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Algebraic Expressions for Stochastic Dynamics in Populations: From Strategy Profile to Aggregate State

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Appendix A Preliminaries

For ease of statement, the notations used in this study are listed in Table A1.

Table A1 Notations used in this study

Symbol	Meaning	Symbol	Meaning
$\mathbb{R}$	The set of real numbers	$\mathbb{R}^n_{\geqslant 0}$	The set of n-dimensional non-negative real column vectors
$\mathbb{N}$	The set $\{0, 1, 2, \dots\}$	$[i : j]$	The set $\{k \in \mathbb{N} : i \leqslant k \leqslant j\}$
$\lvert N \rvert$	The cardinality of the set N	$N \backslash M$	The set $\{i : i \in N, i \notin M\}$
$\mathfrak{S}_N$	The symmetric group on set N	$\mathcal{M}_{m\times n}$	The set of $m \times n$ matrices
$A^\top$	The transpose of matrix A	$A_{i,j}$	The (i, j)-th entry of matrix A
$\mathrm{Col}(A)$	The set of columns of matrix A	$\mathrm{Col}_i(A)$	The i-th column of matrix A
I_m	The $m \times m$ identity matrix	δ^i_m	The column vector $\mathrm{Col}_i(I_m)$
Δ_m	The set $\mathrm{Col}(I_m)$	$\mathcal{L}_{m\times n}$	The set $\{A \in \mathcal{M}_{m\times n} : \mathrm{Col}(A) \subset \Delta_m\}$
$\mathbf{1}_n$	The column vector $[1, 1, \dots, 1]^\top \in \mathbb{R}^n$	$\mathbf{0}_n$	The column vector $[0, 0, \dots, 0]^\top \in \mathbb{R}^n$
Υ_m	The set $\{\mu \in \mathbb{R}^m_{\geqslant 0} : \mathbf{1}^\top_m \mu = 1\}$	Υ^n_m	The set $\{[\mu_1, \dots, \mu_m]^\top \in \mathbb{N}^m : \mathbf{1}^\top_m \mu = n\}$
$\mathbb{P}\mathrm{rob}(\cdot\vert\cdot)$	Conditional probability	$\mathbb{E}(\cdot\vert\cdot)$	Conditional expectation
$\sim$	An equivalence relation	k	$\prod_{i=1}^n k_i$

Definition 1. [1] The semi-tensor product of matrices $A \in \mathcal{M}^{m\times n}$, $B \in \mathcal{M}^{p\times q}$ is

$$A \ltimes B = (A \otimes I_{l/n})(B \otimes I_{l/p}),$$

where $\otimes$ is Kronecker product, and $l = \mathrm{lcm}(n, p)$ is the least common multiple of n and p.

Lemma A1. [2] Let $f : \prod_{i=1}^n \Delta_{k_i} \to \mathbb{R}$ be a pseudo-logical function. Then there exists a unique k-dimensional row vector V_f such that

$$f(a_1, a_2, \cdots, a_n) = V_f \ltimes_{i=1}^n a_i,$$

where $a_i \in \Delta_{k_i}, i \in [1 : n]$ denotes the k_i-dimensional logical vector, and V_f is termed as the structure vector of f.

Lemma A2. [3] Let $x_i \in \Upsilon_m,\ i = [1 : n]$. Define the projection matrices as $\Phi_i = \mathbf{1}^\top_{m^{i-1}} \otimes I_m \otimes \mathbf{1}^\top_{m^{n-i}},\ i \in [1 : n]$. Then, for each $i \in [1 : n]$, the following relation holds:

$$\Phi_i \ltimes_{j=1}^n x_j = x_i.$$

Definition 2. [4] For column vectors $a_i \in \Delta_{k_i},\ i \in [1 : n]$, the matrix $W_\sigma \in \mathcal{M}_{k\times k},\ \sigma \in \mathfrak{S}_N$ is called σ-permutation matrix if

$$W_\sigma \ltimes_{i=1}^n a_i = \ltimes_{i=1}^n a_{\sigma(i)}. \tag{A1}$$

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Lemma A3. [4] For column vectors $a_i \in \Delta_{k_i},\ i \in [1:n]$, the σ-permutation matrix $W_\sigma \in \mathcal{M}_{k\times k}$ satisfies (A1) if and only if

$$\begin{aligned} W_\sigma = [&\delta^1_{k_{\sigma(1)}} \ltimes \delta^1_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(n)}},\ \delta^2_{k_{\sigma(1)}} \ltimes \delta^1_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(n)}},\ \cdots,\ \delta^{k_{\sigma(1)}}_{k_{\sigma(1)}} \ltimes \delta^1_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(n)}},\\ &\delta^1_{k_{\sigma(1)}} \ltimes \delta^2_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(n)}},\ \delta^2_{k_{\sigma(1)}} \ltimes \delta^2_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(1)}},\ \cdots,\ \delta^{k_{\sigma(1)}}_{k_{\sigma(1)}} \ltimes \delta^2_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^1_{k_{\sigma(n)}},\\ &\cdots,\\ &\delta^1_{k_{\sigma(1)}} \ltimes \delta^{k_{\sigma(2)}}_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^{k_{\sigma(n)}}_{k_{\sigma(n)}},\ \delta^2_{k_{\sigma(1)}} \ltimes \delta^{k_{\sigma(2)}}_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^{k_{\sigma(n)}}_{k_{\sigma(n)}},\ \cdots,\ \delta^{k_{\sigma(1)}}_{k_{\sigma(1)}} \ltimes \delta^{k_{\sigma(2)}}_{k_{\sigma(2)}} \ltimes \cdots \ltimes \delta^{k_{\sigma(n)}}_{k_{\sigma(n)}}]. \end{aligned}$$

