

Coevolutionary Systems and PageRank^{☆,☆☆}

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Abstract

Coevolutionary systems have been used successfully in various problem domains involving situations of strategic decision-making. Central to these systems is a mechanism whereby finite populations of agents compete for reproduction and adapt in response to their interaction outcomes. In competitive settings, agents choose which solutions to implement and outcomes from their behavioral interactions express preferences between the solutions. Recently, we have introduced a framework that provides both qualitative and quantitative characterizations of competitive coevolutionary systems. Its two main features are: (1) A directed graph (digraph) representation that fully captures the underlying structure arising from pairwise preferences over solutions. (2) Coevolutionary processes are modelled as random walks on the digraph. However, one needs to obtain prior, qualitative knowledge of the underlying structures of these coevolutionary digraphs to perform quantitative characterizations on coevolutionary systems and interpret the results. Here, we study a deep connection between coevolutionary systems and PageRank to address this issue. We develop a principled approach to measure and rank the performance (importance) of solutions (vertices) in a given coevolutionary digraph. In PageRank formalism, B transfers part of its authority to A if A dominates B (there is an arc from B to A in the digraph). In this manner, PageRank authority indicates the importance of a vertex. PageRank authorities with suitable normalization have a natural interpretation of long-term visitation probabilities over the digraph by the coevolutionary random walk. We derive closed-form expressions to calculate PageRank authorities for any coevolutionary digraph. We can precisely quantify changes to the authorities due to modifications in restart probability for any coevolutionary system. Our empirical studies demonstrate how PageRank authorities characterize coevolutionary digraphs with different underlying structures.

Keywords: Coevolutionary systems, PageRank, Markov chains

1. Introduction

Coevolutionary systems that are inspired by natural evolutionary processes have been applied extensively and shown remarkable success in problem areas involving situations of strategic decision-making. These include simulation tools involving a collection of interacting, adaptive agents to understand conditions for the emergence of complex, intelligent behaviors in the real-world [1, 2] and algorithms to generate high performance agents with minimal preprogrammed knowledge in competitive settings [3, 4].

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Competitive coevolutionary systems share a common framework and are specified by: (1) The *problem* whereby the solutions are the set of all alternatives (strategies in a two-player game) with a pairwise preference relation indicating the superior alternative. (2) The *process* whereby the finite population of agents (each implementing a strategy to play) goes through a process of selection and variation guided only by their interaction (game play) outcomes. This framework allows for various design choices and parameters in strategy representation (finite state machines, neural networks, etc.), variation approaches (recombination and mutation) to generate new distinct strategies, and selection operations that favours higher performing strategies for reproduction.

All coevolutionary systems implement a mechanism that requires the population of agents to compete for reproduction [5]. This can be double-edged in competitive settings. The system could exploit interactions to search increasingly superior strategies or succumb to the deleterious effects of using relative fitness evaluations in the search process. These *pathologies* have been studied [6, 7, 8] and include formal methods [9, 10] characterizing cyclic coevolutionary dynamics due to the choice of selection mechanism in an evolutionary game theoretic setting in the framework of continuous dynamical systems.

Other studies have found that problem structures induced by pairwise relations can affect coevolutionary search [11]. We [12] have introduced a new framework that specifies and models coevolutionary systems formally. It uses a digraph representation of coevolutionary problem where the vertex set corresponds to the strategy set and the arc set captures preferences over all pairs of strategies. Coevolutionary processes are modelled as discrete time Markov chains operating on the digraph. A distinct population-one coevolutionary algorithm corresponds to a specific implementation of random walk on digraphs. Other learning algorithms involving self play for any problem in the form of a two-player game can be modelled within this framework. In this manner, complete qualitative characterization of cycle structures underlying coevolutionary problems as well as quantitative characterizations of coevolutionary processes are obtained.

As in the case of evolutionary algorithms [13], the expected hitting times of the absorbing class for coevolutionary Markov chains (CMCs) operating on reducible digraphs can be formulated. However, other relevant quantitative characterizations can be made since CMCs operate on both reducible and irreducible digraphs. The stationary distribution of a CMC can be formulated but the associated quantitative analysis and interpretation of subsequent results require prior knowledge of the digraph’s underlying structure. For example, the entire probability mass will be concentrated on the absorbing class for a CMC operating on a reducible digraph but the immediate consequence is that one would have no knowledge about the structures underlying the dominated subset of vertices. As such, one might ask if other useful quantitative characterizations could be obtained that incorporate some knowledge of these digraph structures commonly found in coevolutionary problems? Our study to address this issue has led us to establish a direct connection between coevolutionary systems and large network analysis methodologies [14] particularly PageRank (used originally to measure webpage importance [15, 16]). In the PageRank formalism, strategies transfer part of their authorities to those that dominate them at pairwise interactions level and these authorities give indication of strategies’ performances. Crucially, these authorities are linked to the underlying structures of the digraph that capture the relationships (connectivities) between strategies that we will derive explicitly. This allows us to show how PageRank authorities with a suitable normalization are quantity-wise the same as the long-term visitation probabilities given by the stationary distribution associated to the CMC that incorporates a restart operating over the same digraph.

This connection allows us to develop a principled approach to measure and rank the performance of individual strategies that correspond to the vertex set for any digraph representation of the coevolutionary problem. In Section 2, we establish several theoretical results supporting this approach. We prove that PageRank for any coevolutionary system exists, derive closed-form expressions to calculate PageRank authorities, and quantify their changes due to varying restart probability. Section 3 introduces a benchmark of coevolutionary digraphs having different structures that is used in the controlled empirical studies to demonstrate how PageRank authorities provide quantitative characterizations of the digraphs. Section 4 concludes with remarks for future studies.

2. Coevolutionary Systems and PageRank

The framework in [12] provides a formal approach to model and construct coevolutionary systems as random walks on digraphs. We consider a wide range of problems modelled as two-player strategic game $C = (S, R)$ where S is the set of pure strategies and R corresponds to the dominance relation on S . For any game $C = (S, R)$, its full underlying structures are captured by a coevolutionary digraph $D_C = (V_S, A_R)$. V_S is a non-empty, finite vertex set that corresponds to S . $A_R \subset V_S \times V_S$ is a finite arc set of ordered pairs of distinct vertices that represents R . The arc $(u, v) \in A_R$ (uv or $u \rightarrow v$) indicates v dominating u . Note that standard digraph terminology reverses our domination definition [17]. The exposition of this study makes use of digraph theory, finite Markov chains, and matrix analysis, for which we would follow the standard notations associated with the primary texts of the respective areas [17, 18, 19]. In general, we introduce terms and notations before their first use, or at times, where appropriate, immediately after their first appearance.

2.1. Structural Characterizations of Coevolutionary Digraphs

There are unique structures underlying coevolutionary digraphs D_C that allow us to characterize them. The underlying graph $UG(D_C) = (V_S, E)$ of D_C is obtained by replacing arcs for all pairs of vertices by single edges. It is complete. One characterization relates to edge biorientation, e.g., either the orientation uv or vu (win-lose) or both $\{uv, vu\} \in A_R$ (draw). Let $V_{S(n)}$ be the vertex set with $n = |V_{S(n)}|$ number of vertices. For $n \geq 2$, we obtain two coevolutionary digraph classes: (1) tournament $T(V_{S(n)}) \in \mathcal{T}(V_{S(n)})$ as orientations of $UG(D_C)$, and (2) semicomplete digraph $SD(V_{S(n)}) \in \mathcal{SD}(V_{S(n)})$ as biorientations of $UG(D_C)$ [17]. $\mathcal{T}(V_S)$ represents all coevolutionary games with win-lose outcomes and $\mathcal{SD}(V_S)$ generalizes further by allowing draws.

