\Big)\Big(\sum_{j=0}^{N-1} u^j\Big)\Bigg] \\ &- \Big(\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big). \end{aligned} \tag{10}$$

We also have

$$f(x)g(x) = (1+u)\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) := Q(u).$$

Note that $x + \beta a = \beta\theta > 0$ and$f(x)g(x) > 0$. It follows that if $f(x)g'(x) - f'(x)g(x) \le 0$ then $E_r'(\theta) > 0$. Consider the case $f(x)g'(x) - f'(x)g(x) > 0$. Let $u = e^x$ and define

$$F(u) := \frac{Q(u)}{uP(u)} - \log(u). \tag{11}$$

Then

$$\frac{2}{N^2}E_r'(\theta) = \frac{1}{\beta}\frac{1}{g(x)^2}(f(x)g'(x) - f'(x)g(x))\Big(F(u) - \beta a\Big).$$

The next step is to understand the sign of the term $F(u) - \beta a$, which requires to understand the polynomials P and Q. In the next section, we analyse the polynomial P (Q is explicit and much simpler). $\square$

1.3 The polynomial P

In this section, we will compute the coefficients of the polynomial P and study its positive roots. To this end, we will need the following auxiliary lemma.

Lemma 1.4. *It holds that*

$$\sum_{j=m}^{n} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big) j$$
$$= 4(n+1-m) + (k+2-N) \sum_{j=N+m-k-2}^{N+n-k-2} \frac{1}{j} + (k-N+1) \sum_{j=N+m-k-1}^{N+n-k-1} \frac{1}{j} - 2(N-1) \sum_{j=N-1-n}^{N-1-m} \frac{1}{j}. \tag{12}$$

In particular, we have

$$\sum_{j=1}^{k} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big) j$$
$$= 4k + (k+2-N) \sum_{j=N-1-k}^{N-2} \frac{1}{j} + (k-N+1) \sum_{j=N-k}^{N-1} \frac{1}{j} - 2(N-1) \sum_{j=N-1-k}^{N-2} \frac{1}{j}. \tag{13}$$

and

$$\sum_{j=k-N+3}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big) j$$
$$= 4(2N-k-4) + (k+2-N) \sum_{j=1}^{2N-k-4} \frac{1}{j} + (k-N+1) \sum_{j=2}^{2N-k-3} \frac{1}{j} - 2(N-1) \sum_{j=1}^{2N-4-k} \frac{1}{j}$$
$$= 4(2N-k-4) - (4N-2k-5) \sum_{j=1}^{2N-k-4} \frac{1}{j} + (k-N+1)\Big(\frac{1}{2N-k-3} - 1\Big). \tag{14}$$

Proof. By changing of variable $\bar{j} := N+j-k-2$, we have

$$\begin{aligned}
\sum_{j=m}^{n} \frac{j}{N+j-k-2} &= \sum_{\bar{j}=N+m-k-2}^{N+n-k-2} \frac{k+2-N+\bar{j}}{\bar{j}} \\
&= \sum_{\bar{j}=N+m-k-2}^{N+n-k-2} \Big(1 + \frac{k+2-N}{\bar{j}}\Big) \\
&= (n-m+1) + (k+2-N) \sum_{\bar{j}=N+m-k-2}^{N+n-k-2} \frac{1}{\bar{j}}.
\end{aligned}$$

Similarly we have

$$\begin{aligned}\sum_{j=m}^{n}\frac{j}{N+j-k-1} &= \sum_{\bar{j}=N+m-k-1}^{N+n-k-1}\frac{k-N+1+\bar{j}}{\bar{j}}\\ &= \sum_{\bar{j}=N+m-k-1}^{N+n-k-1}\Big(1+\frac{k-N+1}{\bar{j}}\Big)\\ &= (n-m+1)+(k-N+1)\sum_{\bar{j}=N+m-k-1}^{N+n-k-1}\frac{1}{\bar{j}}.\end{aligned}$$

and

$$\begin{aligned}\sum_{j=m}^{n}\frac{j}{N-1-j} &= \sum_{\bar{j}=N-1-n}^{N-1-m}\frac{N-1-\bar{j}}{\bar{j}}\\ &= \sum_{\bar{j}=N-1-n}^{N-1-m}\Big(\frac{N-1}{\bar{j}}-1\Big)\\ &= (N-1)\sum_{\bar{j}=N-1-n}^{N-1-m}\frac{1}{\bar{j}}-(n+1-m).\end{aligned}$$

Thus

$$\begin{aligned}&\sum_{j=m}^{n}\Big(\frac{1}{N+j-k-2}+\frac{1}{N+j-k-1}-\frac{2}{N-1-j}\Big)j\\ &\quad= 4(n+1-m)+(k+2-N)\sum_{j=N+m-k-2}^{N+n-k-2}\frac{1}{j}\\ &\quad+(k-N+1)\sum_{j=N+m-k-1}^{N+n-k-1}\frac{1}{j}-2(N-1)\sum_{j=N-1-n}^{N-1-m}\frac{1}{j}.\end{aligned}$$

□

The next lemma provides a sharp estimates for the harmonic number that will be used later.

Lemma 1.5. *[Young, 1991] The harmonic number satisfies the followings estimates*

$$\log(n)+\gamma+\frac{1}{2n+1}\le\sum_{j=1}^{n}\frac{1}{j}\le\log(n)+\gamma+\frac{1}{2n-1}, \tag{15}$$

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

In the next proposition we compute the coefficients of the polynomial P in terms of the harmonic number. This proposition is the most technical result but is the key to the analysis of this paper.

Proposition 1.6. *Let $P(u)$ be the polynomial defined in (10). Then its coefficients are given by*

explicitly by

$$p_k = \begin{cases} -(H_N + \frac{1}{N-2}) \quad k=0, \\ 4(k+1) + (2k+4-4N)\sum_{j=N-1-k}^{N-1} \frac{1}{j} - \frac{k+1}{N-k-2} - H_N(k+1) \quad 1 \le k \le N-3, \\ 4(N-1) - 2NH_N \quad k = N-2, \\ 4N-5-\frac{1}{N-1} - NH_N \quad k = N-1, \\ 8N-4k-9-(2N-k-1)H_N + (4N-2k-4)\sum_{j=2N-k-1}^{N-1} \frac{1}{j} - \frac{1}{2N-k-2} \quad N \le k \le 2N-5, \\ H_N + \frac{1}{2} \quad k = 2N-4. \end{cases} \tag{16}$$

Furthermore, P has exactly one positive root which is bigger than 1.

Proof. The proof is rather technical and lengthy. To obtain the formula for p_k we apply a general formula for coefficients of a product of two polynomials and use Lemma 1.4. Then we apply Decarte's rule of signs to show that P has exactly one positive root.

Let $a_j := H_N + \frac{1}{N-1-j}$ for $j = 0, \dots, N-2$. Suppose that $P(u) = \sum_{j=0}^{2N-4} p_j u^j$. Using the following formula of product of two polynomials:

$$\Big(\sum_{j=0}^{m} a_j x^j\Big)\Big(\sum_{j=0}^{n} b_j x^j\Big) = \sum_{k=0}^{m+n}\Big(\sum_{j=\max\{0,k-n\}}^{\min\{m,k\}} a_j b_{k-j}\Big)x^k,$$

we have

$$\begin{aligned}
(i)\quad \Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1} j u^{j-1}\Big) &= \Big(\sum_{j=0}^{N-2} a_j u^j\Big)\Big(\sum_{j=1}^{N-2}(j+1)u^j\Big) \\
&= \sum_{k=0}^{2N-4}\Big(\sum_{j=\max(k-N+2,0)}^{\min(k,N-2)} a_j(k-j+1)\Big)u^k \\
(ii)\quad \Big(\sum_{j=1}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)j u^{j-1}\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) &= \Big(\sum_{j=0}^{N-3} a_{j+1}(j+1)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) \\
&= \sum_{k=0}^{2N-4}\Big(\sum_{j=\max(0,k-N+1)}^{\min(k,N-3)} a_{j+1}(j+1)\Big)u^k. \\
(iii)\quad \Big(\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) &= \Big(\sum_{j=0}^{N-2} a_j u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) \\
&= \sum_{k=0}^{2N-3}\Big(\sum_{j=\max(0,k-N+1)}^{\min(N-2,k)} a_j\Big)u^k.
\end{aligned}$$

Hence

$$(iii)\quad \left[\Big(\sum_{j=0}^{N-2}(H_N+\frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1}ju^{j-1}\Big)-\Big(\sum_{j=1}^{N-2}\Big(H_N+\frac{1}{N-1-j}\Big)ju^{j-1}\Big)\Big(\sum_{j=0}^{N-1}u^j\Big)\right](1+u)$$

$$=\left(\sum_{k=0}^{2N-4}\Big(\sum_{j=\max(k-N+2,0)}^{\min(k,N-2)}a_j(k-j+1)-\sum_{j=\max(0,k-N+1)}^{\min(k,N-3)}a_{j+1}(j+1)\Big)u^k\right)(1+u)$$

$$=\Big(\sum_{k=0}^{2N-4}b_ku^k\Big)(1+u)$$

$$=\sum_{k=0}^{2N-3}\Big(\sum_{j=\max(0,k-1)}^{\min(k,2N-4)}b_j\Big)u^k$$

$$=b_0+\sum_{k=1}^{2N-4}(b_{k-1}+b_k)u^k+b_{2N-4}u^{2N-3}$$

where for $k=0,\dots,2N-4$

$$b_k:=\sum_{j=\max(k-N+2,0)}^{\min(k,N-2)}a_j(k-j+1)-\sum_{j=\max(0,k-N+1)}^{\min(k,N-3)}a_{j+1}(j+1) \tag{17}$$

$$=\sum_{j=\max(k-N+3,1)}^{\min(k+1,N-1)}a_{k-j+1}j-\sum_{j=\max(1,k-N+2)}^{\min(k+1,N-2)}a_jj$$

$$=\begin{cases}\sum_{j=1}^{k+1}(a_{k-j+1}-a_j)j & k\le N-3,\\ \sum_{j=1}^{N-1}a_{k-j+1}j-\sum_{j=1}^{N-2}a_jj & k=N-2,\\ \sum_{j=k-N+3}^{N-1}a_{k-j+1}j-\sum_{j=k-N+2}^{N-2}a_jj & N-1\le k\le 2N-4.\end{cases}$$

$$=\begin{cases}\sum_{j=1}^{k+1}(a_{k-j+1}-a_j)j & k\le N-3,\\ \sum_{j=1}^{N-2}(a_{k-j+1}-a_j)j+H_N(N-1)+1 & k=N-2,\\ \sum_{j=k-N+3}^{N-2}(a_{k-j+1}-a_j)j+a_{k-N+2}(2N-3-k) & N-1\le k\le 2N-5,\\ a_{N-2} & k=2N-4.\end{cases}$$

Therefore, we obtain

$$P(u)=\sum_{k=0}^{2N-3}\Big(\sum_{j=\max(0,k-1)}^{\min(k,2N-4)}b_j-\sum_{j=\max(0,k-N+1)}^{\min(N-2,k)}a_j\Big)u^k,$$

that is for $k=0,\dots,2N-3$

$$p_k=\sum_{j=\max(0,k-1)}^{\min(k,2N-4)}b_j-\sum_{j=\max(0,k-N+1)}^{\min(N-2,k)}a_j \tag{18}$$

$$=\begin{cases}b_0-a_0 & k=0,\\ b_{k-1}+b_k-\sum_{j=0}^{k}a_j & 1\le k\le N-2,\\ b_{k-1}+b_k-\sum_{j=k-N+1}^{N-2}a_j & N-1\le k\le 2N-4,\\ b_{2N-4}-a_{N-2} & k=2N-3.\end{cases} \tag{19}$$