Lemma A4. [5] Let $\sigma \in \mathfrak{S}_N$. The σ-permutation matrix $W_\sigma \in \mathcal{M}_{k\times k}$ satisfies the following property:

$$W_{\sigma^{-1}} = W_\sigma^{-1}, \quad W_\sigma^\top = W_\sigma^{-1}.$$

Definition 3. [6] Let $\mathfrak{S}_N$ be the set of all permutations of N equipped with composition of mappings, called the symmetric group on N. The pointwise stabilizer of subset $M \subset N$ in $\mathfrak{S}_N$ is defined as

$$\mathfrak{S}_M = \{\sigma \in \mathfrak{S}_N : \sigma(i) = i,\ i \in M\}.$$

Lemma A5. [7] Let $\{s(t)\}_{t\in\mathbb{N}}$ be a Markov process on state space $Z = \{1, 2, \cdots, z\}$ with a transition probability matrix P, where $P_{\tilde{s},s}$ denotes the transition probability from state s to state $\tilde{s}$. The process $\{s(t)\}_{t\in\mathbb{N}}$ is lumpable with respect to the partition $S = \{S_1, S_2, \cdots, S_\tau\}$ if and only if, for any $S_m \in S$, and any $s, \tilde{s} \in S_m$,

$$\mathbb{P}\text{rob}\big(S_n|s\big) = \mathbb{P}\text{rob}\big(S_n|\tilde{s}\big), \quad S_n \in S,$$

where $\mathbb{P}\text{rob}\big(S_n|s\big) = \sum_{\tilde{s}\in S_n} P_{\tilde{s},s}$ denotes the probability of moving from the state s to the subset S_n. In this case, the common value $\tilde{P}_{S_n,S_m} = \mathbb{P}\text{rob}\big(S_n|s\big),\ s \in S_m$ is well-defined and constitutes the transition probability for the aggregated process after aggregating $\{s(t)\}_{t\in\mathbb{N}}$ with respect to the partition S.

Remark 1. Lumpability guarantees that the aggregated process is also a Markov process, referred to as the aggregated Markov process [7].

Appendix B Remark of Equation (2)

Remark 2. Given a strategy profile $s \in \Delta_{m^n}$, the conditional distribution of the next profile, denoted by $r \in \Upsilon_{m^n}$, can be expressed as

$$\begin{aligned} r &= \mathbb{E}\big(s(t+1)|s(t) = s\big)\\ &= \mathbb{E}(F^\Pi_\omega s|s)\\ &= \sum_{\kappa=1}^{m^n-1} \delta^\kappa_{m^n}\big((\Gamma s)_{\kappa+1} - (\Gamma s)_\kappa\big) + \delta^{m^n}_{m^n}\big(1 - (\Gamma s)_{m^n}\big)\\ &= \sum_{\kappa=1}^{m^n-1} \delta^\kappa_{m^n}\big((U\Pi s)_{\kappa+1} - (U\Pi s)_\kappa\big) + \delta^{m^n}_{m^n}\big(\mathbf{1}^\top_{m^n}\Pi s - (U\Pi s)_{m^n}\big)\\ &= \sum_{\kappa=1}^{m^n-1} \delta^\kappa_{m^n}\big((\delta^{\kappa+1}_{m^n})^\top U\Pi s - (\delta^\kappa_{m^n})^\top U\Pi s)\big) + \delta^{m^n}_{m^n}\big(\mathbf{1}^\top_{m^n}\Pi s - (\delta^{m^n}_{m^n})^\top U\Pi s\big)\\ &= \sum_{\kappa=1}^{m^n-1} \delta^\kappa_{m^n}\big((\delta^{\kappa+1}_{m^n})^\top - (\delta^\kappa_{m^n})^\top\big)U\Pi s + \delta^{m^n}_{m^n}\big(\mathbf{1}^\top_{m^n} - (\delta^{m^n}_{m^n})^\top\big)U\Pi s\\ &= \sum_{\kappa=1}^{m^n} \delta^\kappa_{m^n}\big(\delta^\kappa_{m^n}\big)^\top\Pi s\\ &= \Pi s. \end{aligned}$$

Consequently, $\{s(t),\ t \in \mathbb{N}\}$ is governed by the transition rule:

$$P\big(s(t+1)|s(t)\big) = s(t+1)^\top\Pi s(t), \tag{B1}$$

which is a probabilistic m^n-valued logical dynamic system [3]. Furthermore, let $r(t) = \mathbb{P}\text{rob}\big(s(t)|s(0)\big) \in \Upsilon_{m^n}$ be the probability distribution of $s(t)$. Then, we have $r(t+1) = \Pi r(t),\ t \in \mathbb{N}$, with the initial condition $r(0) = s(0)$.