Further characterizations relate to global structures on reducibility (grouping of related vertices) and connectivity (reachability of vertices). A reducible $D_C(V_{S(n)})$ admits a vertex partition on $V_{S(n)}$ into two disjoint, nonempty subsets $(V_S^1 \cap V_S^2 = \emptyset, V_S^1 \cup V_S^2 = V_{S(n)})$ whereby $V_S^1 \mapsto V_S^2$ (each $v \in V_S^2$ dominates all $u \in V_S^1$ only). Consider $D_C(V_{S(n)})$ with vertices v_i and arcs a_i labelled so that a_i means $v_i v_{i+1}$ for every $i = 1, 2, 3, \dots, k-1$. A (v_1, v_k) -path is a (v_1, v_k) -walk in $D_C(V_{S(n)})$ given by $v_1 a_1 v_2 a_2 v_3 \dots a_{k-1} v_k$ such that all vertices are distinct. A k -cycle is Hamilton if it is a closed (v_1, v_k) -walk (i.e. $v_1 = v_k$) of length $k = n$ on the (v_1, v_{k-1}) -path. A digraph is strongly connected (or strong) if for every pair $v_i, v_j \in V_{S(n)}$, $i, j = 1, 2, 3, \dots, n$ and $i \neq j$, there exist both (v_i, v_j) -path and (v_j, v_i) -path [17]. Coevolutionary digraphs $D_C(V_{S(n)})$ are either reducible or irreducible. Any irreducible $D_C(V_{S(n)})$ on $n \geq 3$ vertices cannot be vertex-partitioned, is hamiltonian and strongly connected [12].

2.2. CMCs

We focus on population-one coevolutionary systems with processes described by random walks on digraphs. A distinct population-one coevolutionary algorithm corresponds to a specific implementation of random walk on digraphs, i.e., it is a single population coevolution where at every generation the single parent generates and competes with the single offspring for selection. They also naturally represent learning algorithms based on self play [20]. A standard random walk on a labelled D_C starts at a random vertex, and in each subsequent step, jumps to one of the out-neighbours $N_D^+(u) = \{v \in V_S \setminus \{u\} : uv \in A_R\}$ of the current vertex u randomly with equal probability. They are modelled as a specific type of discrete time Markov chain $\Phi = \{\Phi_t : t \in \mathbb{N}_0\}$, each Φ_t takes values from the countable state space $X = V_{S(n)}$. By exploiting time homogeneity and memory loss [18], we can construct the CMC Φ as the random walk on $D_C(V_{S(n)})$ with initial distribution μ over X and Markov transition matrix P on X satisfying: (1) $\mu = (\mu_x : x \in X)$, $0 \leq \mu_x \leq 1$ and $\sum_{x \in X} \mu_x = 1$, and (2) $P = (P(x, z) : x, z \in X)$, where every row is a distribution with $0 \leq P(x, z) \leq 1$ and $\sum_{y \in X} P(x, y) = 1$. The distribution describing Φ can be obtained from μ and P .

There is an intimate connection between qualitative characterizations of global connectivity structures in D_C and quantitative characterizations of Φ [12]. A random walk on a reducible D_C leads to an absorbing Φ . In the same manner, an irreducible Φ operates on a strongly connected D_C . One can obtain the long-term limiting distribution of Φ that satisfies the invariant property $\pi P = \pi$. $\pi = (\pi_x : x \in X)$ on X is the stationary distribution of Φ . Each π_x describes the long-term fraction of time spent on x by Φ . For

105 absorbing Φ , the probability mass is concentrated on the absorbing class with all other states having zero probabilities [21].

2.3. PageRank Authority for Coevolutionary Digraphs

We reformulate the PageRank authority [22] using digraph-theoretic notations to make explicit its link to digraph structures. Let $u, v \in V_S$, the in-neighbourhood of u is $N_D^-(u) = \{v \in V_S \setminus \{u\} : vu \in A_R\}$, and the out-degree (number of outgoing arcs) of v is $d_D^+(v) = |\{(u, v) \in A_R : v \in V_S \setminus \{u\}\}|$. The PageRank authority of u is $\varphi_u = \alpha + (1 - \alpha) \sum_{v \in N_D^-(u)} \varphi_v / d_D^+(v)$ where $\alpha \in (0, 1)$. The parameter α has several interpretations depending on the context in which PageRank is formulated. Here, it is used for the convex combination of the free authority that each vertex (node) has and those as a result of connectivity structures to calculate PageRank authorities [22].

115 Let vertices in $D_C(V_{S(n)})$ be labelled as $v_1, v_2, v_3, \dots, v_n$. The PageRank authorities are $\boldsymbol{\varphi} = [\varphi_1, \varphi_2, \varphi_3, \dots, \varphi_n]$ (we write φ_{v_i} as the i th element φ_i of $\boldsymbol{\varphi}$), and given by $\boldsymbol{\varphi} = \alpha \mathbf{e} + (1 - \alpha) \boldsymbol{\varphi} \mathbf{M}$, where $\mathbf{e} = [1, 1, 1, \dots, 1]$ and the matrix $\mathbf{M} = (m_{ij} : i, j \in \{1, 2, 3, \dots, n\})$ with $m_{ij} = \frac{1}{d_D^+(v_j)}$ if $j \rightarrow i$, $m_{ij} = 0$ if $j \nrightarrow i$. The influence of the digraph structure can be seen from non-zero entries of \mathbf{M} that corresponds to the domination matrix associated with $D_C(V_{S(n)})$.

120 2.4. CMC and PageRank Connection

Actual PageRank computation requires reformulation as an eigensystem or an equivalent linear system if $\boldsymbol{\psi}$ is suitably normalized ($\boldsymbol{\psi} \mathbf{e}^T = 1$) [14]. PageRank is a Markov chain with a primitive probability transition matrix \mathbf{P}_{PR} (non-negative, irreducible matrix having one eigenvalue $r = \rho(\mathbf{P}_{PR})$ on its spectral circle [19]). Similarly, setting the usual adjustment $\mathbf{P}_{PR} = \alpha \mathbf{e}^T \mathbf{s} + (1 - \alpha) \mathbf{P}$ where \mathbf{s} is a general probability vector (e.g. uniform $\frac{1}{n} \mathbf{e}$) [23] makes CMC irreducible and akin to a PageRank on $D_C(V_{S(n)})$, but also crucially introduces restart into the coevolutionary process with probability α . $\mathbf{P} = \mathbf{M}$ if standard random walk is used. $\boldsymbol{\psi}$ is the solution to $\boldsymbol{\psi} \mathbf{P}_{PR} = \boldsymbol{\psi}$. This gives two natural interpretations to $\boldsymbol{\psi}$: (1) It indicates how coevolution measures the importance (authority) of individual $v \in V_{S(n)}$ and provides the means to rank them. (2) It gives long-term visitation probabilities over the digraph by coevolutionary search (random walk).

130 We will establish several theoretical results connecting CMC and PageRank, which are reflected by the relationship between the stationary distributions $\boldsymbol{\pi}$ and $\boldsymbol{\psi}_\alpha$ associated with CMC and PageRank (CMC with restart probability α) [24]. In the following, we provide guarantees on the existence of a PageRank vector associated with a coevolutionary system and a linear systems formulation that allows us to uncover several properties related to the coefficient matrix. A lazy random walk with the modified probability transition matrix $\mathbf{Z} = (\mathbf{I} + \mathbf{P})/2$ is used with stationary distribution $\boldsymbol{\pi}$ since $\boldsymbol{\pi} = \boldsymbol{\pi} \mathbf{Z}$. The claim that $\boldsymbol{\pi}$ is the limiting invariant distribution of a CMC operating on a strongly connected digraph $D_C(V_{S(n)})$ that is aperiodic follows from the Perron-Frobenius Theorem. The modification introduced in the lazy random walker ensures that \mathbf{Z} is aperiodic [25].

Lemma 1. *Let $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be a coevolutionary digraph. Let \mathbf{P} be the probability transition matrix associated with a CMC operating on $D_C(V_{S(n)})$ and $\mathbf{Z} = (\mathbf{I} + \mathbf{P})/2$ its lazy version. The row vector \mathbf{s} is the probability distribution over the set vertices $V_{S(n)}$. Given $\alpha \in (0, 1)$ and $\beta = \frac{2\alpha}{1-\alpha}$, the personalized PageRank vector is the unique solution to the linear system defined as*

$$\boldsymbol{\psi}_\alpha(\mathbf{s}) = \alpha \mathbf{s} + (1 - \alpha) \boldsymbol{\psi}_\alpha(\mathbf{s}) \mathbf{Z} \quad (1)$$

and can be computed as

$$\boldsymbol{\psi}_\alpha(\mathbf{s}) = \beta \mathbf{s} (\beta \mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1}. \quad (2)$$

Proof: Equation 1 is formulated in [26]. We can rewrite it as

$$\boldsymbol{\psi}_\alpha(\mathbf{s}) (\beta \mathbf{I} + (\mathbf{I} - \mathbf{P})) = \beta \mathbf{s} \quad (3)$$

140 where $\beta > 0$ (see Appendix A). $\mathbf{W} = \beta\mathbf{I} + (\mathbf{I} - \mathbf{P})$ is a strictly dominant diagonal matrix and is invertible [27]. \square

Let $\mathbf{R}^{n \times n}$ be the set of real, square $n \times n$ matrices. $\mathbf{A} \in \mathbf{R}^{n \times n}$ is an M-matrix with the form $\mathbf{A} = c\mathbf{I} - \mathbf{B}$, where $\mathbf{B} \geq \mathbf{0}$ ($b_{ij} \geq 0 : 1 \leq i, j \leq n$) and $c \geq \rho(\mathbf{B})$ with $\rho(\cdot)$ denoting the spectral radius [28]. $\|\mathbf{A}\|_\infty$ is the ∞ -norm on \mathbf{A} and $\kappa_\infty(\mathbf{A}) = \|\mathbf{W}\|_\infty \|\mathbf{W}^{-1}\|_\infty$ is the condition number with respect to the ∞ -norm for \mathbf{A} [19].