In particular, the coefficient of u^{2N-3} in $P(u)$ is

$$p_{2N-3}=b_{2N-4}-a_{N-2}=\Big(a_{N-2}(N-1)-a_{N-2}(N-2)\Big)-a_{N-2}=0, \tag{20}$$

thus $P(u)$ is a polynomial of degree $2N-4$.

$$p_0 = b_0 - a_0 = (a_0 - a_1) - a_0 = -a_1 < 0.$$

For $1 \le k \le N-3$:

$$\begin{aligned}
b_{k-1} + b_k &= \sum_{j=1}^{k} (a_{k-j} - a_j) j + \sum_{j=1}^{k+1} (a_{k-j+1} - a_j) j \\
&= \sum_{j=1}^{k} (a_{k-j} - 2a_j + a_{k-j+1}) j + (a_0 - a_{k+1})(k+1) \\
&= \sum_{j=1}^{k} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j} \Big) j + (\frac{1}{N-1} - \frac{1}{N-k-2})(k+1)
\end{aligned}$$

Therefore,

$$\begin{aligned}
p_k &= b_{k-1} + b_k - \sum_{j=0}^{k} a_j \\
&= \sum_{j=1}^{k} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j} \Big) j + (\frac{1}{N-1} - \frac{1}{N-k-2})(k+1) \\
&\quad - H_N(k+1) - \sum_{j=0}^{k} \frac{1}{N-1-j} \\
&= \sum_{j=1}^{k} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j} \Big) j - H_N(k+1) - \sum_{j=0}^{k} \frac{1}{N-1-j} \\
&\quad - \frac{(k+1)^2}{(N-1)(N-k-2)} \\
&= 4k + (k+2-N) \sum_{j=N-1-k}^{N-2} \frac{1}{j} + (k-N+1) \sum_{j=N-k}^{N-1} \frac{1}{j} - 2(N-1) \sum_{j=N-1-k}^{N-2} \frac{1}{j} \\
&\quad - H_N(k+1) - \sum_{j=0}^{k} \frac{1}{N-1-j} + (\frac{1}{N-1} - \frac{1}{N-k-2})(k+1) \\
&= 4(k+1) + (2k+4-4N) \sum_{j=N-1-k}^{N-1} \frac{1}{j} - \frac{k+1}{N-k-2} - H_N(k+1).
\end{aligned}$$

For $k = N-2$

$$
\begin{aligned}
b_{k-1} + b_k &= b_{N-3} + b_{N-2} \\
&= \sum_{j=1}^{N-2} (a_{k-j} - a_j) j + \sum_{j=1}^{N-2} (a_{k-j+1} - a_j) j + H_N(N-1) + 1 \\
&= \sum_{j=1}^{N-2} (a_{k-j} - 2a_j + a_{k-j+1}) j + H_N(N-1) + 1 \\
&= \sum_{j=1}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j} \Big) j + 1 + H_N(N-1) \\
&= \sum_{j=1}^{N-2} \Big(\frac{1}{j} + \frac{1}{1+j} - \frac{2}{N-1-j} \Big) j + 1 + H_N(N-1) \\
&= (N-2) + \sum_{j=1}^{N-2} (1 - \frac{1}{1+j}) - 2 \sum_{j=1}^{N-2} \frac{j}{N-1-j} + H_N(N-1) + 1 \\
&= 2(N-2) - (H_N - 1) - 2[(N-1)H_N - (N-1)] + H_N(N-1) + 1 \\
&= 4(N-1) - NH_N,
\end{aligned}
$$

where we have used the relation

$$
\begin{aligned}
\sum_{j=1}^{N-2} \frac{j}{N-1-j} &= \sum_{j=1}^{N-2} \frac{N-1-j}{j} = (N-1) \sum_{j=1}^{N-2} \frac{1}{j} - (N-2) = (N-1)(H_N - \frac{1}{N-1}) - (N-2) \\
&= (N-1)(H_N - 1). \qquad (21)
\end{aligned}
$$

We also have

$$
\sum_{j=0}^{N-2} a_j = (N-1)H_N + \sum_{j=0}^{N-2} \frac{1}{N-1-j} = NH_N.
$$

Thus

$$
\begin{aligned}
p_{N-2} &= b_{N-3} + b_{N-2} - \sum_{j=0}^{N-2} a_j \\
&= 4(N-1) - 2NH_N < 0,
\end{aligned}
$$

where the last inequality follows from the fact that

$$
H_N = \sum_{j=1}^{N-1} \frac{1}{j} > 1 + \frac{N-2}{N} = \frac{2(N-1)}{N}. \qquad (22)
$$

For $k = N-1$:

$$
\begin{aligned}
b_{k-1} + b_k &= b_{N-2} + b_{N-1} \\
&= \sum_{j=1}^{N-2} (a_{N-1-j} - a_j)j + H_N(N-1) + 1 + \sum_{j=2}^{N-2} (a_{N-j} - a_j)j + a_1(N-2) \\
&= \sum_{j=2}^{N-2} \Big(\frac{1}{j} + \frac{1}{j-1} - \frac{2}{N-1-j}\Big)j + (1 - \frac{1}{N-2}) + H_N(2N-3) + 2 \\
&= \Big(N - 3 + \sum_{j=1}^{N-3} \frac{j+1}{j}\Big) - 2\sum_{j=2}^{N-2} \frac{j}{N-1-j} + H_N(2N-3) + 3 - \frac{1}{N-2} \\
&= 2(N-3) + \Big(H_N - \frac{1}{N-2} - \frac{1}{N-1}\Big) - 2\Big((N-1)(H_N-1) - \frac{1}{N-2}\Big) + (2N-3)H_N + 3 - \frac{1}{N-2} \\
&= 4N - 5 - \frac{1}{N-1}
\end{aligned}
$$

Thus

$$
\begin{aligned}
p_{N-1} &= b_{N-2} + b_{N-1} - \sum_{k=0}^{N-2} a_j \\
&= 4N - 5 - \frac{1}{N-1} - NH_N
\end{aligned}
$$

For $N \le k \le 2N-5$:

$$
\begin{aligned}
b_{k-1} + b_k &= \sum_{j=k-N+2}^{N-2} (a_{k-j} - a_j)j + a_{k-N+1}(2N-2-k) + \sum_{j=k-N+3}^{N-2} (a_{k-j+1} - a_j)j + a_{k-N+2}(2N-3-k) \\
&= \sum_{j=k-N+3}^{N-2} (a_{k-j+1} - 2a_j + a_{k-j})j + (a_{N-2} - a_{k-N+2})(k-N+2) \\
&\quad + a_{k-N+1}(2N-2-k) + a_{k-N+2}(2N-3-k) \\
&= \sum_{j=k-N+3}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big)j + (H_N+1)(k-N+2) \\
&\quad + (H_N + 1/(2N-k-2))(2N-k-2) + (3N-2k-5)(H_N + 1/(2N-k-3)) \\
&= \sum_{j=k-N+3}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big)j \\
&\quad + (4N-2k-5)H_N + k - N + 3 + \frac{3N-2k-5}{2N-k-3}.
\end{aligned}
$$

We also have

$$
\begin{aligned}
\sum_{j=k-N+1}^{N-2} a_j &= (2N-k-2)H_N + \sum_{j=k-N+1}^{N-2} \frac{1}{N-1-j} \\
&= (2N-k-2)H_N + \sum_{j=1}^{2N-k-2} \frac{1}{j}.
\end{aligned}
$$

Thus using Lemma 1.4 we obtain

$$
\begin{aligned}
p_k &= b_{k-1} + b_k - \sum_{j=k-N+1}^{N-2} a_j \\
&= \sum_{j=k-N+3}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k-1} - \frac{2}{N-1-j}\Big) j + (4N-2k-5)H_N \\
&\quad + k - N + 3 + \frac{3N-2k-5}{2N-k-3} - (2N-k-2)H_N - \sum_{j=1}^{2N-k-2} \frac{1}{j} \\
&= \sum_{j=k-N+3}^{N-2} \Big(\frac{1}{N+j-k-2} + \frac{1}{N+j-k} - \frac{2}{N-1-j}\Big) j + (2N-k-3)H_N \\
&\quad + k - N + 3 + \frac{3N-2k-5}{2N-k-3} - \sum_{j=1}^{2N-k-2} \frac{1}{j} \\
&= 4(2N-k-4) - (4N-2k-5) \sum_{j=1}^{2N-k-4} \frac{1}{j} + (k-N+1)\Big(\frac{1}{2N-k-3} - 1\Big) \\
&\quad + (2N-k-3)H_N + k - N + 3 + \frac{3N-2k-5}{2N-k-3} - \sum_{j=1}^{2N-k-2} \frac{1}{j} \\
&= 8N - 4k - 13 + (2N-k-3)H_N - (4N-2k-4) \sum_{j=1}^{2N-k-4} \frac{1}{j} \\
&\quad - \frac{2}{2N-k-3} - \frac{1}{2N-k-2} \\
&= 8N - 4k - 9 - (2N-k-1)H_N + (4N-2k-4) \sum_{j=2N-k-1}^{N-1} \frac{1}{j} - \frac{1}{2N-k-2}
\end{aligned}
$$

In particular, for $k = N$

$$p_N = 4N - 9 - (N-1)H_N + (2N-4)\frac{1}{N-1} - \frac{1}{N-2}.$$

Finally, for $k = 2N-4$

$$p_{2N-4} = b_{2N-5} + b_{2N-4} - (a_{N-3} + a_{N-2}) = 2a_{N-3} + a_{N-2} - (a_{N-3} + a_{N-2}) = a_{N-3} = H_N + \frac{1}{2}.$$

In conclusion, we obtain

$$
p_k = \begin{cases}
-(H_N + \frac{1}{N-2}) \quad k = 0, \\
4(k+1) + (2k+4-4N)\sum_{j=N-1-k}^{N-1} \frac{1}{j} - \frac{k+1}{N-k-2} - H_N(k+1) \quad 1 \le k \le N-3, \\
4(N-1) - 2NH_N \quad k = N-2, \\
4N - 5 - \frac{1}{N-1} - NH_N \quad k = N-1, \\
8N - 4k - 9 - (2N-k-1)H_N + (4N-2k-4)\sum_{j=2N-k-1}^{N-1} \frac{1}{j} - \frac{1}{2N-k-2} \quad N \le k \le 2N-5, \\
H_N + \frac{1}{2} \quad k = 2N-4.
\end{cases}
\tag{23}
$$

Now we prove that there is only one change of signs in the sequence $\{p_k, 0 \le k \le 2N-4\}$.