Alternatively, instead of the transition rule (B1), the same dynamics can be written as a stochastic logical dynamics $s(t+1) = F^\Pi_{\omega(t)}s(t),\ t \in \mathbb{N}$, where $\omega(t)$ acts as a switching signal [8].

Appendix C Proof of Lemma 1

Given a permutation $\sigma \in \mathfrak{S}_N$ and arbitrary states $s, \tilde{s} \in \Delta_{m^n}$, we have

$$P\big(\sigma(\tilde{s})|\sigma(s)\big) = \sigma(s)^\top \Pi^\top \sigma(\tilde{s}) = \big(W_\sigma s\big)^\top \Pi^\top W_\sigma \tilde{s} = s^\top W_\sigma^\top \Pi^\top W_\sigma \tilde{s}, \tag{C1}$$

where W_σ is the σ-permutation matrix. Therefore, for any permutation $\sigma \in \mathfrak{S}_N$,

$$P\big(\sigma(\tilde{s})|\sigma(s)\big) = P\big(\tilde{s}|s\big),\ s, \tilde{s} \in \Delta_{m^n} \quad \Longleftrightarrow \quad s^\top W_\sigma^\top \Pi^\top W_\sigma \tilde{s} = s^\top \Pi^\top \tilde{s},\ s, \tilde{s} \in \Delta_{m^n} \quad \Longleftrightarrow \quad W_\sigma^\top \Pi W_\sigma = \Pi.$$

This completes the proof.

Appendix D Proof of Lemma 2

By Lemma A2, each s_i can be rewritten via the projection matrix, which yields:

$$\mu^s = \sum_{i=1}^{n} s_i = \sum_{i=1}^{n} \Phi_i \ltimes_{j=1}^{n} s_j = V_\mu \ltimes_{j=1}^{n} s_j.$$

For the m-dimensional pseudo-logical function $\mu : \Delta_{m^n} \to \Upsilon_m^n$ that satisfies $\mu(s) = \mu^s$, the uniqueness of V_μ is a direct consequence of Lemma A1. This concludes the proof.

Appendix E Proof of Lemma 3

Necessity $\Longrightarrow$: For each $k \in \mathcal{D}$, define $N_k(s) = \{i \in N : s_i = \delta_m^k\}$, which denotes the set of players using δ_m^k in the profile s. Since $|N_k(s)| = \mu_k^s$, the condition $\mu_k^s = \mu_k^{\tilde{s}}$ implies that

$$|N_k(\tilde{s})| = |N_k(s)|.$$

Define functions $f_k : N_k(s) \to N_k(\tilde{s}),\ k \in \mathcal{D}$ such that

$$f_k(i_\kappa) = \tilde{i}_\kappa, \quad \kappa \in [1 : \mu_k^s],$$

where $i_\kappa,\ \tilde{i}_\kappa$ denote the κ-th largest elements in the sets $N_k(s),\ N_k(\tilde{s})$, respectively. By construction, the function f_k is bijective. Then a bijective function $\sigma : N \to N$ is introduced by setting

$$\sigma(i) = f_k(i), \quad i \in N_k(s), \quad k \in \mathcal{D},$$

which corresponds to a permutation on N satisfying $s_i = \tilde{s}_{\sigma(i)}$. Then we have

$$\ltimes_{i=1}^{n} s_i = \ltimes_{i=1}^{n} \tilde{s}_{\sigma(i)} = W_\sigma \tilde{s}. \tag{E1}$$

Rearranging (E1) gives

$$\tilde{s} = W_\sigma^{-1} s = W_{\sigma^{-1}} s,$$

where the last equality follows directly from Lemma A4, and the proof of the necessity is finished.

Sufficiency $\Longleftarrow$: Given that every permutation $\sigma \in \mathfrak{S}_N$ can be expressed as the composition of at most $\lfloor n^2/4 \rfloor$ adjacent transpositions [9], W_σ can be decomposed into as a series of adjacent transpositions:

$$W_\sigma = \prod_{k=1}^{k_{\max}} W_{\sigma_{[i_k \leftrightarrow i_k+1]}}, \quad k_{\max} \leqslant \lfloor n^2/4 \rfloor,$$

where $\sigma_{[i \leftrightarrow i+1]}$ denotes the adjacent transposition that interchanges i and $i+1$, defined by

$$\sigma_{[i \leftrightarrow i+1]}(j) = \begin{cases} i+1, & j = i, \\ i, & j = i+1, \\ j, & \text{otherwise}. \end{cases}$$

Based on this assertion, it is enough to prove that

$$V_\mu W_{\sigma_{[i \leftrightarrow i+1]}} = V_\mu, \quad i \in [1 : n-1].$$

Following Lemma A3, the expression for $W_{\sigma_{[i \leftrightarrow i+1]}}$ is given by

$$W_{\sigma_{[i \leftrightarrow i+1]}} = I_{m^{i-1}} \otimes W_{[m,m]} \otimes I_{m^{n-1-i}}, \tag{E2}$$

where $W_{[m,m]} = [\delta_m^1 \ltimes \delta_m^1, \delta_m^2 \ltimes \delta_m^1, \cdots, \delta_m^m \ltimes \delta_m^1, \cdots, \delta_m^m \ltimes \delta_m^2, \cdots, \delta_m^m \ltimes \delta_m^m]$ a special permutation matrix that exchanges factors s_i and s_{i+1} in $s_i \ltimes s_{i+1}$, referred to as the swap matrix [2].