Lemma 2. Let $\psi_\alpha(\mathbf{s})(\beta\mathbf{I} + (\mathbf{I} - \mathbf{P})) = \beta\mathbf{s}$ be the formulation of the PageRank problem as a linear system. The coefficient matrix $\mathbf{W} = \beta\mathbf{I} + (\mathbf{I} - \mathbf{P})$ has the following properties:

- | | |
|---|---|
| 1. \mathbf{W} is an M-matrix. | 5. $\mathbf{W}^{-1} \geq \mathbf{0}$. |
| 2. \mathbf{W} is nonsingular. | 6. The row sums of \mathbf{W}^{-1} are $\frac{1}{\beta}$. |
| 3. The row sums of \mathbf{W} are β . | 7. $\ \mathbf{W}^{-1}\ _\infty = \frac{1}{\beta}$. |
| 4. $\ \mathbf{W}\ _\infty = 2 + \beta$. | 8. $\kappa_\infty(\mathbf{W}) = \frac{2+\beta}{\beta} = \frac{1}{\alpha}$. |

Proof: The main idea uses the fact that by definition, $\mathbf{W} = c\mathbf{I} - \mathbf{B}$ is an M-matrix with $c = 1 + \beta$ and $\mathbf{B} = \mathbf{P}$ a stochastic matrix. Various properties can be shown such as *inverse-positivity* (Theorem 2.3, [28]). See Appendix A for complete details. \square

$\kappa_\infty(\mathbf{W})$ in Lemma 2 indicates the sensitivity of the solution to PageRank to perturbations in \mathbf{W} . It quantifies the extent \mathbf{W} is ill-conditioned with respect to machine precision when direct computation based on Gaussian elimination is used. For a machine precision \mathbf{u} , this quantity is taken to be $\mathbf{u}\kappa_\infty(\mathbf{W})$ (Chapter 3, [29]). For example, $\mathbf{u}\kappa_\infty(\mathbf{W}) \leq 1$ would indicate a loss of a single decimal digit of precision for $\alpha = 0.1$. In practice, iterative methods are used for PageRank computation (see Theorem 2.2 [14] for error characterizations of these methods).

165 2.5. CMC and PageRank - Stationary Distributions

Given the connection between CMC and PageRank, the immediate issues are (1) characterization of introducing restart in random walks on D_C and (2) how changes to α impact the long-term limiting distribution of CMC. Our theoretical results address these issues qualitatively and quantitatively, for (1) and (2), respectively. We use recent results from random walks generalized to digraphs in [30]. Let \mathbf{P} be associated with a CMC operating on irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ with stationary vector $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3, \dots, \pi_n)$ where $\boldsymbol{\pi}\mathbf{P} = \boldsymbol{\pi}$. Let the diagonal matrix be $\boldsymbol{\Pi} = \text{diag}(\pi_i)$. The normalized digraph Laplacian is $\tilde{\mathcal{L}} = \boldsymbol{\Pi}^{\frac{1}{2}}(\mathbf{I} - \mathbf{P})\boldsymbol{\Pi}^{-\frac{1}{2}}$, with its individual element given by

$$\tilde{\mathcal{L}}_{ij} = \begin{cases} 1 - p_{ii} & \text{if } i = j \\ -\pi_i^{1/2} p_{ij} \pi_j^{1/2} & \text{if } (i, j) \in A \\ 0 & \text{otherwise.} \end{cases}$$

The Green's function for digraphs $\tilde{\mathcal{Z}} = \tilde{\mathcal{L}}^+$ is the Moore-Penrose pseudoinverse of $\tilde{\mathcal{L}}$ with $\tilde{\mathcal{Z}}\tilde{\mathcal{L}} = \tilde{\mathcal{L}}\tilde{\mathcal{Z}} = \mathbf{I} - \tilde{\mathcal{J}}$, where $\tilde{\mathcal{J}} = (\boldsymbol{\pi}^{1/2})^T \boldsymbol{\pi}^{1/2}$. The next theorem shows the relationship between PageRank and stationary vectors of CMC.

Theorem 3. Let $\boldsymbol{\pi}$ be the stationary vector associated with a CMC operating on an irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$. The personalized PageRank vector is given by

$$\boldsymbol{\psi}_\alpha(\mathbf{s}) = \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}}). \quad (4)$$

Furthermore,

$$\lim_{\beta \rightarrow 0} \tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} = \tilde{\mathcal{L}}(\tilde{\mathcal{L}})^+ = \tilde{\mathcal{L}}\tilde{\mathcal{Z}}$$

170 where $\beta = \frac{2\alpha}{1-\alpha}$ and $\tilde{\mathcal{Z}} = \tilde{\mathcal{L}}^+$ is the Moore-Penrose pseudoinverse of $\tilde{\mathcal{L}}$. For small values of α (subsequently, small values of β), the PageRank vector is approximated by the stationary vector, i.e., $\boldsymbol{\psi}_\alpha(\mathbf{s}) \approx \boldsymbol{\pi}$ with equality ($\boldsymbol{\psi}_0(\mathbf{s}) = \boldsymbol{\pi}$) for any \mathbf{s} .

Proof: Appendix A gives the full proof while we summarize the main ideas here. Using various identities involving the normalized digraph Laplacian and the generalized identity for the inverse of a sum of matrices [31], we can rewrite Equation 2 so that

$$\psi_\alpha(\mathbf{s}) = \mathbf{s}(\mathbf{I} - \Pi^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}\Pi^{\frac{1}{2}})$$

can be calculated where $(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}$ is nonsingular (Theorem 1.2.17, [27]).

We can reformulate the linear system as

$$\psi_\alpha(\mathbf{s}) = \boldsymbol{\pi} + \beta(\mathbf{s} - \boldsymbol{\pi})(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}, \quad (5)$$

which indicates that $\psi_0(\mathbf{s}) = \boldsymbol{\pi}$ for any \mathbf{s} as we let $\alpha \rightarrow 0 \Rightarrow \beta \rightarrow 0$.

We can directly calculate $\psi_0(\mathbf{s})$. Let $\mathbf{N}_\beta = \beta(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}$. We will apply results from [30] (Theorem 1 and Lemma 1) involving identities relating the normalized digraph Laplacian and its Moore-Penrose pseudoinverse. As $\beta \rightarrow 0$, we have $\mathbf{N}_0 = \mathbf{N}_0\tilde{\mathcal{J}}$. Given that $\tilde{\mathcal{J}}$ is singular, the solutions to the equality $\mathbf{N}_0 = \mathbf{N}_0\tilde{\mathcal{J}}$ are $\mathbf{N}_0 = \mathbf{0}$ and $\mathbf{N}_0 = \tilde{\mathcal{J}}^k = \tilde{\mathcal{J}}$, $k = 1, 2, 3, \dots$. Then, $\tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} = \tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\mathbf{I} - \beta(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1})$ reduces to $\tilde{\mathcal{L}}(\tilde{\mathcal{L}})^+ = \tilde{\mathcal{L}}\tilde{\mathcal{Z}}$, implying that

$$\lim_{\beta \rightarrow 0} \tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} = \tilde{\mathcal{L}}\tilde{\mathcal{Z}}.$$

□

175 Theorem 3 shows a direct relationship between $\boldsymbol{\pi}$ and $\psi_\alpha(\mathbf{s})$ as a result of introducing restart in CMC. Crucially, the connection between structures in D_C and quantities arising from random walks on D_C is made explicit through the digraph Laplacian. For small $\alpha > 0$, how the long-term fraction of time the random walker spends on each vertices that is redistributed is represented by the perturbed normalized digraph Laplacian $(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}$. What is the difference between $\boldsymbol{\pi}$ and $\psi_\alpha(\mathbf{s})$ due to restart with probability α ? The
180 following results answer this quantitatively.