Consider first $1 \le k \le N-3$. Since

$$\sum_{j=N-1-k}^{N-1} \frac{1}{j} \ge \frac{k+1}{N-1},$$

we have,

$$\begin{aligned}
p_k &\le 4(k+1) - (4N-2k-4)\frac{k+1}{N-1} - \frac{k+1}{N-k-2} - H_N(k+1) \\
&\le (k+1)\Big(4 - \frac{4N-2k-4}{N-1} - \frac{1}{N-k-2} - H_N\Big) \\
&= (k+1)\Big(\frac{2k}{N-1} - H_N - \frac{1}{N-k-2}\Big) < 0,
\end{aligned}$$

where to obtain the last inequality we have used (22) so that

$$H_N \ge \frac{2(N-1)}{N} > \frac{2(N-3)}{N-1} \ge \frac{2k}{N-1}.$$

Thus $p_k < 0$ for all $0 \le k \le N-3$. Next we consider $p_m =$ with $N \le m \le 2N-5$. It will be more convenient to set $m = 2N-4-k$ and consider instead p_{2N-4-k}. We have

$$\begin{aligned}
p_{2N-4-k} &= 8N - 4(2N-4-k) - 9 - (2N-(2N-4-k)-1)H_N \\
&\quad + (4N - 2(2N-4-k) - 4)\sum_{j=k+3}^{N-1}\frac{1}{j} - \frac{1}{k+2}. \\
&= 4k+7-(k+3)H_N + (2k+4)\sum_{j=k+3}^{N-1}\frac{1}{j} - \frac{1}{k+2} \\
&= 4k+7-(k+3)H_N + (2k+4)(H_N - H_{k+3}) - \frac{1}{k+2} \\
&= 4k+7+(k+1)H_N - (2k+4)H_{k+3} - \frac{1}{k+2}.
\end{aligned}$$

By lemma 1.5

$$\log(k+2)+\gamma+\frac{1}{2(k+2)+1} \le H_{k+3} = \sum_{j=1}^{k+2}\frac{1}{j} \le \log(k+2)+\gamma+\frac{1}{2(k+2)-1},$$

we have

$$\begin{aligned}
4k+7+(k+1)H_N - (2k+4)(\log(k+2)+\gamma+\frac{1}{2k+3}) - \frac{1}{k+2} &\le p_{2N-k-4} \\
&\le 4k+7+(k+1)H_N - (2k+4)(\log(k+2)+\gamma+\frac{1}{2k+5}) - \frac{1}{k+2} \qquad (24)
\end{aligned}$$

Consider the equation

$$4x+7+(x+1)H_N - 2(x+2)(\log(x+2)+\gamma+\frac{1}{2x+5}) - \frac{1}{x+2} = 0 \quad \text{for} \quad x \ge 0, \qquad (25)$$

which is equivalent to

$$h(x) := 2\log(x+2) + \frac{1}{x+2} + \frac{H_N}{x+2} + \frac{1}{(x+2)^2} + \frac{2}{2x+5} = 4 + H_N - 2\gamma.$$

We have

$$h'(x) = \frac{8x^4 + (64-4H_N)x^3 + (182-28H_N)x^2 + (207-65H_N)x + (68-50H_N)}{(x+2)^3(2x+5)^2}.$$

Let $r(x) := 8x^4 + (64-4H_N)x^3 + (182-28H_N)x^2 + (207-65H_N)x + (68-50H_N) := r_4x^4 + r_3x^3 + r_2x^2 + r_1x + r_0$, where $r_4 := 8, r_3 = 64-4H_N, r_2 := 182-28H_N, r_1 = 207-65H_N, r_0 := 68-50H_N$, be the enumerator of $h'(x)$. Since $N \ge 2$, $H_N \ge 1.5$, it follows that $r_0 < 0$. There is only one change of signs in the coefficients of $r(x)$ since:

(i) if $H_N \le 207/65$ then $r_0 < 0 < r_1, r_2, r_3, r_4$,

(ii) if $207/65 < H_N < 182/28$, then $r_0, r_1 < 0$ while $r_2, r_3, r_4 > 0$,

(iii) if $182/28 < H_N \le 16$, then $r_0, r_1, r_2 < 0$ while $r_3, r_4 > 0$,

(iv) $16 < H_N$ then $r_0, r_1, r_2, r_3 < 0$, while $r_4 > 0$.

Thus, by Decarte's rule of signs, $r(x)$ has a unique positive solution $x_0 > 0$. It follows that $h'(x) < 0$ when $x < x_0$ and $h'(x) > 0$ when $x > x_0$. Hence $h(x)$ is decreasing when $x < x_0$, increasing when $x > x_0$ and attains a global minimum at $x = x_0$. Since $f(0) = 2\log(2) + 1/2 + H_N/2 + 1/4 + 2/5 < 4 + H_N - 2\gamma$, Equation (25) has a unique solution $x^* > x_0$. If $k \ge x^* > x_0$ then, since $h(x)$ is increasing for $x > x_0$, $4 + H_N - 2\gamma \le h(k) = 2\log(k+2) + \frac{1}{k+2} + \frac{H_N}{k+2} + \frac{1}{(k+2)^2} + \frac{2}{2k+5}$, that is

$$4k + 7 + (k+1)H_N - (2k+4)(\log(k+2) + \gamma + \frac{1}{2k+5}) - \frac{1}{k+2} \le 0.$$

Hence if $k > x^*$ then

$$p_{2N-4-k} < 4k + 7 + (k+1)H_N - (2k+4)(\log(k+2) + \gamma + \frac{1}{2k+5}) - \frac{1}{k+2} < 0.$$

Similarly, let

$$\bar{g}(x) := 2\log(x+2) + \frac{1}{x+2} + \frac{H_N}{x+2} + \frac{1}{(x+2)^2} + \frac{2}{2x+3},$$

and consider the equation

$$\bar{g}(x) = 4 + H_N - 2\gamma. \tag{26}$$

$\bar{g}'(x) = 0$ has a unique positive solution; $\bar{g}(x)$ is decreasing when $x < x_1$, increasing when $x > x_1$ and attains a global minimum at $x = x_1$; equation (26) has a unique solution $\hat{x}$.

If $k \le \hat{x}$ then $h(k) \le 4 + H_N - 2\gamma$, that is

$$4k + 7 + (k+1)H_N - (2k+4)(\log(k+2) + \gamma + \frac{1}{2k+5}) - \frac{1}{k+2} \ge 0.$$

Hence if $k \le \hat{x}$ then $p_{2N-k-4} > 0$. Since

$$\bar{g}(\hat{x}) = h(x^*) < \bar{g}(x^*)$$

and $\bar{g}$ is increasing in (x_1, ∞), we have $\hat{x} < x^*$. We now prove that they are closed together.

$$\bar{g}(x^*) - h(x^*) = \bar{g}(x^*) - \bar{g}(\hat{x}) + \bar{g}(\hat{x}) - h(x^*) = \bar{g}(x^*) - \bar{g}(\hat{x}).$$

Hence

$$\begin{aligned}
\frac{4}{(2x^*+3)(2x^*+5)} &= 2(\log(x^*+2) - \log(\hat{x}+2)) + (H_N+1)\Big(\frac{1}{x^*+2} - \frac{1}{\hat{x}+2}\Big) \\
&\quad + \Big(\frac{1}{(x^*+2)^2} - \frac{1}{(\hat{x}+2)^2}\Big) + \Big(\frac{2}{2x^*+3} - \frac{2}{2\hat{x}+3}\Big) \\
&= (x^* - \hat{x})\Big(\frac{2}{\xi+2} - \frac{H_N+1}{(x^*+2)(\hat{x}+2)} - \frac{1}{(\hat{x}+2)^2(x^*+2)} - \frac{1}{(\hat{x}+2)(x^*+2)^2} \\
&\quad - \frac{4}{(2x^*+3)(2\hat{x}+3)}\Big),
\end{aligned} \tag{27}$$

where $\hat{x} < \xi < x^*$. Since

$$\bar{g}(H_N - 1) = 2\log(H_N+1) + 1 + \frac{1}{H_N+1} + \frac{2}{2H_N+1} < 4 + H_N - 2\gamma = \bar{g}(\hat{x}),$$

we have $m := H_N - 1 < \hat{x} < x^*$. For $N \geq 5$, we have $x^* > \hat{x} > m \geq \frac{77}{60}$. Hence

$$\begin{aligned}
&\frac{H_N+1}{(\hat{x}+2)(x^*+2)} + \frac{1}{(\hat{x}+2)^2(x^*+2)} + \frac{1}{(\hat{x}+2)(x^*+2)^2} + \frac{4}{(2x^*+3)(2\hat{x}+3)} \\
&\quad < \frac{1}{x^*+2} + \frac{1}{(m+2)^2(x^*+2)} + \frac{1}{(m+2)^2(x^*+2)} + \frac{4}{(2m+3)(2x^*+3)}.
\end{aligned}$$

It follows that

$$\begin{aligned}
&\frac{2}{\xi+2} - \frac{H_N+1}{(x^*+2)(\hat{x}+2)} - \frac{1}{(\hat{x}+2)^2(x^*+2)} - \frac{1}{(\hat{x}+2)(x^*+2)^2} - \frac{4}{(2x^*+3)(2\hat{x}+3)} \\
&\quad > \frac{2}{x^*+2} - \Big(\frac{1}{x^*+2} + \frac{1}{(m+2)^2(x^*+2)} + \frac{1}{(m+2)^2(x^*+2)} + \frac{4}{(2m+3)(2x^*+3)}\Big) \\
&\quad = \frac{(4m^3+18m^2+16m-4)x^* + (6m^3+25m^2+16m-14)}{(m+2)^2(2m+3)(x^*+2)(2x^*+3)}. \qquad (28)
\end{aligned}$$

From (27) and (28) we deduce

$$\begin{aligned}
0 < (x^* - \hat{x}) &< \frac{4(m+2)^2(2m+3)(x^*+2)}{(2x^*+5)(4m^3+18m^2+16m-4)x^* + (6m^3+25m^2+16m-14)} \\
&< \frac{2(m+2)^2(2m+3)}{(4m^3+18m^2+16m-4)x^* + (6m^3+25m^2+16m-14)} \\
&< \frac{2(m+2)^2(2m+3)}{(4m^3+18m^2+16m-4)m + (6m^3+25m^2+16m-14)} \\
&< 1,
\end{aligned}$$

where the last inequality is because $m > 1.28$.

Let k_0 be the position of change of signs in the coefficients $\{p_k, 0 \leq k \leq 2N-4\}$, that is $p_k < 0$ for $0 \leq k \leq k_0$ and $p_k > 0$ for $k_0 + 1 \leq k \leq 2N-4$. Since $p_N > 0$ for $N \geq 27$, we have

$$k_0 = \begin{cases} N-2 & N \leq 25, \\ N-1 & N \in \{26, 27\}, \\ 2N-4-\lfloor 2N - x^* - 4 \rfloor & N \geq 27. \end{cases} \qquad (29)$$

Since there is only one change of signs in the sequence of coefficients of P, by Decarte's rule of signs, P has a unique positive root. This root is bigger than 1 since we have

$$\begin{aligned}
P(1) &= 2\Big[\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{N-1-j})\Big)(\sum_{j=1}^{N-1} j) - N\sum_{j=1}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)j\Big] \\
&\quad - N\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big) \\
&= \Big[(N-1)N\Big((N-1)H_N + \sum_{j=0}^{N-2}\frac{1}{N-1-j}\Big) - N\Big((N-2)(N-1)H_N + 2\sum_{j=1}^{N-2}\frac{N-1-j}{j}\Big)\Big] \\
&\quad - N\Big((N-1)H_N + \sum_{j=0}^{N-2}\frac{1}{N-1-j}\Big) \\
&= \Big[(N-1)N^2H_N - N((N-2)(N-1)H_N + 2(N-1)H_N - 2 - 2(N-2))\Big] - N^2H_N \\
&= 2N(N-1) - N^2H_N < 0
\end{aligned}$$

where the first inequality follows from (22). □

1.4 The function F

Next we study the function F defined in (11). We will need the following lemma, which establishes a relation between the polynomials P and Q.

Lemma 1.7. *For $u > 0$, we have*

$$Q(u) \geq (1+u)uP(u). \tag{30}$$

As a consequence, for $\beta \leq \frac{1}{a}$ we have $\frac{d}{d\theta}E_r(\theta) \geq 0$.

Proof. The statement (30) is equivalent to

$$\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{N-1-j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1}u^j\Big) = \sum_{k=0}^{2N-3}\Big(\sum_{j=\max(0,k-N+1)}^{\min(N-2,k)} a_j\Big)u^k \geq uP(u), \tag{31}$$

which we now prove. Let

$$\begin{aligned} h_k := \sum_{j=\max(0,k-N+1)}^{\min(N-2,k)} a_j &= \begin{cases} \sum_{j=0}^{k} a_j & 0 \leq k \leq N-2, \\ \sum_{j=k-N+1}^{N-2} a_j & N-1 \leq k \leq 2N-3 \end{cases} \\ &= \begin{cases} (k+1)H_N + \sum_{j=N-1-k}^{N-2}\frac{1}{j} & 0 \leq k \leq N-2, \\ (2N-k-2)H_N + \sum_{j=1}^{2N-k-2}\frac{1}{j} & N-1 \leq k \leq 2N-3 \end{cases} \end{aligned}$$

Now we show that $h_{k+1} \geq p_k$ for all $k = 0, \ldots, 2N-4$.