For $i \in [1:n-1]$, by substituting (E2) into $V_\mu = \sum_{j=1}^{n} \mathbf{1}_{m^{j-1}}^\top \otimes I_m \otimes \mathbf{1}_{m^{n-j}}^\top$, we get

$$\begin{aligned}
V_\mu W_{\sigma_{[i\leftrightarrow i+1]}} &= \sum_{j=1}^{n} \left(\mathbf{1}_{m^{j-1}}^\top \otimes I_m \otimes \mathbf{1}_{m^{n-j}}^\top\right)\left(I_{m^{i-1}} \otimes W_{[m,m]} \otimes I_{m^{n-i-1}}\right) \\
&= \sum_{j=1}^{i-1} \left(\mathbf{1}_{m^{j-1}}^\top I_{m^{j-1}}\right) \otimes \left(I_m\right) \otimes \left(\mathbf{1}_{m^{i-j-1}}^\top I_{m^{i-j-1}}\right) \otimes \left(\mathbf{1}_{m^2}^\top W_{[m,m]}\right) \otimes \left(\mathbf{1}_{m^{n-i-1}}^\top I_{m^{n-i-1}}\right) \\
&\quad + \left(\mathbf{1}_{m^{i-1}}^\top I_{m^{i-1}}\right) \otimes \left[\left(I_m \otimes \mathbf{1}_m^\top\right) W_{[m,m]}\right] \otimes \left(\mathbf{1}_{m^{n-i-1}}^\top I_{m^{n-i-1}}\right) \\
&\quad + \left(\mathbf{1}_{m^{i-1}}^\top I_{m^{i-1}}\right) \otimes \left[\left(\mathbf{1}_m^\top \otimes I_m\right) W_{[m,m]}\right] \otimes \left(\mathbf{1}_{m^{n-i-1}}^\top I_{m^{n-i-1}}\right) \\
&\quad + \sum_{j=i+2}^{n} \left(\mathbf{1}_{m^{i-1}}^\top I_{m^{i-1}}\right) \otimes \left(\mathbf{1}_{m^2}^\top W_{[m,m]}\right) \otimes \left[\left(\mathbf{1}_{m^{j-i-2}}^\top \otimes I_m \otimes \mathbf{1}_{m^{n-j}}^\top\right) I_{m^{n-i-1}}\right] \\
&= \sum_{j=1}^{i-1} \mathbf{1}_{m^{j-1}}^\top \otimes I_m \otimes \mathbf{1}_{m^{i-j-1}}^\top \otimes \mathbf{1}_{m^2}^\top \otimes \mathbf{1}_{m^{n-i-1}}^\top \\
&\quad + \mathbf{1}_{m^{i-1}}^\top \otimes \mathbf{1}_m^\top \otimes I_m \otimes \mathbf{1}_{m^{n-i-1}}^\top + \mathbf{1}_{m^{i-1}}^\top \otimes I_m \otimes \mathbf{1}_m^\top \otimes \mathbf{1}_{m^{n-i-1}}^\top \\
&\quad + \sum_{j=i+2}^{n} \mathbf{1}_{m^{i-1}}^\top \otimes \mathbf{1}_{m^2}^\top \otimes \mathbf{1}_{m^{j-i-2}}^\top \otimes I_m \otimes \mathbf{1}_{m^{n-j}}^\top \\
&= \sum_{j=1}^{n} \mathbf{1}_{m^{j-1}}^\top \otimes I_m \otimes \mathbf{1}_{m^{n-j}}^\top \\
&= V_\mu,
\end{aligned}$$

which accomplishes the proof.

Appendix F Remark of Lemma 3

Remark 3. For any $s, \tilde{s} \in S_\mu$, there exists a permutation $\sigma \in \mathfrak{S}_N$ such that

$$\tilde{s}^\top W_\sigma s = 1.$$

Moreover, for any strategy profiles $s \in S_\mu, \tilde{s} \notin S_\mu$, the following equality holds:

$$\tilde{s}^\top W_\sigma s = 0, \quad \sigma \in \mathfrak{S}_n.$$

Appendix G Identify μ by index n_μ

For the set Υ_m^n, all its elements are lexicographic ordered. For any element $\mu \in \Upsilon_m^n$, its index n_μ is defined as the position of μ in this ordered sequence. Specifically, n_μ takes values within $[0:\tau]$, where τ is equal to $\frac{(n+m-1)!}{n!(m-1)!}$ [10].

To illustrate this indexing, we take Υ_3^3 as a simple example. Table G1 explicitly enumerates the full lexicographic ordering of Υ_3^3. For instance, $\mu = [1,2,0]^\top$ occupies the 6-th position, so $n_\mu = 6$.