Lemma 4. *Let a CMC operating on irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be associated with a probability transition matrix \mathbf{P} , stationary distribution $\boldsymbol{\pi}$, and the fundamental matrix \mathbf{Z} . Correspondingly, the personalized PageRank on $D_C(V_{S(n)})$ is a CMC with probability transition matrix \mathbf{P}_{PR} and stationary distribution $\psi_\alpha(\mathbf{s})$. Then*

$$\begin{aligned} \boldsymbol{\pi} - \psi_\alpha(\mathbf{s}) &= -\psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})\mathbf{Z} \\ &= \beta(\boldsymbol{\pi} - \mathbf{s})(\beta\mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1}. \end{aligned}$$

Proof: Applying results from Perturbation theory on finite Markov chains (Theorems 1 and 2, [32]), we obtain

$$\boldsymbol{\pi} - \psi_\alpha(\mathbf{s}) = -\psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})\mathbf{Z}.$$

We can show that the vector $\boldsymbol{\pi} - \psi_\alpha(\mathbf{s})$ is invariant under multiplication of the matrix $(\mathbf{I} - \mathbf{P})\mathbf{Z}$, i.e., $(\boldsymbol{\pi} - \psi_\alpha(\mathbf{s}))(\mathbf{I} - \mathbf{P})\mathbf{Z} = \boldsymbol{\pi} - \psi_\alpha(\mathbf{s})$. Furthermore, $((\mathbf{I} - \mathbf{P})\mathbf{Z})^k = (\mathbf{I} - \mathbf{P})\mathbf{Z}$, $k = 1, 2, 3, \dots$. From Equation 5, we obtain the following

$$\boldsymbol{\pi} - \psi_\alpha(\mathbf{s}) = \beta(\boldsymbol{\pi} - \mathbf{s})(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}.$$

Multiplying $(\mathbf{I} - \mathbf{P})\mathbf{Z}$ on both sides of the equality above completes the proof (see Appendix A for details). □

Corollary 5. *For $\boldsymbol{\pi}$ and $\psi_\alpha(\mathbf{s})$ associated with CMC on an irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$, the following inequality is given for restart probabilities $\alpha_1 \leq \alpha_2$*

$$\|\boldsymbol{\pi} - \psi_{\alpha_1}(\mathbf{s})\| \leq \|\boldsymbol{\pi} - \psi_{\alpha_2}(\mathbf{s})\| \quad (6)$$

where $\alpha_1, \alpha_2 \in (0, 1)$.

Proof: Let $\mathbf{y} = \boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})$, which consists of entries that are differentiable functions of a real variable α [19].

185 We can show that $\|\mathbf{y}(\alpha)\|$ is monotonically increasing for α in $(0, 1)$. See Appendix A for complete details. \square

Corollary 6. *Associated to each irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ is CMC with stationary distribution $\boldsymbol{\psi}_\alpha(\mathbf{s})$ for $\alpha \in (0, 1)$ and $\boldsymbol{\pi}$ with the following perturbation bound*

$$\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_\infty \leq \|\boldsymbol{\pi} - \mathbf{s}\|_\infty \quad (7)$$

with equality when $\alpha = 1$.

Proof: Since $\|(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}\|_\infty = \frac{1}{\beta}$ from Lemma 2, we obtain $\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_\infty \leq \beta\|\boldsymbol{\pi} - \mathbf{s}\|_\infty \|(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}\|_\infty = \|\boldsymbol{\pi} - \mathbf{s}\|_\infty$. See Appendix A for details. \square

In this paper, we adopt a centrality measure approach [14] and take \mathbf{s} to be uniform for a global digraph analysis. For a given norm, $\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|$ is monotonic with α (Corollary 5). $\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_\infty$ is upper-bounded by $\|\boldsymbol{\pi} - \mathbf{s}\|_\infty$ (Corollary 6). A general upper-bound of $\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_1$ can be obtained for probability vectors associated with random walks on labelled (isomorphic) tournaments [33, 34], taking into account their unilateral and directional duals [17, 35] (see Appendix A)

$$\|\boldsymbol{\pi}_1 - \boldsymbol{\pi}_2\|_1 \leq 2\left(1 - \frac{1}{n}\right). \quad (8)$$

190 Although characterizing $\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_1$ against changes in α is more useful, tight bounds are difficult to obtain (e.g. $\frac{2}{\alpha}$) [22, 23, 36]. We combine a coupling approach [36] with digraph-theoretic arguments to improve the bound to $\frac{2}{1-\alpha}$ for irreducible D_C (see Lemma 5, Appendix A).

3. Computational Results

We present results from controlled empirical studies on CMCs operating on coevolutionary tournaments $T_C(V_{S(n)})$ having specific structures [12, 17, 33]. They are selected based on known internal cycle structures that let us test current understanding of those structures and evaluate their impact on the visitation probabilities of vertices by the coevolutionary random walkers using quantitative measures we develop earlier. We also compute differences on PageRank orderings [37] that we describe in detail later. We adapt the standard Power Method approach [23] to compute the PageRank vectors $\boldsymbol{\psi}_\alpha(\mathbf{s})$, using the lazy version of the CMCs with uniform (teleportation vector) \mathbf{s} .
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3.1. Generating Coevolutionary Tournaments

The set of coevolutionary digraphs for the experiments includes irreducible, reducible, and random $T_C(V_{S(n)})$. All irreducible $T_C(V_{S(n)})$ are pancyclic [12]. The vertex-pancyclic $T_C(V_{S(n)})$ with the least number of 3-cycles [38] can be obtained from the transitive tournaments of order n indexed by its score sequences and then just reversing the arc v_1v_n to v_nv_1 . It has a single transitive subtournament induced from a maximal, disjoint vertex partition of $n - 2$ vertices. We will refer to these tournaments as *pancyclic (maximal transitive subtournament)*. Other vertex-pancyclic (or simply pancyclic) $T_C(V_{S(n)})$ that we use are those where we further reverse the arc v_2v_{n-1} to $v_{n-1}v_2$.

For reducible cases, we use two approaches to generate reducible $T_C(V_{S(n)})$ with various degrees of cycle structures in a controlled manner. The first approach exploits known digraph-theoretic structures. Every reducible $T_C(V_{S(n)}) \in \mathcal{T}_C(V_{S(n)})$, $n \geq 2$ has a strong decomposition $V(T^{(1)}) \cup V(T^{(2)}) \cup V(T^{(3)}) \cup \dots \cup V(T^{(l)})$ with a unique ordering $T^{(1)}, T^{(2)}, T^{(3)}, \dots, T^{(l)}$ whereby $T^{(i)} \mapsto T^{(j)}$ when $i < j$ for $i, j = 1, 2, 3, \dots, l$. $T^{(1)}$ ($T^{(l)}$) is the initial (terminal) strong component [12]. We generate reducible $T_C(V_{S(n)})$ with odd number of components so that each odd-numbered- i th component is a single vertex and even-numbered- i th component consists of a strong component of known structures, e.g., vertex-pancyclic (maximal transitive subtournament) and regular [17].
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The second approach uses a network-growth-based methodology via preferential attachment [12, 39]. A hierarchy of $T_C(V_{S(n)})$ where a control parameter is used to move between two complexity extremes – irreducible $T_C(V_{S(n)})$ and reducible $T_C(V_{S(n)})$ with prominent transitive structures – can be generated. We use the same settings in [12]: an initial transitive T_C of order ten is used as a seed and attachment probabilities $P_i^- = (1 + \exp(-\gamma(x_i - \bar{x})))^{-1}$ of nodes v_i are computed with $\{x_i\}_1^m$ being the ranks of v_i sorted according to the score sequences, $\bar{x} = m/2$, and γ that plays the role of the inverse temperature. We control the generator to produce reducible T_C of order $n = m + 1$ by introducing at the final iteration a single dominant node v_n .