For $k = 0$: $h_1 > 0 > p_0$.

For $1 \leq k \leq N-3$, we have

$$h_{k+1} = (k+2)H_N + \sum_{j=N-k-2}^{N-2}\frac{1}{j}, \quad p_k = 4(k+1) + (2k+4-4N)\sum_{j=N-1-k}^{N-1}\frac{1}{j} - \frac{k+1}{N-k-2} - H_N(k+1).$$

Since $H_N \geq 2$ $(N \geq 4)$, $(2k+3)H_N \geq 4(k+1)$. It follows that $h_{k+1} \geq p_k$.

For $k = N-2$

$$h_{N-1} = (N-1)H_N + \sum_{j=1}^{N-1}\frac{1}{j} = NH_N > 4(N-1) - 2NH_N$$

since according to (22), $3NH_N > 6(N-1) > 4(N-1)$.

For $k = N-1$,

$$h_N = (N-2)H_N + \sum_{j=1}^{N-2}\frac{1}{j} = (N-1)H_N - \frac{1}{N-1} > 4N-5 - \frac{1}{N-1} - NH_N = p_{N-1}$$

since $H_N \geq 2$ $(N \geq 4)$, $(2N-1)H_N \geq 4N-2 > 4N-5$.

For $N \leq k \leq 2N-5$. We have

$$\begin{aligned} h_{k+1} &= (2N-k-3)H_N + \sum_{j=1}^{2N-k-3}\frac{1}{j}, \\ p_k &= 8N-4k-9-(2N-k-1)H_N + (4N-2k-4)\sum_{j=2N-k-1}^{N-1}\frac{1}{j} - \frac{1}{2N-k-2} \\ &= 8N-4k-9-(2N-k-1)H_N + (4N-2k-4)[H_N - H_{2N-k-1}] - \frac{1}{2N-k-2}. \end{aligned}$$

Thus, we obtain

$$h_{k+1} - p_k = (4N - 2k - 3)H_{2N-k-1} - (8N - 4k - 9).$$

Since $2N - k - 1 \geq 4$, we have $H_{2N-k-1} \geq 2$, thus

$$h_{k+1} - p_k \geq 2(4N - 2k - 3) - (8N - 4k - 9) = 3 > 0,$$

i.e., $h_{k+1} > p_k$ for all $N \leq k \leq 2N - 5$

Finally for $k = 2N - 4$, we have

$$h_{2N-3} = H_N + 1 > H_N + \frac{1}{2} = p_{2N-4}.$$

In conclusion, we have proved that $h_{k+1} > p_k$ for all $k = 0, \ldots, 2N - 4$.

As a consequence, if $\beta a \leq 2$, then

$$0 < x + \beta a \leq x + 2 \leq e^x + 1 = 1 + u,$$

thus

$$(x + \beta a)(f(x)g'(x) - f'(x)g(x)) = (x + \beta a)uP(u) \leq (1 + u)uP(u) \leq Q(u) = f(x)g(x),$$

which implies that $E'(x) \geq 0$. This completes the proof of the lemma. □

Let $u^0 > 1$ be the unique positive root of P obtained in Proposition 1.6. Then

$$\{u \in \mathbb{R} : \ P(u) > 0\} = \{u > u_0\}.$$

Lemma 1.7 provides an upper bound $\bar{\beta}$ of β such that $E(\theta) \geq 0$ for all $\beta \leq \bar{\beta}$. To obtain the optimal bound we need to study the minimization problem

$$\min\{F(u) \mid u > u^0\}.$$

Proposition 1.8. *F has a global minimizer on $(u^0, +\infty)$. Furthermore, for $N \leq N_0 = 100$, F has a unique minimizer u^* and F is decreasing when $u^0 < u < u^*$ and is increasing when $u > u^*$.*

Proof. It follows from Lemma 1.7 that F is bounded below on $(u^0, +\infty)$. Further more, it is continuous and coercive in this interval since

$$\lim_{u \to (u^0)^+} F(u) = \lim_{u \to +\infty} F(u) = +\infty.$$

Therefore F has a global minimizer on $(u^0, +\infty)$. We have

$$F'(u) = \frac{uQ'(u)P(u) - Q(u)(P(u) + uP'(u))}{u^2 P(u)^2} - \frac{1}{u} =: \frac{M(u)}{u^2 P(u)^2},$$

where

$$M(u) := uQ'(u)P(u) - Q(u)(P(u) + uP'(u)) - uP(u)^2. \tag{32}$$

Then M is a polynomial of degree $4N - 6$. The leading coefficient m_{4N-6} of M is

$$m_{4N-6} = q_{2N-2}p_{2N-4} > 0.$$

The sign of F' is the same as that of M. Thus the number of changes of signs of F' is equal to the number of positive roots of M. Since $Q(0) > 0$ while $P(0) < 0$, we have

$$M(0) = -Q(0)P(0) > 0$$

In addition, since P is a polynomial whose coefficient of the highest degree is positive and u^0 is the unique positive root of P, it follows that $P'(u^0) > 0$. Hence

$$M(u^0) = -u^0 Q(u^0)P'(u^0) < 0.$$

Since $\lim_{u\to+\infty} M(u) = +\infty$, M has at least two positive roots, one is belong to $(0, u^0)$ and one is in $(u^0, +\infty)$. To determine the number of positive roots of M we can use Sturm's theorem. To this end, we construct the Sturm sequence of M as follows

$$\begin{aligned} M_0 &= M, \\ M_1 &= M', \\ M_{i+1} &= -\mathrm{rem}(M_{i-1}, M_i), \end{aligned}$$

for $i \geq 1$, where M' is the derivative of M and $\mathrm{rem}(M_{i-1}, M_i)$ is the remainder of the Euclidean division of M_{i-1} by M_i. The number of changes of signs at ξ of the Sturm sequence of M, denoted by $s(\xi)$, is the number of sign changes, by ignoring zeros, in the sequence of real numbers

$$M_0(\xi), M_1(\xi), \ldots$$

According to Sturm theorem, the number of distinct positive real roots of M is $s(0) - s(+\infty)$, where the sign at $+\infty$ of a polynomial is the sign of its leading coefficient. Sturm' algorithm is rather analytically intricate but is easily implemented using mathematical softwares such as Mathematica.

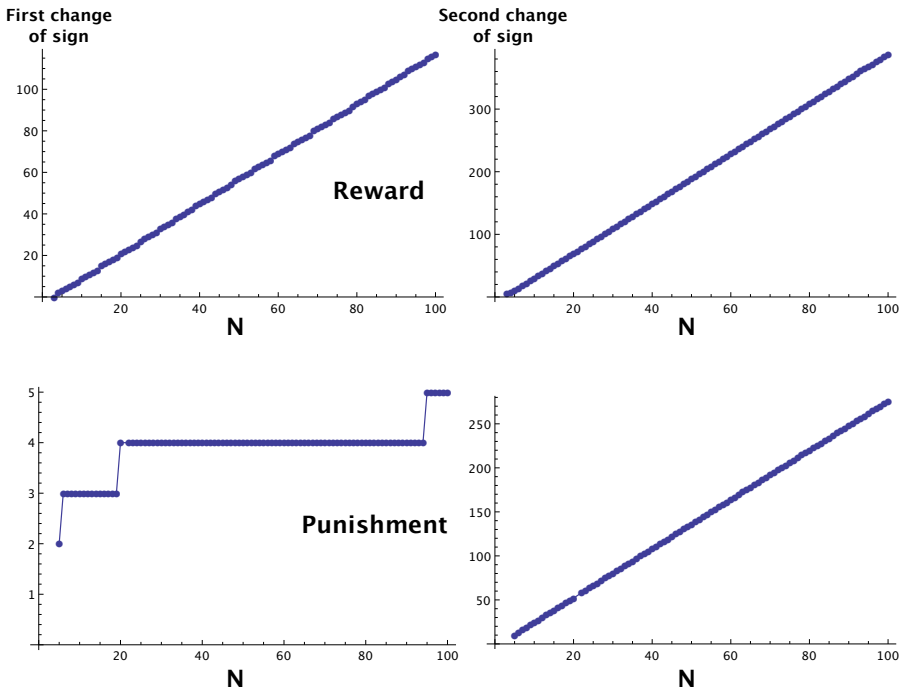

Figure 2: **Numerical results showing there are always two changes of sign in the sequence of coefficients of M, for N up to 100.** We show the positions at which the changes of signs occur, for reward (top row) and punishment (bottom row).

We conjecture that M actually has exactly two roots. One possible way to prove this conjecture is to show that there are two changes of signs in the sequence of coefficients of M. This is because if there are two changes of signs in the sequence of coefficients of M then M has either 2 or none positive roots according to Descartes' rule of signs, which follows that M has exactly 2 positive roots since we already proved above that M has at least two positive roots. However, finding the signs of coefficients of M is analytically challenging since formulas for the coefficients of M is extremely intricate. By direct computations (using Mathematica) we verify that this conjecture is true for $N \leq N_0 = 100$. As a consequence, for $N \leq N_0$, F' has only one zero, denoted by u^*, on $(u^0, +\infty)$. Then u^* is the unique minimizer of F on $(u^0, +\infty)$. Furthermore, F is decreasing on (u^0, u^*) and is increasing on $(u^*, +\infty)$. $\square$

1.5 Finite population estimates

In this section, we establish the finite population estimates for $E_r(\theta)$. To this end, we need the following auxiliary lemma.

Lemma 1.9. *For all $x \in \mathbb{R}$, we have*

$$0 \le \frac{e^x + \ldots + e^{(N-2)x}}{1 + e^x + \ldots + e^{(N-1)x}} \le \frac{N-2}{N}. \tag{33}$$

Proof. Let $u = e^x$ and $z(u) := \frac{u+\ldots+u^{N-2}}{1+u+\ldots+u^{N-1}}$. Then

$$z(u) = \begin{cases} \frac{N-2}{N} & u = 1, \\ \frac{u^{N-1}-u}{u^N-1} & u \neq 1. \end{cases}$$

For $u \neq 1$, we have

$$z'(u) = \frac{(N-1)u^N - u^{2N-2} - (N-1)u^{N-2} + 1}{(u^N-1)^2}.$$

To find the roots of $f'(u)$ we need to factorize the enumerator in the above expression.

$$\begin{aligned}
&(N-1)u^N - u^{2N-2} - (N-1)u^{N-2} + 1 \\
&\quad = (1-u^{2N-2}) - (N-1)u^{N-2}(1-u) \\
&\quad = (1-u)(1+u+\ldots+u^{2N-3} - (N-1)u^{N-2} - (N-1)u^{N-1}) \\
&\quad = (1-u)\Big[(1-u^{N-2}) + u(1-u^{N-3}) + \ldots + u^{N-3}(1-u) - u^{N-1}(1-u) \\
&\qquad\qquad - u^{N-1}(1-u^2) - \ldots - u^{N-1}(1-u^{N-2})\Big] \\
&\quad = (1-u)\Big[(1-u)(u^{N-3}-u^{N-1}) + (1-u^2)(u^{N-4}-u^{N-1}) + \ldots + (1-u^{N-2})(1-u^{N-1})\Big] \\
&\quad = (1-u)\Big[(1-u)u^{N-3}(1-u^2) + (1-u^2)u^{N-4}(1-u^3) + \ldots + (1-u^{N-2})(1-u^{N-1})\Big] \\
&\quad = (1-u)^3\Big[u^{N-3}(1+u) + u^{N-4}(1+u)(1+u+u^2) + \ldots + (1+u+\ldots+u^{N-3})(1+u+\ldots+u^{N-2})\Big].
\end{aligned}$$