Table G1 The relationship between n_μ and μ

Lexicographic index n_μ	1	2	3	4	5	6	7	8	9
Aggregate state μ	$\begin{bmatrix}0\\0\\3\end{bmatrix}$	$\begin{bmatrix}0\\1\\2\end{bmatrix}$	$\begin{bmatrix}0\\2\\1\end{bmatrix}$	$\begin{bmatrix}1\\0\\2\end{bmatrix}$	$\begin{bmatrix}1\\1\\1\end{bmatrix}$	$\begin{bmatrix}1\\2\\0\end{bmatrix}$	$\begin{bmatrix}2\\0\\1\end{bmatrix}$	$\begin{bmatrix}2\\1\\0\end{bmatrix}$	$\begin{bmatrix}3\\0\\0\end{bmatrix}$

To construct elements of the class S_{n_μ}, it is necessary to map each index n_μ to its corresponding aggregate state μ. Algorithm G1 provides the procedure for this index-to-state conversion.

Appendix H Proof of Lemma 4

Let $\sigma = \sigma_1 \circ \sigma_2 \circ \cdots \circ \sigma_m$ and $\tilde{s} = W_\sigma s$, where $\sigma_k \in \mathfrak{S}_{N\setminus N_k(s)}$ for each $k \in \mathcal{D}$. For any $i \in N_k(s)$, the pointwise stabilizer of $N\setminus N_k(s)$ guarantees that there exists $\tilde{i} \in N_k(s)$ satisfying $\sigma_k(i) = \tilde{i}$. By the definition of $N_k(s)$, this implies $s_i = s_{\sigma(i)}$. Moreover, for any $j \notin N_k(s)$, every element of the pointwise stabilizer $\mathfrak{S}_{N\setminus N_k(s)}$ fixes j, i.e., $\sigma_k(j) = j$.

Algorithm G1 Identify μ by index n_μ

Require: n, m, n_μ;
Ensure: $\mu = (\mu_1; \mu_2; \cdots; \mu_m)$;
$x \Leftarrow n_\mu - 1$;
$i \Leftarrow 1$;
while $x \neq 0$ and $i \neq m$ **do**
  $\mu_i = \max\left\{k \in [0:n] : \sum_{\kappa=0}^{k} \frac{(n-\kappa+m-i-1)!}{(n-\kappa)!(m-i-1)!} <= x\right\}$;
  if $\mu_i > 0$ **then**
    $x \Leftarrow x - \sum_{\kappa=0}^{\mu_i - 1} \frac{(n-\kappa+m-i-1)!}{(n-\kappa)!(m-i-1)!}$;
  end if
  $n \Leftarrow n - \mu_i$;
  $i \Leftarrow i + 1$;
end while
if $i <= m$ **then**
  $j \Leftarrow i$
  while $j < m$ **do**
    $\mu_j \Leftarrow 0$;
    $j \Leftarrow j + 1$;
  end while
  $\mu_j = n$;
end if

Combining these properties, the following equivalence holds:

$$s_{\sigma(i)} = \begin{cases} s_{\sigma_1(i)} = s_i, & i \in N_1(s), \\ \quad\vdots & \\ s_{\sigma_m(i)} = s_i, & i \in N_m(s), \end{cases} \iff s_{\sigma(i)} = s_i, \quad i \in N.$$

Necessity $\Longrightarrow$: Given that $\tilde{s}_i = s_i$ holds for all $i \in N$, we have

$$\tilde{s}_i = s_{\sigma(i)} = s_i, \quad i \in N,$$

which ensures the necessity.

Sufficiency $\Longleftarrow$: By the chain of equalities:

$$\tilde{s} = \ltimes_{i=1}^{n} s_{\sigma(i)} = \ltimes_{i=1}^{n} s_i = s,$$

the sufficiency follows.

Appendix I Proof of Proposition 1

Let $s \in S_{n_\mu}$, and $\tilde{s} \notin S_{n_\mu}$. By Lemma 4, there are $\prod_{k=1}^{m} |\mathfrak{S}_{N \setminus N_k(s)}| = \mu_1!\mu_2! \cdots \mu_m!$ stabilizers of s, which implies

$$s^\top \sum_{\sigma \in \mathfrak{S}_{N\setminus N_1} \circ \mathfrak{S}_{N\setminus N_2} \circ \cdots \circ \mathfrak{S}_{N\setminus N_m}} W_\sigma s = \mu_1!\mu_2! \cdots \mu_m!,$$

and

$$s^\top \sum_{\sigma \notin \mathfrak{S}_{N\setminus N_1} \circ \mathfrak{S}_{N\setminus N_2} \circ \cdots \circ \mathfrak{S}_{N\setminus N_m}} W_\sigma s = 0.$$