Finally, random $T_C(V_{S(n)})$ is generated by orienting each edge $\{v_i, v_j\} \in E$ of its underlying, complete graph $G_C(V_{S(n)}, E)$ randomly with equal probability for each direction. However, a random $T_C(V_{S(n)})$ is likely to be irreducible (e.g. more than half the chance for a generated random tournament of order five [33]). Irreducibility test on random $T_C(V_{S(n)})$ can be done using their score sequences following a well-known result of Moser and Harary (1966) [17].

3.2. Results For $\|\pi - \psi_\alpha(\mathbf{s})\|$

We evaluate both max and one norms and study the impact of the restart probability α on $\|\pi - \psi_\alpha(\mathbf{s})\|$ as the structure and size of $T_C(V_{S(n)})$ are varied in a controlled manner. Fig. 1 shows the results for $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$. For reducible $T_C(V_{S(n)})$, they all have one absorbing state v_n so that $\pi = (0, 0, 0, \dots, 1)$. Following Theorem 3, $\psi_\alpha(\mathbf{s})$ is a redistribution of π and amounts to leakages of the probability mass concentrated on v_n . Essentially, the max norm takes the value $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty = |\pi_{v_n} - \psi_{v_n}|$. Since there are leakages to a maximal subset $V_{S(n)} \setminus \{v_n\}$ of $n - 1$ vertices, $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ for reducible cases would be larger in comparison with the irreducible cases where there are no leakages.

$\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ becomes larger and gets closer to the upper bound $(1 - \frac{1}{n})$ (bold line in Fig. 1) as a result of increasing number of 3-cycles that leads to fewer transitive components in the reducible $T_C(V_{S(n)})$. This is achieved by setting the dominated strong component parts with specific cycle structures from pancyclic with the least number of 3-cycles in B to regular with the most number of 3-cycles (corollary of Theorem 4, [33]) in C.

For irreducible cases, both stationary and PageRank vectors will be nonnegative (all entries > 0) so that $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ are substantially lower than $(1 - \frac{1}{n})$. Intuition suggests that as the number of 3-cycles increases, i.e., towards tournaments with regular cycle structures that have maximum number of 3-cycles and uniform π [12], $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ will decrease. This can be observed by comparing results in D for pancyclic $T_C(V_{S(n)})$ with the least number of 3-cycles and results in E and particularly in F where random $T_C(V_{S(n)})$ become increasingly more regular-like as the number of vertices increases (inset of F).

Computational results indicate that $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ is monotonic with α (see the higher-valued dotted lines in Fig. 1 representing results where larger α values are used for reducible and irreducible cases). $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ gets closer to the upper bound $\|\pi - \mathbf{s}\|_\infty \leq \|\pi_{\text{tran}} - \mathbf{s}\|_\infty = (1 - \frac{1}{n})$ for the reducible A-C cases and $\|\pi - \mathbf{s}\|_\infty$ for the irreducible D-E cases. Although this property was shown explicitly only for irreducible CMCs in Corollary 5, one can argue from the point of leakages and setting a uniform \mathbf{s} that $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ is monotonic for reducible CMCs too.

Sharp bounds can be obtained for CMCs operating on $T_C(V_{S(n)})$ with specific structures in D that consist of pancyclic (maximal transitive subtournament). We note that $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty = |\pi_{v_1} - \psi_{v_1}| \leq \|\pi - \mathbf{s}\|_\infty = |\pi_{v_1} - \frac{1}{n}|$. This coincides with our intuitive understanding how this structure affects PageRank calculation. Redistribution affects vertex v_1 , which shares most of the probability mass with v_n . As in [22], the PageRank authority of v_1 is obtained from a single link $v_n \rightarrow v_1$ even though v_n has the highest authority.

We can calculate this bound directly using digraph-theoretic arguments (see notes after Corollary 8, Appendix A). We have these identities: $H_n = \sum_{k=1}^n \frac{1}{k}$ (n th Harmonic number), $\sum_{i=1}^n H_i = (n+1)(H_{n+1} - 1)$ [40], and $\mathbb{E}(\eta_{V_{S(n-2)}}) = \frac{1}{n-2} \sum_{i=1}^{n-2} H_i$. We apply these identities with $m = n - 2, n \geq 3$ on Equation A.9 in Appendix A to obtain

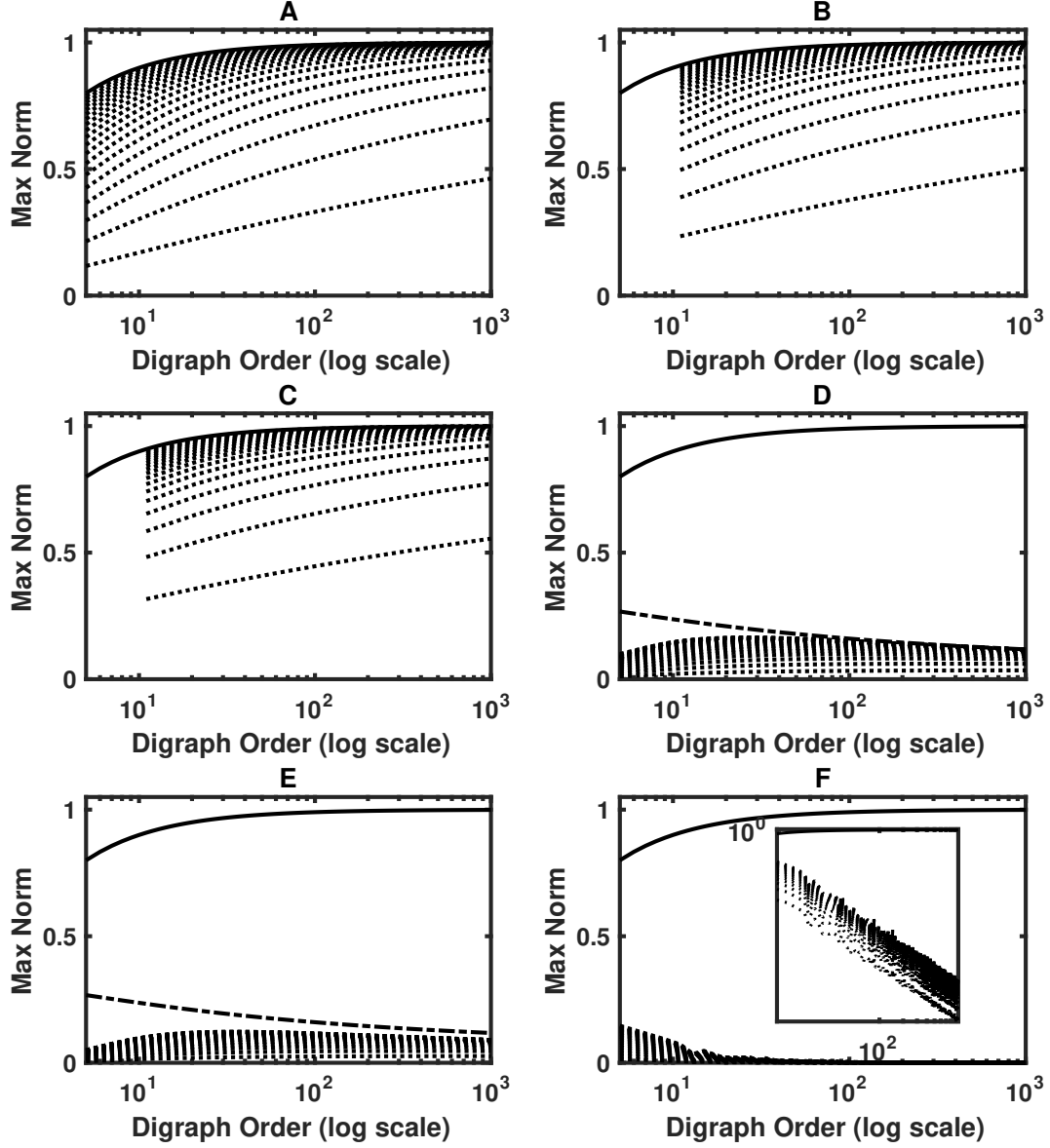


Figure 1: $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ of CMCs operating on tournaments that are (A) transitive, (B) with pancyclic (maximal transitive subtournament) components of order 9, (C) with regular components of order 9, (D) pancyclic (maximal transitive subtournament), (E) pancyclic, and (F) random tournaments of odd order $n \in [5, 999]$. All plots are semilog except the inset of F, which is log-log. Dotted lines indicate $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ for $\alpha \in [0.05, 0.95]$ in steps of 0.05. Upper bounds: $(1 - \frac{1}{n})$ (bold lines) and $(\frac{a_1}{a_2 + H_{m+1}} - \frac{1}{m+2})$ (dash-dot lines in D-E).