It follows that $z'(u) > 0$ in $(0,1)$ and $z'(u) < 0$ in $(1,+\infty)$. Hence $\max z(u) = f(1) = \frac{N-2}{N}$. In addition, we have

$$z(0) = 0 = \lim_{u\to+\infty} f(u).$$

Thus $0 \le z(u) \le \frac{N-2}{N}$ for all $u > 0$, which is the required statement. □

Lemma 1.10. *It holds that*

$$\frac{N^2\theta}{2}\Big(H_N + \frac{1}{N-1}\Big) \le E_r(\theta) \le N(N-1)\theta\Big(H_N + 1\Big). \tag{34}$$

Proof. We have

$$\frac{(1+e^x)(1+e^x+\ldots+e^{(N-2)x})}{1+e^x+\ldots+e^{(N-1)x}} = 1 + \frac{e^x+\ldots+e^{(N-2)x}}{1+e^x+\ldots+e^{(N-1)x}}.$$

Using Lemma 1.9, we get

$$1 \le \frac{(1+e^x)(1+e^x+\ldots+e^{(N-2)x})}{1+e^x+\ldots+e^{(N-1)x}} \le \frac{2(N-1)}{N}.$$

Since

$$\frac{1}{N-1}\sum_{j=0}^{N-2} e^{jx} \le e^{(N-1)x}\sum_{j=1}^{N-1}\frac{e^{-jx}}{j} = \sum_{j=0}^{N-2}\frac{e^{jx}}{N-1-j} \le \sum_{j=0}^{N-2} e^{jx}.$$

we obtain the following estimates

$$\frac{1}{N-1} \leq \frac{1}{N-1}\frac{(1+e^x)(1+e^x+\ldots+e^{(N-2)x})}{1+e^x+\ldots+e^{(N-1)x}} \leq \frac{(1+e^x)}{1+e^x+\ldots+e^{(N-1)x}} e^{(N-1)x}\sum_{j=1}^{N-1}\frac{e^{-jx}}{j}$$
$$\leq \frac{(1+e^x)(1+e^x+\ldots+e^{(N-2)x})}{1+e^x+\ldots+e^{(N-1)x}} \leq \frac{2(N-1)}{N}.$$

Thus for $\theta > 0$ we have

$$\frac{N^2\theta}{2}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+\frac{1}{N-1}\Big) \leq E_r(\theta) \leq \frac{N^2\theta}{2}\frac{2(N-1)}{N}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+1\Big) = N(N-1)\theta\Big(\sum_{j=1}^{N-1}\frac{1}{j}+1\Big).$$

As a consequence, since E is smooth as a function of θ, by the extreme value theorem, it attains a minimum in any bounded interval $[\theta_0, \theta_1]$ where $\theta_0 \geq 0$. □

1.6 Asymptotic limits

In this section, we will establish the asymptotic limits of $E_r(\theta)$ as $N \to +\infty$, $\beta \to 0$ and $\beta \to +\infty$ where N is the population size and β is the selection intensity.

Proposition 1.11 (Infinite population limit)**.** *We have*

$$\lim_{N\to+\infty}\frac{E_r(\theta)}{\frac{N^2\theta}{2}(\ln N+\gamma)} = \begin{cases} 1+e^{-\beta|\theta-c|} & \textit{for DG}, \\ 1+e^{-\beta|\theta-c|}e^{\beta c\frac{r}{n}} & \textit{for PGG}. \end{cases} \tag{35}$$

Proof.

$$\frac{N^2\theta}{2}\frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+\frac{1}{N-1}\Big) \leq E_r(\theta)$$
$$\leq \frac{N^2\theta}{2}\frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+1\Big)$$

Hence

$$\frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\frac{\Big(\sum_{j=1}^{N-1}\frac{1}{j}+\frac{1}{N-1}\Big)}{\ln N+\gamma} \leq \frac{E_r(\theta)}{\frac{N^2\theta}{2}(\ln N+\gamma)}$$
$$\leq \frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\frac{\Big(\sum_{j=1}^{N-1}\frac{1}{j}+1\Big)}{\ln N+\gamma} \tag{36}$$

We recall that $x = \beta(\theta+\delta)$, where

$$\delta = \delta(N) = \begin{cases} -(c+\frac{b}{N-1}) & \text{for DG}, \\ -c(1-\frac{r(N-n)}{n(N-1)}) & \text{for PGG}. \end{cases}$$

Let

$$w(\theta) := \frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}.$$

Then we have

$$w(\theta) = 1+\frac{e^x+\ldots e^{(N-2)x}}{1+\ldots+e^{(N-1)x}} = \begin{cases} \frac{2(N-1)}{N} & \text{if} \quad x=0, \\ 1+e^x\frac{1-e^{(N-3)x}}{1-e^{(N-1)x}} & \text{if} \quad x\neq 0. \end{cases}$$

Since for fixed θ, x equals to 0 for only one value of N, we can consider $x \neq 0$ when we study the limit $N \to +\infty$. We have

$$\lim_{N\to+\infty} e^x = \lim_{N\to+\infty} e^{\beta(\theta+\delta(N))} = \begin{cases} e^{\beta(\theta-c)} & \text{for DG,} \\ e^{\beta(\theta-c(1-\frac{r}{n}))} & \text{for PGG.} \end{cases}$$

For DG:

$$\lim_{N\to+\infty} \frac{1-e^{(N-3)x}}{1-e^{(N-1)x}} = \lim_{N\to+\infty} \frac{1-e^{-\beta b(N-3)/(N-1)}e^{\beta(\theta-c)(N-3)}}{1-e^{-\beta b}e^{\beta(\theta-c)(N-1)}} = \begin{cases} 1 & \text{if} \quad \theta \leq c, \\ e^{-2\beta(\theta-c)} & \text{if} \quad \theta > c. \end{cases}$$

For PGG:

$$\lim_{N\to+\infty} \frac{1-e^{(N-3)x}}{1-e^{(N-1)x}} = \lim_{N\to+\infty} \frac{1-e^{(N-3)\beta cr\frac{(N-n)}{n(N-1)}}e^{\beta(\theta-c)(N-3)}}{1-e^{\beta cr\frac{(N-n)}{n}}e^{\beta(\theta-c)(N-1)}} = \begin{cases} 1 & \text{if} \quad \theta \leq c, \\ e^{-2(\theta-c)} & \text{if} \quad \theta > c. \end{cases}$$

It follows that for DG

$$\begin{aligned} \lim_{N\to+\infty} w(\theta) &= \begin{cases} 1+e^{\beta(\theta-c)} & \text{if} \quad \theta \leq c, \\ 1+e^{-\beta(\theta-c)} & \text{if} \quad \theta > c \end{cases} \\ &= 1+e^{-\beta|\theta-c|}. \end{aligned} \tag{37}$$

and for PGG

$$\begin{aligned} \lim_{N\to+\infty} w(\theta) &= \begin{cases} 1+e^{\beta(\theta-c)}e^{\beta c\frac{r}{n}} & \text{if} \quad \theta \leq c, \\ 1+e^{-\beta(\theta-c)}e^{\beta c\frac{r}{n}} & \text{if} \quad \theta > c \end{cases} \\ &= 1+e^{-\beta|\theta-c|}e^{\beta c\frac{r}{n}}. \end{aligned} \tag{38}$$

From Lemma 1.5, we deduce that

$$\lim_{N\to+\infty} \frac{\left(\sum_{j=1}^{N-1}\frac{1}{j}+\frac{1}{N-1}\right)}{\ln N+\gamma} = \lim_{N\to+\infty} \frac{\left(\sum_{j=1}^{N-1}\frac{1}{j}+1\right)}{\ln N+\gamma} = 1 \tag{39}$$

From (36), (37), (38) and (39) we obtain, for DG

$$\lim_{N\to+\infty} \frac{E_r(\theta)}{\frac{N^2\theta}{2}(\ln N+\gamma)} = 1+e^{-\beta|\theta-c|}.$$

and for PGG

$$\lim_{N\to+\infty} \frac{E_r(\theta)}{\frac{N^2\theta}{2}(\ln N+\gamma)} = 1+e^{-\beta|\theta-c|}e^{\beta c\frac{r}{n}}.$$

□

Proposition 1.12. *We have*

(i) (weak selection limit)

$$\lim_{\beta\to 0} E_r(\theta) = N^2\Big(\sum_{j=1}^{N-1}\frac{1}{j}\Big)\theta. \tag{40}$$

(ii) (large selection limit)

$$\lim_{\beta\to+\infty} E_r(\theta) = \begin{cases} \frac{N^2}{2}\theta\Big(\frac{1}{N-1}+H_N\Big) & \textit{for} \quad \theta < -\delta, \\ N^2\theta H_N & \textit{for} \quad \theta = -\delta, \\ \frac{N^2}{2}\theta\Big(1+H_N\Big) & \textit{for} \quad \theta > -\delta. \end{cases} \tag{41}$$

Proof. We recall that the total expected cost function is

$$E_r(\theta) = \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\left[\left(1+e^x+\ldots+e^{(N-2)x}\right)\sum_{j=1}^{N-1}\frac{1}{j}+\sum_{j=1}^{N-1}\frac{e^{(N-1-j)x}}{j}\right]$$
$$= \frac{N^2\theta}{2}\frac{\sum\limits_{j=0}^{N-1}\eta_j e^{jx}}{\sum\limits_{j=0}^{N-1}e^{jx}},$$

where

$$\eta_0 := \frac{1}{N-1}+H_N, \quad \eta_j := \frac{1}{N-j-1}+2H_N+\frac{1}{N-j}, \quad j=1,\ldots,N-2 \quad \text{and} \quad \eta_{N-1}=1+H_N.$$

We recall that $x=\beta(\theta+\delta)$. Since $\beta\to 0$ implies $x\to 0$, it follows from the formula of $E_r(\theta)$ that

$$\lim_{\beta\to 0} E_r(\theta) = N^2\Big(\sum_{j=1}^{N-1}\frac{1}{j}\Big)\theta.$$

Now we consider the limit $\beta\to+\infty$. If $\theta=-\delta$, then $x=0$. Hence we also have

$$\lim_{\beta\to+\infty} E_r(\theta) = N^2\theta\frac{\sum_{j=0}^{N-1}\eta_j}{N} = N^2\theta H_N.$$

If $\theta>-\delta$, then $\lim_{\beta\to+\infty}\left(e^{-j(\theta+\delta)}\right)^\beta = 0$ for all $1\le j\le N-2$. Hence

$$\lim_{\beta\to+\infty} E_r(\theta) = \frac{N^2\theta}{2}\lim_{\beta\to+\infty}\frac{\sum_{j=0}^{N-1}\eta_j\left(e^{j(\theta+\delta)}\right)^\beta}{\sum_{j=0}^{N-1}\left(e^{j(\theta+\delta)}\right)^\beta}$$
$$= \frac{N^2\theta}{2}\lim_{\beta\to+\infty}\frac{\sum_{j=0}^{N-1}\eta_j\left(e^{(j-N+1)(\theta+\delta)}\right)^\beta}{\sum_{j=0}^{N-1}\left(e^{(j-N+1)(\theta+\delta)}\right)^\beta}$$
$$= \frac{N^2\theta}{2}\frac{\eta_{N-1}}{1} = \frac{N^2\theta}{2}(1+H_N).$$

If $\theta<-\delta$, then $\lim_{\beta\to+\infty}\left(e^{j(\theta+\delta)}\right)^\beta = 0$ for all $j=1,\ldots,N-1$. Hence

$$\lim_{\beta\to+\infty} E_r(\theta) = \frac{N^2\theta}{2}\lim_{\beta\to+\infty}\frac{\sum_{j=0}^{N-1}\eta_j\left(e^{j(\theta+\delta)}\right)^\beta}{\sum_{j=0}^{N-1}\left(e^{j(\theta+\delta)}\right)^\beta}$$
$$= \frac{N^2\theta}{2}\frac{\eta_0}{1} = \frac{N^2}{2}\theta\Big(\frac{1}{N-1}+H_N\Big).$$

□

1.7 Phase transition

In this section, we prove Theorem 3.2 for reward incentive.