Next, by Lemma 3, there exists a permutation $\tilde{\sigma} \in \mathfrak{S}_N$ such that $s = W_{\tilde{\sigma}} s_0^\mu$. Using the expression of $\mathrm{Col}_{n_\mu}(\Psi)$, we obtain

$$\begin{aligned} s^\top \mathrm{Col}_{n_\mu}(\Psi) &= \frac{1}{\mu_1!\mu_2! \cdots \mu_m!} s^\top \sum_{\sigma \in \mathfrak{S}_N} W_\sigma s_0^\mu \\ &= \frac{1}{\mu_1!\mu_2! \cdots \mu_m!} s^\top \sum_{\sigma \in \mathfrak{S}_N} W_{\sigma \circ \tilde{\sigma}^{-1}} W_{\tilde{\sigma}} s_0^\mu \\ &= \frac{1}{\mu_1!\mu_2! \cdots \mu_m!} s^\top \sum_{\sigma \in \mathfrak{S}_N} W_{\sigma \circ \tilde{\sigma}^{-1}} s. \\ &= 1. \end{aligned}$$

On the other hand, by Remark 3, we get

$$\tilde{s}^\top \mathrm{Col}_{n_\mu}(\Psi) = \frac{1}{\mu_1!\mu_2! \cdots \mu_m!} \tilde{s}^\top \sum_{\sigma \in \mathfrak{S}_N} W_\sigma s_0^\mu = 0.$$

Indeed, since Δ_{m^n} forms a basis of $\mathbb{R}^m$, $\mathrm{Col}_{n_\mu}(\Psi) \in \mathbb{R}^{m^n}$ admits a unique expansion

$$\mathrm{Col}_{n_\mu}(\Psi) = \sum_{i=1}^{m^n} c_i \delta_{m^n}^i = \sum_{\hat{s}\in\Delta_{m^n}} \big(\hat{s}^\top \mathrm{Col}_{n_\mu}(\Psi)\big)\hat{s} = \sum_{\hat{s}\in S_{n_\mu}} 1\cdot\hat{s} + \sum_{s\notin S_\mu} 0\cdot\hat{s} = \sum_{\hat{s}\in S_{n_\mu}} 1\cdot\hat{s},$$

which confirms the expression of $\mathrm{Col}_{n_\mu}(\Psi)$.

Finally, for any permutation $\sigma \in \mathfrak{S}_N$, the bijectivity of σ implies

$$W_\sigma \mathrm{Col}_{n_\mu}(\Psi) = \sum_{\hat{s}\in S_{n_\mu}} W_\sigma \hat{s} = \sum_{\hat{s}\in S_\mu} \hat{s} = \mathrm{Col}_{n_\mu}(\Psi),$$

which further yields

$$W_\sigma \Psi = [W_\sigma \mathrm{Col}_1(\Psi), W_\sigma \mathrm{Col}_2(\Psi), \cdots, W_\sigma \mathrm{Col}_\tau(\Psi)] = \Psi. \tag{I1}$$

This completes the proof.

Appendix J Proof of Theorem 1

Before proving the theorem, it is worthwhile to note that the stochastic dynamics $s(t+1) = F^\Pi_{\omega(t)}s(t)$ is equivalent to the Markov process $\{s(t)\}_{t\in\mathbb{N}}$ endowed with the transition probability matrix Π, which can be specifically expressed as:

$$s(t+1) = F^\Pi_{\omega(t)}s(t) \quad \sim \quad s(t+1) \vDash \Pi s(t), \tag{J1}$$

where $\vDash$ represents the next state $s(t+1)$ is randomly generated according to the probability distribution $\Pi s(t)$.

Proof of Theorem 1. Given $n_\mu \in [1:\tau]$, and $s, \tilde{s} \in S_{n_\mu}$, let $\tilde{\sigma}$ be the permutation satisfying $\tilde{s} = W_{\tilde{\sigma}}s$. For any $S_{n_{\tilde{\mu}}} \in S$, the equivalent description (J1) yields

$$\mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|\tilde{s}) = \sum_{\hat{s}\in S_{n_{\tilde{\mu}}}} \hat{s}^\top \Pi \tilde{s} = \big(\Psi\delta_\tau^{n_{\tilde{\mu}}}\big)^\top \Pi W_{\tilde{\sigma}} s = \big(\Psi\delta_\tau^{n_{\tilde{\mu}}}\big)^\top W_{\tilde{\sigma}} W_{\tilde{\sigma}}^{-1} \Pi W_{\tilde{\sigma}} s = \big(W_{\tilde{\sigma}}\Psi\delta_\tau^{n_{\tilde{\mu}}}\big)^\top W_{\tilde{\sigma}}^\top \Pi W_{\tilde{\sigma}} s = \big(\Psi\delta_\tau^{n_{\tilde{\mu}}}\big)^\top \Pi s,$$

where the second-to-last equality follows from Lemma A4, and the last equality is holds by Lemma 1 and (I1). Then, the key equality holds:

$$\mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|\tilde{s}) = \mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|s), \quad s, \tilde{s} \in S_{n_\mu}. \tag{J2}$$

By combining (J2) with Lemma A5, we confirm that the aggregated process $\{x(t)\}_{t\in\mathbb{N}}$ is Markovian.