$$\pi_{v_1} = \frac{1}{2} \left(1 - \frac{\frac{1}{m} \sum_{i=1}^m H_i}{2 + \frac{1}{m} \sum_{i=1}^m H_i} \right)$$

$$\begin{aligned}
&= \frac{1}{2} \left(1 - \frac{\frac{1}{m}(m+1)(H_{m+1}-1)}{2 + \frac{1}{m}(m+1)(H_{m+1}-1)} \right) \\
&= \frac{a_1}{a_2 + H_{m+1}}
\end{aligned}$$

where $a_1 = \frac{m}{m+1}$ and $a_2 = \frac{m-1}{m+1}$. Then,

$$\|\pi - \psi_\alpha(\mathbf{s})\|_\infty \leq \left(\frac{a_1}{a_2 + H_{m+1}} - \frac{1}{m+2} \right).$$

For these tournaments with large but finite number of vertices $n = m+2$, the right-hand side of the inequality is dominated by the reciprocal of H_{m+1} (since H_{m+1} grows logarithmically) and is bounded away from zero [40]. Equality is obtained only for $m = 1$ where the right-hand side of the inequality is zero. This corresponds to the isomorphic pancyclic tournament of $n = 3$ vertices, which is regular and has $\|\pi - \psi_\alpha(\mathbf{s})\| = 0$.

Fig. 2 shows the results for $\|\pi - \psi_\alpha(\mathbf{s})\|_1$ for the same set of experiments. The upper-bound $\|\pi - \psi_\alpha(\mathbf{s})\|_1 \leq 2(1 - \frac{1}{n})$ is plotted as a bold line while $\|\pi - \psi_\alpha(\mathbf{s})\|_1 \leq \frac{2}{1-\alpha} \left(1 - (\pi_{v_n} - \frac{1}{n}) \right)$ is plotted as a dash-dot line in Fig. 2. For reducible A-C cases with one absorbing state v_n , we can verify numerically that $\|\pi - \psi_\alpha(\mathbf{s})\|_1 = 2\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$. Any leakage that is measured by the max norm would be redistributed over all other states. The one norm cumulatively adds these leakages in addition to that given by the max norm for v_n . Crucially, this leakage relationship extends to that between the digraph-theoretic-derived upper-bounds since $\|\pi - \psi_\alpha(\mathbf{s})\|_1 \leq 2(1 - \frac{1}{n})$ and $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty \leq (1 - \frac{1}{n})$.

We now turn our attention to experiments involving reducible $T_C(V_{S(n)})$ generated from the network-growth-based methodology and consider $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ only. Fig. 3 shows results where the temperature $1/\gamma$ for the system is increased from A to D. At a lower temperature in A, random orientations of edges generated as a result of introducing a new node at each iteration of the method are biased towards existing nodes with higher scores. This leads to more prominent transitive structures in $T_C(V_{S(n)})$, detected by computing its Landau's index ν [12] that gives the number of strong components in $T_C(V_{S(n)})$. ν ranges at [8, 49], [8, 39], [7, 47] for experiments with the final generated $T_C(V_{S(n)})$ at $n = 100, 500$, and 1000 , respectively. At higher temperatures, $T_C(V_{S(n)})$ generated in B-D have two strong components only (a single dominant node and a strong dominated component of $n - 1$ nodes). A higher $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ value is a result of the larger-sized, strong dominated component drawing out more probability mass away from the absorbing dominant node (more leakages).

3.3. Results For PageRanking Coevolutionary Tournaments

The PageRank vector $\psi_\alpha(\mathbf{s})$ gives the visitation probabilities ψ_{v_i} that ranks the importance (performance) of vertices $v_i \in V_{S(n)}$ representative of the underlying structure of their pairwise relations in the coevolutionary digraph $D_C(V_{S(n)})$. We *PageRank* (index) the importance of these vertices in the same manner as their score sequence for consistency. Let $\tau : \{\psi_{v_i}\}_i^n \rightarrow \mathbb{Z}_k^n$ be the PageRanks of the vertices $v_i \in V_{S(n)}$ of $D_C(V_{S(n)})$, with visitation probabilities $\{\psi_{v_i}\}_i^n$ and $\mathbb{Z}_k^n = \{1, 2, 3, \dots, n\}$. Vertices are *PageRanked* in the ascending order from the least important $\tau(v_1) = 1$ to the most important $\tau(v_n) = n$. Ties are handled in the usual manner through fractional (average) ranks [41]. In our experiments, we generate tournaments and strong components of odd orders so that tied ranks can be assigned with the median (integer) value.

For transitive $T_C(V_{S(n)})$, results show that the ranking of vertices from τ is the same as that of score sequences $(d_T^-(v_i))_i^n$ even for high α setting. How about irreducible $T_C(V_{S(n)})$ with prominent transitive structures? In the case of the pancyclic (maximal transitive subtournament) $T_C(V_{S(n)})$, visitation probabilities are sorted as $\psi_{v_2} < \psi_{v_3} < \psi_{v_4} < \dots < \psi_{v_{n-1}} < \psi_{v_1} < \psi_{v_n}$, for reasonably low α settings. Unlike the situation with the stationary probability vector where the two highest ranks are tied since $\pi_{v_1} = \pi_{v_n}$, PageRank is able to distinguish between v_1 and v_n .

If such a structure is embedded within a reducible $T_C(V_{S(n)})$ (as one may encounter in real-world problems with such complex structures), PageRank can be used to uncover this strong component structure for small-sized $T_C(V_{S(n)})$ where the issue of scale does not arise although the analysis can be more nuanced. For