Proof of Theorem 3.2 for reward incentive. First we show the existence of phase transition (i.e., the existence of the threshold value β^*) and study the optimization problem $\min_{\theta\ge\theta_0} E_r$ when the selection is less than or equal the threshold value, $\beta\le\beta^*$. According to Lemma 1.3 we have

$$E_r'(\theta) = \frac{1}{g(x)^2}\left[f(x)g(x)-(x+\beta a)(f(x)g'(x)-f'(x)g(x))\right] = \frac{1}{g(x)^2}\left[Q(u)-(\log u+\beta a)uP(u)\right],$$

where $u = e^x$, $f(x), g(x), P(u)$ and $Q(u)$ are given in Lemma 1.3. By Proposition 1.6, P, which is a polynomial with positive leading coefficient, has a unique positive root $u_0 > 1$. Therefore for $0 < u \leq u_0$, $uP(u) < 0$ and hence $E_r'(\theta) \geq 0$ (since $Q(u) > 0$ and $x + \beta a > 0$). Consider now the case $u > u_0$ (thus $uP(u) > 0$). We write $E_r'(\theta)$ as

$$E_r'(\theta) = \frac{1}{g(x)^2} uP(u) \left[F(u) - \beta a\right],$$

where $F(u) = \frac{Q(u)}{uP(u)} - \log u$, which is also given in Lemma 1.3. By Proposition 1.8, $F(u)$ has a global minimizer on $(u_0, +\infty)$. Let F^* be the global minimum. Let $\beta^* := \frac{F^*}{a}$. Then for $\beta \leq \beta^*$, $\beta a \leq \beta^* a = F^* \leq F(u)$ for all $u > u_0$. Thus $F(u) - \beta a \leq 0$ for all $u > u_0$, which implies that $E'(\theta) \geq 0$ for all $u > u_0$ as well. Hence, for $\beta \leq \beta^*$, $E'(\theta) \geq 0$ for all θ and so, $\min_{\theta \geq \theta_0} E_r(\theta) = E_r(\theta_0)$ and the minimum is attained at $\theta = \theta_0$.

Now we study the optimization problem $\min_{\theta \geq \theta_0} E_r(\theta)$ when the selection is greater than the threshold value, $\beta > \beta^*$. According to Proposition 1.8, F' changes signs at least once when $u > u_0$. Thus $F(u)$ is non-monotonic and the equation $F(u) = \beta a$ has at least two roots which are larger than u_0 for all $\beta > \beta^*$. Hence $F(u) - \beta a$, thus $E_r'(\theta)$, changes sign at least twice for any $\beta > \beta^*$. For $N \leq N_0 = 100$, the equation $F(u) = \beta a$ has exactly two solutions $u_0 < u_1 < u_2$. Hence

$$F(u) - \beta a \begin{cases} > 0 & u > u_1, \\ < 0 & u_1 < u < u_2, \\ > 0 & u > u_2. \end{cases}$$

The statement of the main theorem then follows by setting $\theta_i := \frac{\log u_i}{\beta} + a,\ i = 1, 2.$ □

2 Detailed computations and proof: punishment incentive

In this section we present detailed computations and prove Theorems 3.1-3.2 for the case of punishment incentive. We will only sketch on the parts that are similar to the reward case and focus on the parts that are distinguish from the reward case.

2.1 The cost function and its derivative

Similarly as in the reward case, using Lemma 1.2 we obtain the expected total cost of interference for institutional punishment

$$\begin{aligned}
E_p(\theta) &= \frac{\theta}{2} \sum_{i=1}^{N-1} (n_{1,i} + n_{N-1,i})(N - i) \\
&= \frac{1}{2} \sum_{j=1}^{N-1} \frac{N^2}{(N-j)j} \Big((W^{-1})_{1j} + (W^{-1})_{N-1,j} \Big) (N - j)\theta \\
&= \frac{N^2 \theta (1 + e^x)}{2(e^{Nx} - 1)} \sum_{j=1}^{N-1} \frac{e^{(N-1)x} - e^{(j-1)x} + e^{jx} - 1}{j} \\
&= \frac{N^2 \theta (1 + e^x)}{2(e^{Nx} - 1)} \Big[(e^{(N-1)x} - 1) \sum_{j=1}^{N-1} \frac{1}{j} + (e^x - 1) \sum_{j=1}^{N-1} \frac{e^{(j-1)x}}{j} \Big] \\
&= \frac{N^2 \theta (1 + e^x)}{2(1 + e^x + \ldots + e^{(N-1)x})} \Big[(1 + e^x + \ldots + e^{(N-2)x}) \sum_{j=1}^{N-1} \frac{1}{j} + \sum_{j=1}^{N-1} \frac{e^{(j-1)x}}{j} \Big] \\
&:= \frac{N^2 \theta}{2} \frac{\hat{f}(x)}{g(x)},
\end{aligned} \tag{42}$$

where $g(x) = 1 + e^x + \ldots + e^{(N-1)x}$ is the same as in the reward case, and

$$\hat{f}(x) = (1+e^x)\Big[\big(1 + e^x + \ldots + e^{(N-2)x}\big)H_N + \sum_{j=1}^{N-1} \frac{e^{(j-1)x}}{j}\Big].$$

The derivative of E_p with respect to θ is

$$E_p'(\theta) = \frac{N^2}{2}\frac{1}{g(x)^2}\Big[\hat{f}(x)g(x) - (x+\beta a)(\hat{f}(x)g'(x) - \hat{f}'(x)g(x))\Big]. \tag{43}$$

Using again the notation $u = e^x$, by similar computations as in the reward case, we have

$$\hat{f}(x)g(x) - \hat{f}'(x)g(x) = u\hat{P}(u), \quad \hat{f}(x)g(x) = \hat{Q}(u),$$

where

$$\begin{aligned}\hat{P}(u) := (1+u)\Bigg[\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{1+j})u^j\Big)\Big(\sum_{j=1}^{N-1} ju^{j-1}\Big) - \Big(\sum_{j=1}^{N-2}\Big(H_N + \frac{1}{1+j}\Big)ju^{j-1}\Big)\Big(\sum_{j=0}^{N-1} u^j\Big)\Bigg] \\ - \Big(\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{1+j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big)\end{aligned} \tag{44}$$

and

$$\hat{Q}(u) := (1+u)\Big(\sum_{j=0}^{N-2}(H_N + \frac{1}{j+1})u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big). \tag{45}$$

If $\hat{f}(x)g(x) - \hat{f}'(x)g(x) \le 0$ then $E_p'(\theta) > 0$. We consider the case $\hat{f}(x)g(x) - \hat{f}'(x)g(x) > 0$, and write $E_p'(\theta)$ as

$$E_p'(\theta) = \frac{N^2}{2}\frac{1}{g(x)^2}(\hat{f}(x)g(x) - \hat{f}'(x)g(x))\Big(\hat{F}(u) - \beta a\Big), \tag{46}$$

where

$$\hat{F}(u) := \frac{\hat{Q}(u)}{u\hat{P}(u)} - \log(u). \tag{47}$$

2.2 Concrete examples of small populations

2.3 The polynomial $\hat{P}$

The following proposition establishes interesting relationships between the polynomials P and $\hat{P}$ as well as between Q and $\hat{Q}$. These relationships enable us to obtain properties of the polynomials $\hat{P}$ and $\hat{Q}$ from P and Q without the need to calculate their coefficients, which significantly reduces the complexity of the analysis.

Proposition 2.1. *We have*

$$P(u) = -u^{2N-4}\hat{P}\Big(\frac{1}{u}\Big) \quad \textit{and} \quad Q(u) = u^{2N-2}\hat{Q}\Big(\frac{1}{u}\Big) \tag{48}$$

or equivalently

$$\hat{P}(u) = -u^{2N-4}P\Big(\frac{1}{u}\Big) \quad \textit{and} \quad \hat{Q}(u) = u^{2N-2}Q\Big(\frac{1}{u}\Big). \tag{49}$$

As a consequence, since P has a unique positive root according to Proposition 1.6, $\hat{P}$ also has a unique positive root.

Proof. By change of index $\hat{j} := N - 2 - j$, we have

(i)

$$\sum_{j=0}^{N-2}\Big(H_N+\frac{1}{N-1-j}\Big)u^j=\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)u^{N-2-\hat{j}}$$
$$=u^{N-2}\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)\Big(\frac{1}{u}\Big)^{\hat{j}}$$

(ii)

$$\sum_{j=0}^{N-2}\Big(H_N+\frac{1}{N-1-j}\Big)ju^{j-1}=\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)(N-2-\hat{j})u^{N-3-\hat{j}}$$
$$=u^{N-4}\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)(N-2-\hat{j})\Big(\frac{1}{u}\Big)^{\hat{j}-1}.$$

By change of index $\hat{j}:=N-1-j$ we have

(a)

$$\sum_{j=0}^{N-1}ju^{j-1}=\sum_{\hat{j}=0}^{N-1}(N-1-\hat{j})u^{N-2-\hat{j}}=u^{N-3}\sum_{\hat{j}=0}^{N-1}(N-1-\hat{j})\Big(\frac{1}{u}\Big)^{\hat{j}-1}$$

(b)

$$\sum_{j=0}^{N-1}u^j=\sum_{\hat{j}=0}^{N-1}u^{N-1-\hat{j}}=u^{N-1}\sum_{\hat{j}=0}^{N-1}\Big(\frac{1}{u}\Big)^{\hat{j}}$$

Therefore, by denoting

$$v:=\frac{1}{u},\quad \hat{a}_j:=H_N+\frac{1}{\hat{j}+1}$$

$$
\begin{aligned}
P(u) &= (1+u)\Big[\Big(\sum_{j=0}^{N-2}(H_N+\frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=1}^{N-1}ju^{j-1}\Big)-\Big(\sum_{j=1}^{N-2}\Big(H_N+\frac{1}{N-1-j}\Big)ju^{j-1}\Big)\Big(\sum_{j=0}^{N-1}u^j\Big)\Big]\\
&\quad-\Big(\sum_{j=0}^{N-2}\Big(H_N+\frac{1}{N-1-j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1}u^j\Big)\\
&= u^{2N-4}\Big(1+\frac{1}{u}\Big)\Big[\Big(\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\Big(\sum_{\hat{j}=0}^{N-1}(N-1-\hat{j})\Big(\frac{1}{u}\Big)^{\hat{j}-1}\Big)\\
&\qquad\qquad-\Big(\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)(N-2-\hat{j})\Big(\frac{1}{u}\Big)^{\hat{j}-1}\Big)\Big(\sum_{\hat{j}=0}^{N-1}\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\Big]\\
&\quad-u^{2N-3}\Big(\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\Big(\sum_{\hat{j}=0}^{N-1}\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\\
&= u^{2N-4}\Big\{(1+v)\Big(\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big[(N-1)\sum_{j=0}^{N-1}v^{j-1}-\sum_{j=0}^{N-1}jv^{j-1}\Big]\\
&\qquad\qquad-\Big[(N-2)\sum_{j=0}^{N-2}\hat{a}_jv^{j-1}-\sum_{j=0}^{N-2}a_jjv^{j-1}\Big]\Big(\sum_{j=0}^{N-1}v^j\Big)\Big)-\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-1}v^{j-1}\Big)\Big\}\\
&= u^{2N-4}\Big\{(1+v)\Big[\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-1}v^{j-1}\Big)-\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-2}jv^{j-1}\Big)+\Big(\sum_{j=0}^{N-2}\hat{a}_jjv^{j-1}\Big)\Big(\sum_{j=0}^{N-1}v^j\Big)\Big]\\
&\qquad\qquad-\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-1}v^{j-1}\Big)\Big\}\\
&= u^{2N-4}\Big\{(1+v)\Big[-\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-2}jv^{j-1}\Big)+\Big(\sum_{j=0}^{N-2}\hat{a}_jjv^{j-1}\Big)\Big(\sum_{j=0}^{N-1}v^j\Big)\Big]\\
&\qquad\qquad+\Big(\sum_{j=0}^{N-2}\hat{a}_jv^j\Big)\Big(\sum_{j=0}^{N-1}v^j\Big)\Big\}\Big\}\\
&= -u^{2N-4}\hat{P}(v)\\
&= -u^{2N-4}\hat{P}\Big(\frac{1}{u}\Big).
\end{aligned}
$$

Similarly for $Q(u)$, we obtain

$$
\begin{aligned}
Q(u) &= (1+u)\Big(\sum_{j=0}^{N-2}(H_N+\frac{1}{N-1-j})u^j\Big)\Big(\sum_{j=0}^{N-1}u^j\Big)\\
&= u^{2N-2}\Big(1+\frac{1}{u}\Big)\Big(\sum_{\hat{j}=0}^{N-2}\Big(H_N+\frac{1}{\hat{j}+1}\Big)\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\Big(\sum_{\hat{j}=0}^{N-1}\Big(\frac{1}{u}\Big)^{\hat{j}}\Big)\\
&= u^{2N-2}\hat{Q}\Big(\frac{1}{u}\Big).
\end{aligned}
$$

□

The following lemma, which is the counter-part of Lemma 1.7, establishes a relation between $\hat{P}$ and $\hat{Q}$. It is interesting to notice the appearance of the factor $\frac{3}{4(N-1)}$ on the right-hand side of (50) below.