Following the Proposition 1, the $(n_{\tilde{\mu}}, n_\mu)$-th entry of $\Psi^\top\Pi\Psi$ is given by

$$(\delta_\tau^{n_{\tilde{\mu}}})^\top \Psi^\top \Pi \Psi \delta_\tau^{n_\mu} = \mathrm{Col}_{n_{\tilde{\mu}}}(\Psi)^\top \Pi \,\mathrm{Col}_{n_\mu}(\Psi) = \sum_{s\in S_{n_\mu}} \mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|s). \tag{J3}$$

Noting that $\Psi_{n_\mu}^\top \mathbf{1}_{m^n} = |\sum_{s\in S_{n_\mu}} s^\top \mathbf{1}_{m^n}| = |S_{n_\mu}|$, we normalize (J3):

$$(\Psi_{n_\mu}^\top \mathbf{1}_{m^n})^{-1} \mathrm{Col}_{n_{\tilde{\mu}}}(\Psi)^\top \Pi \,\mathrm{Col}_{n_\mu}(\Psi) = (\Psi_{n_\mu}^\top \mathbf{1}_{m^n})^{-1} \sum_{s\in S_{n_\mu}} \mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|s) = \mathbb{P}\mathrm{rob}(S_{n_{\tilde{\mu}}}|s), \quad s \in S_{n_\mu},$$

which constitutes the $(n_{\tilde{\mu}}, n_\mu)$-th entry of the transition probability matrix $\hat{\Pi}$. Thus, the matrix $\hat{\Pi}$ is explicitly expressed as $\hat{\Pi} = \big(\mathrm{diag}(\Psi^\top \mathbf{1}_{m^n})\big)^{-1}\Psi^\top\Pi\Psi$, and the proof is completed.

Appendix K Illustrative example

In evolutionary game theory, a key criterion for evaluating a mutant strategy is whether it can successfully invade a resident population and ultimately replace it [11]. A common quantitative measure of such success is the fixation probability, defined as the probability that a single mutant introduced by a randomly player eventually takes over the entire population [12].

Consider a simplified version of the model in [13], with parameter $n = 3$ and $m = 2$. Specifically, a well-mixed population $N = \{X, Y, Z\}$ with strategy set $\{L, M\}$, where L denotes the resident strategy and and M denotes the mutant strategy. Mutants have relative payoffs $r > 0$, as compared to residents, whose payoffs are 1. Identify L, and M with δ_2^1, and δ_2^2, respectively. For a strategy profile $s = s_X \ltimes s_Y \ltimes s_Z \in \Delta_{2^3}$, the payoff structure can be described as follows:

$$\pi(\delta_2^k, s) = \begin{cases} 1, & \delta_2^1, \\ r, & \delta_2^2. \end{cases} \tag{K1}$$

At each discrete time step, a player $i \in N$ is selected for reproduction with the probability proportional to its fitness. Then its offspring replaces one of i's neighbors, chosen uniformly at random. This PUSR is called Moran process. After incorporating payoff structure (K1) into the Moran process, the induced dynamics of the strategy profile can be expressed as

$$s(t+1) = F^\Pi_{\omega(t)}s(t), \quad t \in \mathbb{N},$$

where the column stochastic matrix is given by

$$\Pi = \begin{bmatrix} 1 & \frac{1}{2+r} & \frac{1}{2+r} & 0 & \frac{1}{2+r} & 0 & 0 & 0 \\ 0 & \frac{1}{2+r} & 0 & \frac{0.5}{1+2r} & 0 & \frac{0.5}{1+2r} & 0 & 0 \\ 0 & 0 & \frac{1}{2+r} & \frac{0.5}{1+2r} & 0 & 0 & \frac{0.5}{1+2r} & 0 \\ 0 & \frac{0.5r}{1+2r} & \frac{0.5r}{1+2r} & \frac{r}{1+2r} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2+r} & \frac{0.5}{1+2r} & \frac{0.5}{1+2r} & 0 \\ 0 & \frac{0.5r}{2+r} & 0 & 0 & \frac{0.5r}{2+r} & \frac{r}{1+2r} & 0 & 0 \\ 0 & 0 & \frac{1}{2+r} & 0 & \frac{0.5r}{2+r} & 0 & \frac{r}{1+2r} & 0 \\ 0 & 0 & 0 & \frac{r}{1+2r} & 0 & \frac{r}{1+2r} & \frac{r}{1+2r} & 1 \end{bmatrix}.$$

After reordering the profile via the permutation matrix

$$W = \begin{bmatrix} \mathbf{0}_7^\top & 1 \\ I_7 & \mathbf{0}_7 \end{bmatrix},$$

the corresponding stochastic matrix admits the following block form:

$$W \Pi W^\top = \begin{bmatrix} I & R \\ \mathbf{0} & Q \end{bmatrix}.$$

Here, I characterizes transitions among absorbing states, while Q characterizes transitions among transient states. Note that $W^\top = W^{-1}$ [14].