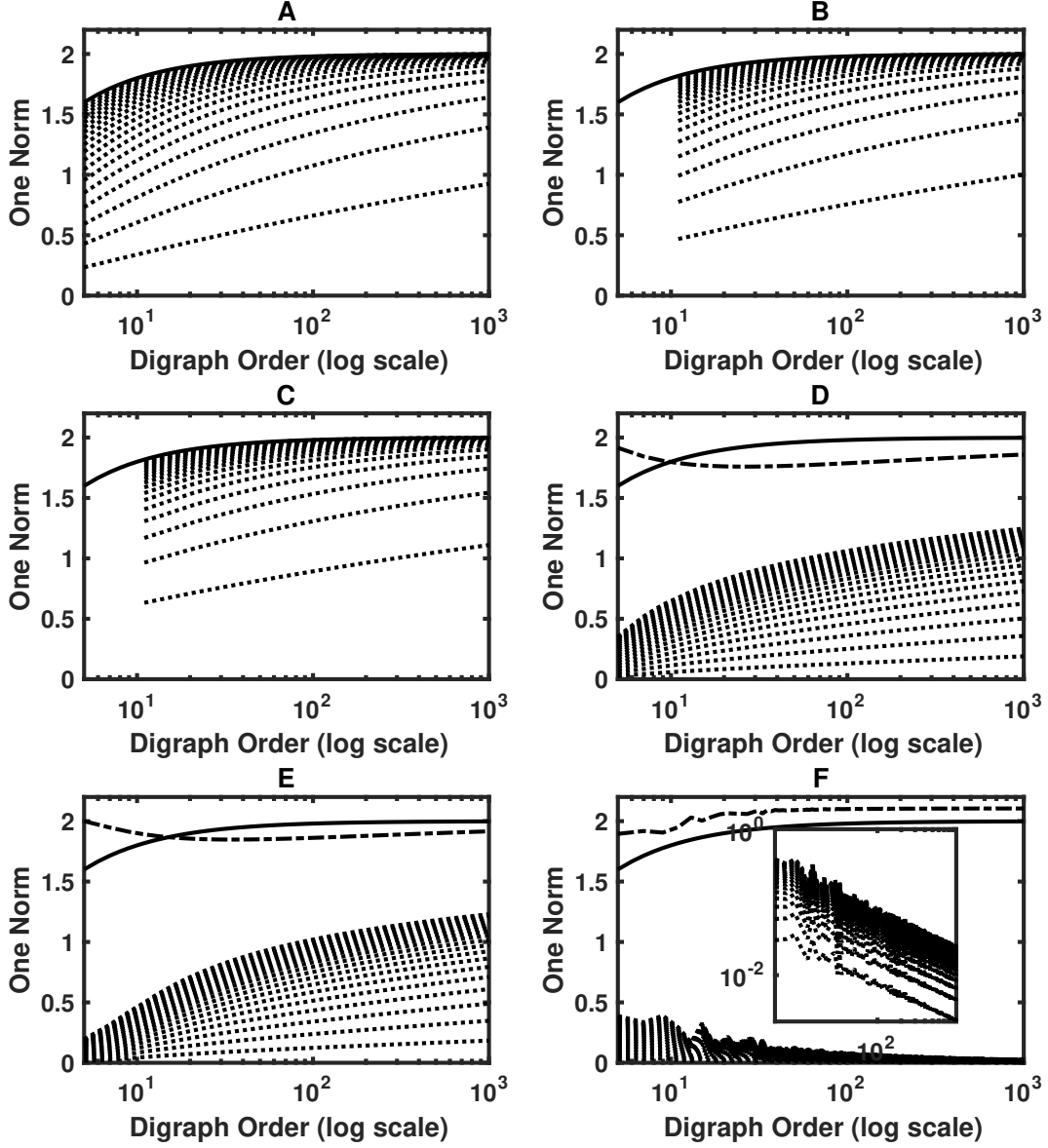


Figure 2: $\|\pi - \psi_\alpha(\mathbf{s})\|_1$ of CMCs operating on tournaments that are (A) transitive, (B) with pancyclic (maximal transitive subtournament) components of order 9, (C) with regular components of order 9, (D) pancyclic (maximal transitive subtournament), (E) pancyclic, and (F) random tournaments of odd order $n \in [5, 999]$. All plots are semilog except the inset of F, which is log-log. Dotted lines indicate $\|\pi - \psi_\alpha(\mathbf{s})\|_1$ for $\alpha \in [0.05, 0.95]$ in steps of 0.05. Upper bounds: $2(1 - \frac{1}{n})$ (bold lines) and $\frac{2}{1-\alpha} \left(1 - (\pi_{v_n} - \frac{1}{n})\right)$ at $\alpha = 0.05$ setting (dash-dot lines in D-F).

example, consider the case whereby the strong component is pancyclic (maximal transitive subtournament). Nodes v_{62} and v_{63} (inset of Fig. 4A) have the same out-degree globally ($d_T^-(v_{62}) = d_T^-(v_{63})$) and within the strong component, the least number of just one outgoing link locally. However, v_{62} has a higher PageRank

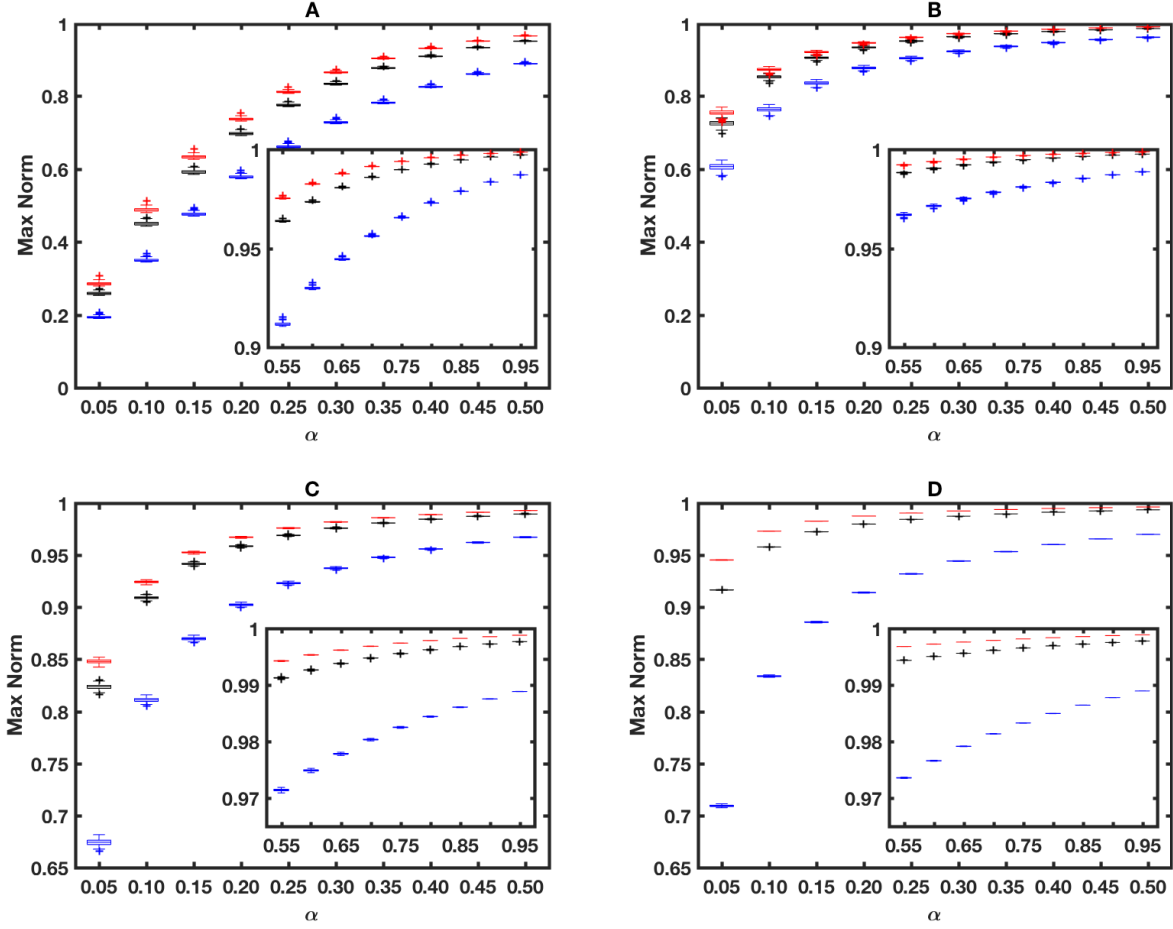


Figure 3: $\|\pi - \psi_\alpha(\mathbf{s})\|_\infty$ of CMCs operating on reducible tournaments that are generated from a network-growth-based methodology with γ set to (A) 2.0, (B) 0.1, (C) 0.05, and (D) 0.01. Box plots in blue (bottom), black (middle), and red (top) represent results where the final generated tournaments are of order 100, 500, and 1000, respectively.

authority than v_{63} . Together both information would indicate that they are part of a strong component that dominates all other vertices $\{v_1, v_2, v_3, \dots, v_{61}\}$. If the strong component is regular, PageRanks are the same for those vertices (inset of Fig. 4B). Regardless, our setting (uniform \mathbf{s}) is to provide a global view [14]. For reducible $T_C(V_{S(n)})$, there would be a general increase in visitation probabilities ψ_{v_i} for vertices with higher scores and that vertices in the absorbing class have significantly larger values (in Fig. 4, both tournaments are reducible with a single dominant vertex).

3.4. Results For Differences in Rank Aggregation

It is known that setting α appropriately can improve the convergence rate of the Power Method (Theorem 5.1 in [23]) to compute PageRanks at the expense of increasing perturbations on PageRank authorities and subsequently the actual PageRank orderings [37]. We study the impact of α on PageRanks by computing the differences between PageRanks at baseline $\alpha = 0.05$ setting and those obtained from using higher α settings. There are various approaches to calculate this difference through rank aggregation. We use a form of the Spearman footrule distance [42].