Lemma 2.2. *We have*

$$\hat{Q}(u) \geq \frac{3}{4(N-1)}(1+u)u\hat{P}(u). \tag{50}$$

Proof. It follows from Proposition 2.1 that $\hat{p}_k = -p_{2N-4-k}$. Hence from Proposition 1.6 we obtain

$$\hat{p}_k = \begin{cases} -(H_N + \frac{1}{2}), \quad k = 0, \\ -(4k+7) + (k+3)H_N - (2k+4)\sum_{j=k+3}^{N-1} \frac{1}{j} + \frac{1}{k+2} \quad 1 \leq k \leq N-4, \\ -4N + 5 + \frac{1}{N-1} + NH_N, \quad k = N-3, \\ 2NH_N - 4(N-1), \quad k = N-2, \\ -8N + 4(k+3) + (2k+4)\sum_{j=k+3-N}^{N-1} \frac{1}{j} + \frac{2N-3-k}{k+2-N} + (2N-k-3)H_N, \quad N-1 \leq k \leq 2N-5, \\ H_N + \frac{1}{2}, \quad k = 2N-4. \end{cases}$$

The statement (50) is equivalent to

$$\sum_{j=0}^{N-2}\Big(H_N + \frac{1}{1+j}\Big)u^j\Big)\Big(\sum_{j=0}^{N-1} u^j\Big) = \sum_{k=0}^{2N-3}\Big(\sum_{j=\max(0,k-N+1)}^{\min(N-2,k)} \hat{a}_j\Big)u^k \geq \frac{3}{4(N-1)}u\hat{P}(u), \tag{51}$$

which we now prove. Let

$$\bar{h}_k := \sum_{j=\max(0,k-N+1)}^{\min(N-2,k)} \hat{a}_j = \begin{cases} \sum_{j=0}^{k} \hat{a}_j & 0 \leq k \leq N-2, \\ \sum_{j=k-N+1}^{N-2} \hat{a}_j & N-1 \leq k \leq 2N-3 \end{cases}$$
$$= \begin{cases} (k+1)H_N + \sum_{j=0}^{k} \frac{1}{j+1} & 0 \leq k \leq N-2, \\ (2N-k-2)H_N + \sum_{j=k-N+1}^{N-2} \frac{1}{j+1} & N-1 \leq k \leq 2N-3 \end{cases}$$

To prove (51) we will prove a slightly stronger statement that $\bar{h}_{k+1} \geq \frac{1}{2}\hat{p}_k$ for $k = 0, \ldots, N-2$ and $k = 2N-4$, and that $\bar{h}_{k+1} \geq \frac{3}{4(N-1)}\hat{p}_k$ for $k = N-1, \ldots, 2N-5$.

For $k = 0 : \bar{h}_1 = 2H_N + 1 + 3/2 > -\frac{1}{2}(H_N + 1/2)$.

For $1 \leq k \leq N-4$, we have

$$\bar{h}_{k+1} - \frac{1}{2}\hat{p}_k = (k+2)H_N + \sum_{j=0}^{k+1}\frac{1}{j+1} + \frac{1}{2}\Big((4k+7) - (k+3)H_N + (2k+4)\sum_{j=k+3}^{N-1}\frac{1}{j} - \frac{1}{k+2}\Big)$$
$$= (k+1)(H_N - H_{k+3}) + \frac{(4k+7)}{2} + \frac{k+3}{2}H_N - \frac{1}{2(k+2)} > 0.$$

For $k = N-3$:

$$\bar{h}_{k+1} - \frac{1}{2}\hat{p}_k = (N-1)H_N + \sum_{j=0}^{N-2}\frac{1}{1+j} - \frac{1}{2}(-4N + 5 + \frac{1}{N-1} + NH_N)$$
$$= \frac{1}{2}((4N-5) + NH_N - \frac{1}{N-1}\Big) > 0.$$

For $k = N-2$

$$\bar{h}_{k+1} - \frac{1}{2}\hat{p}_k = (N-1)H_N + \sum_{j=0}^{N-2}\frac{1}{1+j} - \frac{1}{2}(2NH_N - 4(N-1))$$
$$= 2(N-1) > 0.$$

For $N-1 \le k \le 2N-5$. Let $\alpha > 1$ be chosen later. We have

$$\begin{aligned}
\bar{h}_{k+1} - \frac{1}{\alpha}\hat{p}_k &= (2N-k-3)H_N + \sum_{j=k+3-N}^{N-1} \frac{1}{j} \\
&\quad - \frac{1}{\alpha}\Big(-8N + 4(k+3) + (2k+4) \sum_{j=k+3-N}^{N-1} \frac{1}{j} + \frac{2N-3-k}{k+2-N} + (2N-k-3)H_N \Big) \\
&= (2N-k-3)H_N\Big(1-\frac{1}{\alpha}\Big) + \Big(1 - \frac{2(k+2)}{\alpha}\Big) \sum_{j=k+3-N}^{N-1} \frac{1}{j} - \frac{(2N-3-k)}{\alpha(k+2-N)} \\
&\ge (2N-k-3)\Big(1-\frac{1}{\alpha}\Big)H_N - \Big(\frac{2(k+2)}{\alpha} - 1\Big) \sum_{j=k+2-N}^{N-1} \frac{1}{j}.
\end{aligned}$$

We choose $\alpha > 1$ such that

$$(2N-k-3)\Big(1-\frac{1}{\alpha}\Big) \ge \Big(\frac{2(k+2)}{\alpha} - 1\Big) \quad \text{for all} \quad k = N-1, \dots, 2N-5.$$

The above condition is equivalent to the following condition

$$2N(\alpha-1) \ge (k+2)\alpha + (k+1) \quad \text{for all} \quad k = N-1, \dots, 2N-5.$$

Therefore we only need to choose $\alpha > 1$ such that the above inequality holds true for $k = 2N-5$, that is

$$2N(\alpha-1) \ge (2N-3)\alpha + (2N-4).$$

Hence $\alpha \ge \frac{4(N-1)}{3}$. Therefore, we obtain that for $N-1 \le k \le 2N-5$

$$\bar{h}_{k+1} \ge \frac{3}{4(N-1)}\hat{p}_k.$$

For $k = 2N-4$, we have

$$\bar{h}_{k+1} - \frac{1}{2}\hat{p}_k = H_N + \frac{1}{N-1} - \frac{1}{2}(H_N + \frac{1}{2}) = \frac{1}{2}H_N + \frac{1}{N-1} - \frac{1}{4} > 0.$$

□

Let $\hat{u}^0$ be the unique positive root of $\hat{P}$. Note that $\hat{u}^0 = \frac{1}{u^0}$, where u^0 is the unique positive root of P. We consider the minimisation problem

$$\min\{\hat{F}(u) : \quad u > \hat{u}^0\}, \tag{52}$$

where $\hat{F}$ is defined in (47). The following proposition is the counter-part of Proposition 1.8.

Proposition 2.3. *The minimisation problem (52) has a global minimizer. For $N \le N_0 = 100$ sufficiently small, it has a unique minimizer $\hat{u}^*$ and $\hat{F}$ is decreasing when $\hat{u}^0 < u < \hat{u}^*$ and is increasing when $u > \hat{u}^*$.*

Proof. The proof of this proposition is similar to that of Proposition 1.8 in the reward case. According to Lemma 2.2 we have

$$\hat{F}(u) \ge \frac{3}{4(N-1)}(1+u) - \log(u).$$

It implies that

$$\lim_{u\to+\infty} \hat{F}(u) = +\infty = \lim_{u\to\hat{u}_0^+} \hat{F}(u).$$

From this together with the fact that $\hat{F}$ is smooth on the interval $(\hat{u}^0, +\infty)$, we conclude that $\hat{F}$ has a minimizer on this domain. The rest of the proof is the same as that of Proposition 1.8 where P and Q are replaced by $\hat{P}$ and $\hat{Q}$, respectively and the unique positive root u^0 of P is replaced by that of $\hat{P}$ (i.e., $\hat{u}^0$).

□

2.4 Finite population estimates

Lemma 2.4. *It holds that*

$$\frac{N^2\theta}{2}\Big(H_N + \frac{1}{N-1}\Big) \leq E_p(\theta) \leq N(N-1)\theta\Big(H_N + 1\Big). \tag{53}$$

Proof. We recall that

$$E_p(\theta) = \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\Big[\big(1+e^x+\ldots+e^{(N-2)x}\big)\sum_{j=1}^{N-1}\frac{1}{j} + \sum_{j=1}^{N-1}\frac{e^{(j-1)x}}{j}\Big]. \tag{54}$$

Since we also have the following estimates

$$\frac{1}{N-1}(1+e^x+\ldots+e^{(N-2)x}) \leq \sum_{j=1}^{N-1}\frac{e^{(j-1)x}}{j} \leq (1+e^x+\ldots+e^{(N-2)x}),$$

we can proceed exactly as in the proof of Proposition 1.11 in the reward case to obtain the required estimates. □

2.5 Asymptotic limits

Proposition 2.5. *We have the following limits:*

(i) (Infinite-population limit)

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

(ii) (weak selection limit)

$$\lim_{\beta\to 0} E_p[(\theta) = N^2\theta H_N.$$

(iii) (large selection limit)

$$\lim_{\beta\to+\infty} E_p(\theta) = \begin{cases} \frac{N^2\theta}{2}\Big(1+H_N\Big) & \text{for} \quad \theta < -\delta, \\ N^2\theta H_N & \text{for} \quad \theta = -\delta, \\ \frac{N^2\theta}{2}\Big(H_N + \frac{1}{N-1}\Big) & \text{for} \quad \theta > -\delta. \end{cases}$$

Proof.

(i) We also have

$$\frac{N^2\theta}{2}\frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+\frac{1}{N-1}\Big) \leq E_p(\theta)$$
$$\leq \frac{N^2\theta}{2}\frac{(1+e^x)(1+\ldots+e^{(N-2)x})}{1+\ldots+e^{(N-1)x}}\Big(\sum_{j=1}^{N-1}\frac{1}{j}+1\Big)$$

Hence by proceeding exactly the same as in the reward case, we obtain the desired limit.