For the calculation of the fixation probability of M, three distinct initial strategy profiles are considered, as illustrated in Figure K1. Then we have

$$\begin{aligned} \rho_M &= \lim_{t\to\infty} \frac{1}{3}\Big(\mathbb{P}\mathrm{rob}\big(s(t) = \delta_2^2 \ltimes \delta_2^2 \ltimes \delta_2^2 | s(0) = \delta_2^1 \ltimes \delta_2^1 \ltimes \delta_2^2\big) + \mathbb{P}\mathrm{rob}\big(s(t) = \delta_2^2 \ltimes \delta_2^2 \ltimes \delta_2^2 | s(0) = \delta_2^1 \ltimes \delta_2^2 \ltimes \delta_2^1\big) \\ &\quad + \mathbb{P}\mathrm{rob}\big(s(t) = \delta_2^2 \ltimes \delta_2^2 \ltimes \delta_2^2 | s(0) = \delta_2^2 \ltimes \delta_2^1 \ltimes \delta_2^1\big)\Big) \\ &= \lim_{t\to\infty} \frac{1}{3} \big(\delta_8^8\big)^\top \Pi^t \big(\delta_2^1 \ltimes \delta_2^1 \ltimes \delta_2^2 + \delta_2^1 \ltimes \delta_2^2 \ltimes \delta_2^1 + \delta_2^2 \ltimes \delta_2^1 \ltimes \delta_2^1\big) \\ &= \frac{1}{3} \sum_{i=1}^{3} \big(W \delta_8^8\big)^\top \lim_{t\to\infty} \big(W \Pi W^{-1}\big)^t \big(W \ltimes_{j=1}^{i-1} \delta_2^1 \ltimes \delta_2^2 \ltimes_{h=i+1}^{3} \delta_2^1\big) \\ &= \frac{1}{3} \sum_{i=1}^{3} \delta_8^1 \begin{bmatrix} I & R(I-Q)^{-1} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} W \big(\delta_8^2 + \delta_8^3 + \delta_8^5\big) \\ &= \frac{1}{3} \sum_{i=1}^{3} \delta_8^1 \begin{bmatrix} I & R(I-Q)^{-1} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \big(\delta_8^3 + \delta_8^4 + \delta_8^6\big) \\ &= \frac{1 - r^{-1}}{1 - r^{-3}}, \end{aligned}$$

which aligns with the expression reported in [13].

Computing this fixation probability requires $a = R(I-Q)^{-1}$, which equivalently solving the linear matrix equation $a(I-Q) = R$. A standard approach is to solve this equation via Gaussian elimination, which runs in $O\big((m^n - 2)^3\big)$ times for a population with size n and m strategies.

Following lexicographic ordering, Algorithm G1 implements the index-to-state conversion, which is summarized in Table K1. Moreover, after aggregation, each aggregate state μ can be represented in logical form as $x = \delta_4^{n_\mu}$.

Table K1 Index-to-state Correspondence

Lexicographic index	1	2	3	4
Aggregate state	$\begin{bmatrix} 0 \\ 3 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 2 \end{bmatrix}$	$\begin{bmatrix} 2 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 3 \\ 0 \end{bmatrix}$

Then, the transition probability matrix for x is

$$\hat{\Pi} = \begin{bmatrix} 1 & \frac{1}{2+r} & 0 & 0 \\ 0 & \frac{1}{2+r} & \frac{1}{1+2r} & 0 \\ 0 & \frac{r}{2+r} & \frac{r}{1+2r} & \frac{r}{1+2r} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

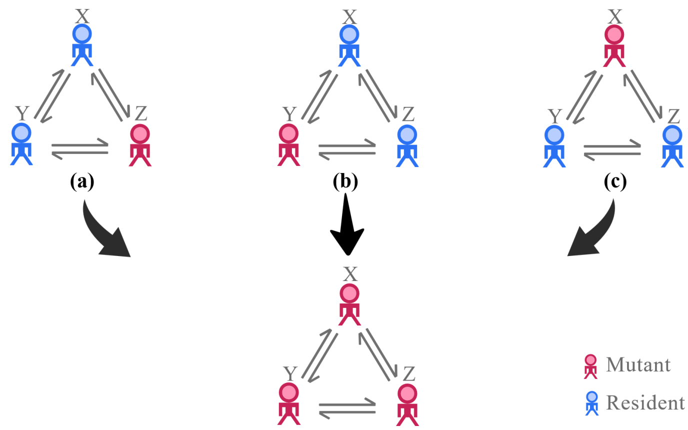

Figure K1 Mutants take over the whole population under three initial conditions: (a) $\delta_2^1 \ltimes \delta_2^1 \ltimes \delta_2^2$, (b) $\delta_2^1 \ltimes \delta_2^2 \ltimes \delta_2^1$, (c) $\delta_2^2 \ltimes \delta_2^1 \ltimes \delta_2^1$.

Similarly, the fixation probability for M is

$$\rho_M = \lim_{t\to\infty} \mathbb{P}\mathrm{rob}\big(x(t) = \delta_4^4 | x(0) = \delta_4^2\big) = \frac{1 - r^{-1}}{1 - r^{-3}}.$$

Using Gaussian elimination, the computational complexity for evaluating the fixation probability is reduced from $O\big((m^n - 2)^3\big)$ to $O\big((\tau - 2)^3\big)$ for n players and m strategies. Importantly, this aggregation preserves the relevant evolutionary dynamics and hence does not affect the fixation probability.

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