(ii) Since $\beta \to 0^+$ implies $x \to 0$, we have

$$\lim_{\beta\to 0^+} E_p(\theta) = N^2\theta\Big(\sum_{j=1}^{N-1}\frac{1}{j}\Big).$$

(iii) We have

$$E_p(\theta) = \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\Big[\big(1+e^x+\ldots+e^{(N-2)x}\big)\sum_{j=1}^{N-1}\frac{1}{j}+\sum_{j=1}^{N-1}\frac{e^{(j-1)x}}{j}\Big].$$
$$= \frac{N^2\theta}{2}\frac{\sum_{j=0}^{N-1}\hat{\eta}_j e^{jx}}{\sum_{j=0}^{N-1}e^{jx}},$$

where

$$\hat{\eta}_0 = H_N+1, \quad \hat{\eta}_j = 2H_N+\frac{1}{j}+\frac{1}{1+j} \quad \text{for } j=1,\ldots,N-2 \quad \text{and} \quad \hat{\eta}_{N-1} = H_N+\frac{1}{N-1}.$$

Proceeding similarly as in Proposition 1.12 we get

$$\lim_{\beta\to+\infty} E_p(\theta) = \begin{cases} \frac{N^2\theta}{2}\frac{\hat{\eta}_0}{1} = \frac{N^2\theta}{2}\Big(1+H_N\Big) & \text{for} \quad \theta<-\delta, \\ N^2\theta H_N \quad \text{for} \quad \theta=-\delta, \\ \frac{N^2\theta}{2}\frac{\hat{\eta}_{N-1}}{1} = \frac{N^2\theta}{2}\Big(H_N+\frac{1}{N-1}\Big) & \text{for} \quad \theta>-\delta. \end{cases}$$

□

2.6 Phase transition

Having obtained Proposition 2.3, the proof of Theorem 3.2 for the case of punishment can be proceeded in the exactly as in the reward case by replacing F^* by $\hat{F}^*$, which is the minimum value of $\hat{F}$ in the interval $(\hat{u}^0,+\infty)$ and β^* by β_p^*, where

$$\beta_p^* := \frac{\hat{F}^*}{a}. \tag{55}$$

Therefore we omit the details.

3 Proof of Theorem 3.4

In this section, we prove Theorem 3.4, that is to establish the relation on the difference between the reward and punishment costs.

Proof of Theorem 3.4. It follows from formulas of E_r and E_p that

$$(E_r-E_p)(\theta) = \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\sum_{j=1}^{N-1}\frac{e^{(N-1-j)x}-e^{(j-1)x}}{j}$$
$$= \frac{N^2\theta(1+e^x)}{2(1+e^x+\ldots+e^{(N-1)x})}\sum_{j=1}^{N-1}e^{(j-1)x}\Big[\frac{1}{N-j}-\frac{1}{j}\Big].$$

Hence the sign of $(E_r-E_p)(\theta)$ depends on the sign of the function

$$r(u) := \sum_{j=1}^{N-1}u^{(j-1)}\Big[\frac{1}{N-j}-\frac{1}{j}\Big]$$

for $u := e^x \in (0,\infty)$. $r(u)$ is a polynomial of degree $N-2$ with a positive leading coefficient. We have

$$r(0) = \frac{1}{N-1}-1<0, \qquad \lim_{u\to+\infty} r(u) = +\infty.$$

Moreover, the sequence of coefficients of r has one change of signs, which happens at $j = \lfloor N/2 \rfloor$. Thus, by Decartes's rule of signs, r has a unique positive solution, which is $u = 1$. Hence $r(u) < 0$ for $u \in (0, 1)$ while $r(u) > 0$ for $u \in (1, +\infty)$. As a consequence, $E_r(\theta) < E_p(\theta)$ for $u < 1$, that is for $\theta < -\delta$ and $E_r(\theta) > E_p(\theta)$ for $\theta > -\delta$.

Finally, we prove the last statement of Theorem 3.4. Suppose $\beta < \min\{\beta_r^*, \beta_p^*\}$. According to Theorem 3.2 we have

$$E_r^* = \min_{\theta \geq \theta_0} E_r(\theta) = E_r(\theta_0) \quad \text{and} \quad E_p^* = \min_{\theta \geq \theta_0} E_p(\theta) = E_p(\theta_0).$$

Thus

$$E_r^* - E_p^* = E_r(\theta_0) - E_p(\theta_0).$$

By definition of θ_0 we have

$$\theta_0 - (-\delta) = \frac{1}{(N-1)\beta} \log\Big(\frac{\omega}{1-\omega}\Big) = \begin{cases} < 0 & \text{if} \quad \omega < 0.5, \\ = 0 & \text{if} \quad \omega = 0.5, \\ > 0 & \text{if} \quad \omega > 0.5. \end{cases}$$

Therefore, according to the first statement of Theorem 3.4, we have

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

This completes the proof of Theorem 3.4. □

4 Explicit computations for some small N

In this section, for the sake of illustration, we will present explicit computations for some small N for the case of reward incentive.

Example 4.1. ($N = 3$). When $N = 3$, the total cost interference for the reward case is given by

$$\begin{aligned} E_r(\theta) &= \frac{9\theta(1+e^x)}{2(1+e^x+e^{2x})}\Big[(1+e^x)(1+1/2) + e^{2x}(e^{-x} + e^{-2x}/2)\Big] \\ &= \frac{9\theta}{4}\Big(5 + \frac{4e^x - 1}{1+e^x+e^{2x}}\Big). \end{aligned}$$

Note that since $x = \beta(\theta - a)$, $\frac{d}{d\theta}E(\theta) = \beta \frac{d}{dx}E(x)$.

$$\begin{aligned} \frac{4}{9}E_r'(\theta) &= \frac{1}{\beta}\Big(5 + \frac{4e^x - 1}{1+e^x+e^{2x}}\Big) + \theta\Big(\frac{4e^x}{1+e^x+e^{2x}} - \frac{(4e^x-1)(e^x+2e^{2x})}{(1+e^x+e^{2x})^2}\Big) \\ &= \frac{1}{\beta}\left[\Big(5 + \frac{4e^x - 1}{1+e^x+e^{2x}}\Big) + (x+\beta a)\Big(\frac{4e^x}{1+e^x+e^{2x}} - \frac{(4e^x-1)(e^x+2e^{2x})}{(1+e^x+e^{2x})^2}\Big)\right] \\ &= \frac{1}{\beta(1+u+u^2)^2}\left[(u+1)(u+4/5)(5u^2+5u+5) - (x+\beta a)u(4u^2-2u-5)\right] \end{aligned} \tag{56}$$

where $a = c + \frac{b}{N-1} > 0$. Note that $x + \beta a = \beta\theta > 0$.

(1) If $x \leq \log\Big(\frac{1+\sqrt{21}}{4}\Big)$, then $4u^2 - 2u - 5 \leq 0$. It follows from (56) that $E'(x) > 0$ for all β. Hence E is increasing for all β.

(2) If $x > \log\left(\frac{1+\sqrt{21}}{4}\right)$, then $4u^2 - 2u - 5 > 0$. Consider the function

$$F(u) := \frac{(u+1)(5u+4)(u^2+u+1)}{u(4u^2-2u-5)} - \log(u) \qquad \text{for } \ u > \frac{1+\sqrt{21}}{4} =: u^0.$$

Then

$$E_r'(x) = \frac{9}{4}\frac{u(4u^2-2u-5)}{\beta(1+u+u^2)^2}\Big[F(u) - (\beta a)\Big].$$

We have $\min_{u>u^0} F(u) = 10.9291 = f^*$ at $u^* = 4.29712$. Moreover, $f(u)$ is decreasing when $u < u^*$ and is increasing when $u > u^*$. The number of solutions of the equation $F(u) = \beta a$ and the sign of $E'(x)$ depends on the value of βa.

(i) If $\beta a < f^*$, then $F(u) = \beta a$ has no solution and $E'(x) > 0$. Hence E is increasing.

(ii) If $\beta a = f^*$, then $F(u) = \beta a$ has a unique solution, and $E'(x) \geq 0$ and E is non-decreasing.

(iii) If $\beta a > f^*$, then $F(u) = \beta a$ has two solutions $(1+\sqrt{21})/4 < u_1 < u_2$.

$$E_r'(\theta) \begin{cases} > 0 & u < u_1, \\ < 0 & u_1 < u < u_2, \\ > 0 & u > u_2. \end{cases}$$

Thus E_r is increasing when $u < u_1$, is decreasing when $u_1 < u < u_2$ and is increasing again when $u > u_2$.

Algorithm for $N = 3$

1. Compute

$$\delta = \begin{cases} -(c + \frac{b}{N-1}) & \text{PD games}, \\ -c\Big(1 - \frac{r(N-n)}{n(N-1)}\Big) & \text{PGG games} \end{cases} \tag{57}$$

2. Compute $\theta_0 = \frac{1}{(N-1)\beta}\log\left(\frac{\omega}{1-\omega}\right) - \delta$;

3. Compute $\beta^* = -\frac{f^*}{\delta} = -\frac{10.9291}{\delta}$.

4. If $\beta \leq \beta^*$ then

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

5. If $\beta > \beta^*$

   (a) Compute $\theta_2 = \frac{\log u_2}{\beta} - \delta$ where u_2 is the largest zero of the equation $F(u) + \beta\delta = 0$.

   (b) If $\theta_0 \geq \theta_2$: $\theta^* = \theta_0, \quad \min E(\theta) = E(\theta_0)$;

   (c) if $\theta_0 < \theta_2$, compare $E(\theta_0)$ and $E(\theta_2)$: if $E(\theta_0) \leq E(\theta_2)$: $\theta^* = \theta_0, \quad \min E(\theta) = E(\theta_0)$; if $E(\theta_2) < E(\theta_0)$: $\theta^* = \theta_2, \quad \min E(\theta) = E(\theta_2)$.

Example 4.2. ($N = 4$) When $N = 4$, the total cost function is $E_r(\theta) = 8\theta\frac{f(x)}{g(x)}$, where

$$\begin{aligned} f(x) &= (1+e^x)\Big[\frac{11}{6}(1+e^x+e^{2x}) + e^{3x}(e^{-x}+e^{-2x}/2+e^{-3x}/3)\Big] \\ &= (1+e^x)(\frac{13}{6} + \frac{14}{6}e^x + \frac{17}{6}e^{2x}) \\ &= (1+u)\Big(13/6 + 14/6u + 17/6u^2\Big), \\ g(x) &= 1 + e^x + e^{2x} + e^{3x} = 1 + u + u^2 + u^3. \end{aligned}$$

In this case,

$$F(u) = \frac{1}{2}\frac{(13+14u+17u^2)(1+u+u^2+u^3)}{u(1+u)(7u^2-4u-7)} - \log(u)$$

Algorithm for $N = 4$

1. Compute
$$\delta = \begin{cases} -(c + \frac{b}{N-1}) & \text{PD games,} \\ -c\Big(1 - \frac{r(N-n)}{n(N-1)}\Big) & \text{PGG games} \end{cases} \tag{58}$$

2. Compute $\theta_0 = \frac{1}{(N-1)\beta} \log\left(\frac{\omega}{1-\omega}\right) - \delta$;

3. Compute $u_0 > 0$ that solves $7u^2 - 4u - 7 = 0$; that is $u_0 = 3.4697$;

4. Compute $f^* = \min\{F(u) : u > u_0\}$, which gives $f^* = 6.64711$;

5. Compute $\beta^* = -\frac{f^*}{\delta}$.

6. If $\beta \leq \beta^*$ then
$$\theta = \theta_0, \quad \min E(\theta) = E(\theta_0).$$

7. If $\beta > \beta^*$
   (a) Compute $\theta_2 = \frac{\log u_2}{\beta} - \delta$ where u_2 is the largest zero of the equation $F(u) + \beta\delta = 0$.
   (b) if $E_r(\theta_0) \leq E_r(\theta_2)$: $\theta^* = \theta_0, \quad \min E_r(\theta) = E(\theta_0)$;
   (c) if $E_r(\theta_2) < E_r(\theta_0)$: $\theta^* = \theta_2, \quad \min E_r(\theta) = E_r(\theta_2)$.

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