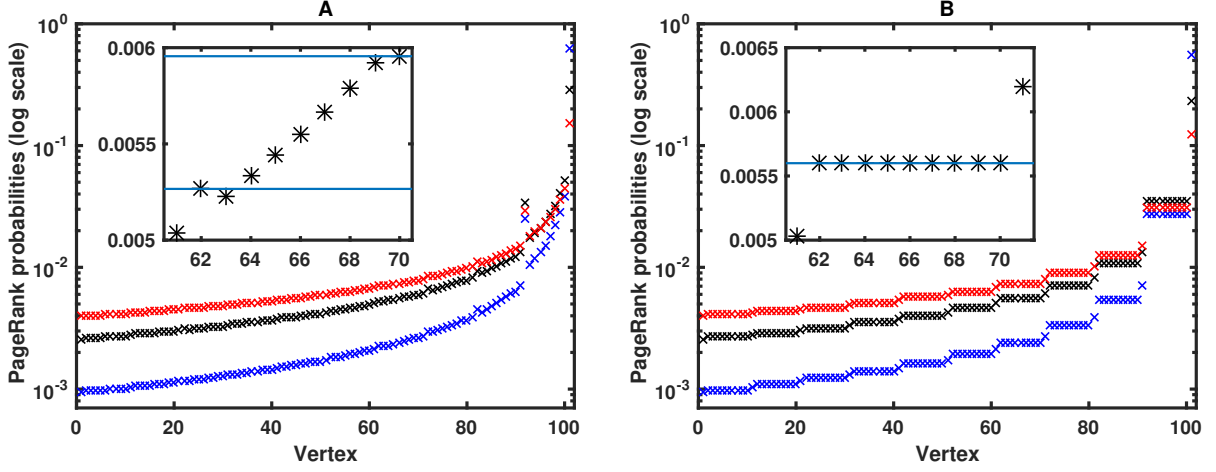


Figure 4: Visitation probabilities (PageRank vector) of the CMC with restart on the vertices of reducible tournaments of order 101 (A) with pancyclic (maximal transitive subtournament) components of order 9 and (B) with regular components of order 9. Plots with blue (bottom), black (middle), and red (top) crosses are for the visitation probabilities where α is set to 0.05, 0.15 and 0.25, respectively. Insets show the visitation probabilities where $\alpha = 0.25$ for one of the strong components. Vertices are sorted according to their score sequences.

For $T_C(V_{S(n)})$ of odd orders n , we can calculate this distance

$$d_{\text{spear}}(\tau_1, \tau_2) = \frac{4}{n^2 - 1} \sum_{i=1}^n |\tau_1(v_i) - \tau_2(v_i)| \quad (9)$$

where the normalizing constant is given by the maximum of the sum of absolute differences $\max d(\tau_1, \tau_2) = \frac{n^2 - 1}{4}$. This can be obtained in the same manner as the Spearman's rank correlation [41] by calculating the distance obtained from completely opposed rankings of $1, 2, 3, \dots, n$ and $n, n-1, n-2, \dots, 1$ that also take into account directional duals of labelled tournaments [35]. The maximum distance is the same as in the case of the distance between that of transitive and regular tournaments. We also compute the average rank difference

$$d_{\text{avg}}(\tau_1, \tau_2) = \frac{1}{n} \sum_{i=1}^n |\tau_1(v_i) - \tau_2(v_i)|. \quad (10)$$

$d_{\text{avg}}(\tau_1, \tau_2)$ would be a useful comparison with $d_{\text{spear}}(\tau_1, \tau_2)$ for experiments where the n^2 factor could mask the effect of small rank differences for certain large tournaments.

In general, higher α settings would lead to more perturbations to PageRanks measured by larger $d(\tau_1, \tau_2)$ values (e.g. the bold lines in Fig. 5). However, increasing the size of the generated $T_C(V_{S(n)})$ leads to lower $d(\tau_1, \tau_2)$ values, indicating that changes to PageRanks are localized to certain vertices. For example, this is usually v_1 for pancyclic (maximal transitive subtournament) $T_C(V_{S(n)})$ in A-B. Beyond specific structures in $T_C(V_{S(n)})$, our results indicate that the presence of prominent transitive structures (A-B) and those that forces reducibility (C-D) would localize perturbations of PageRanks to a small number of vertices, leading to lower $d(\tau_1, \tau_2)$ values as $T_C(V_{S(n)})$ increases in size.

4. Discussion and Conclusion

One important issue dealing with problems in competitive settings is how problem structures can affect the performance of solutions discovered by iterative means. Under some assumptions, coevolutionary processes can be represented as Markov chain models operating on digraphs that capture preference relations

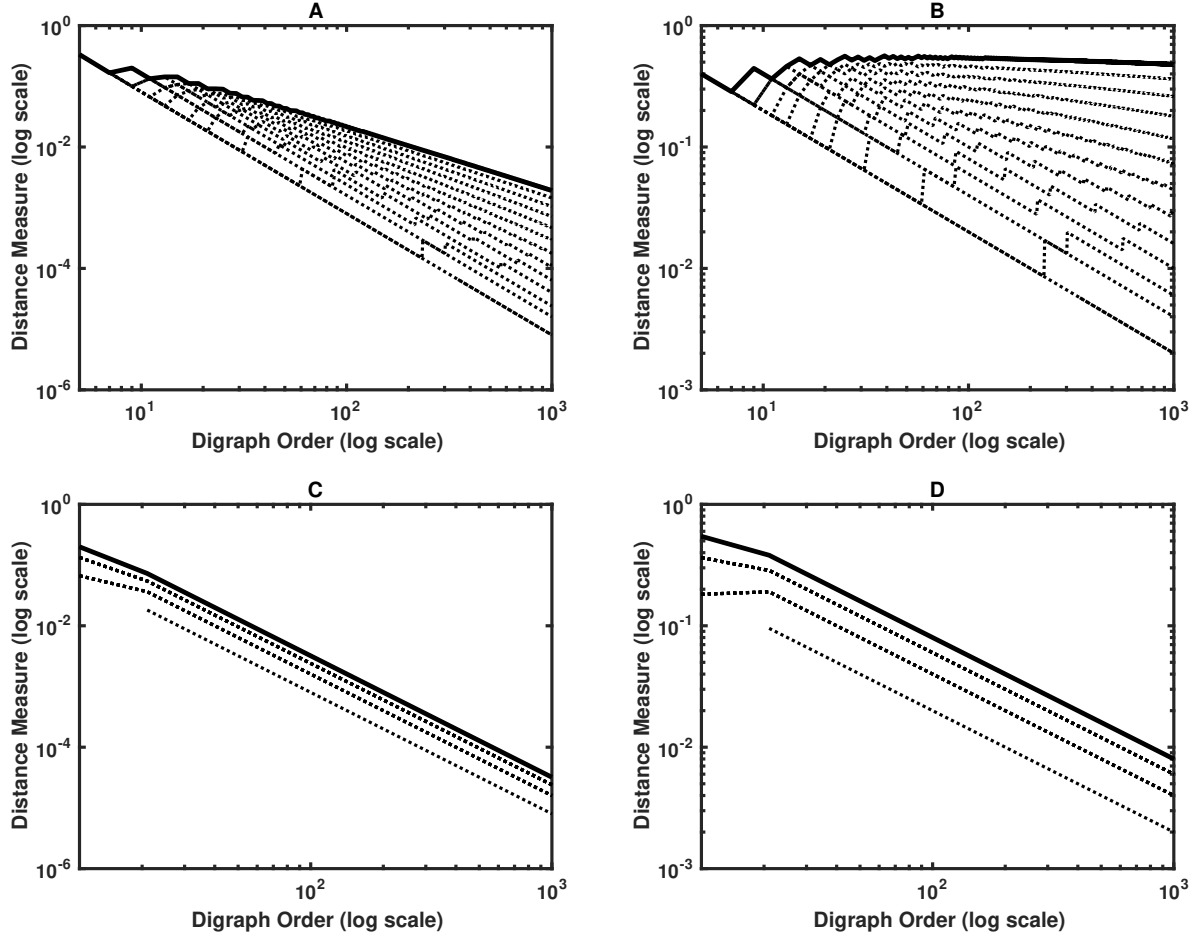


Figure 5: Differences of PageRanks for coevolutionary tournaments that are irreducible having (A)-(B) pancyclic (maximal transitive subtournament) structures and reducible having (C)-(D) pancyclic (maximal transitive subtournament) components of order 9. Plots in (A) and (C) are for $d_{\text{spear}}(\tau_1, \tau_2)$ and (B) and (D) are for $d_{\text{avg}}(\tau_1, \tau_2)$. Dotted lines show difference from baseline PageRanks obtained with $\alpha = 0.05$ to PageRanks obtained from setting higher $\alpha \in [0.10, 0.90]$. Bold lines are the case where $\alpha = 0.95$.

between competing solutions to those problems. As a consequence, we are able to establish a direct and formal connection between the Markov chain model of coevolutionary processes and PageRank operating on such digraphs. This lets us develop a principled approach for quantitative characterization of coevolutionary digraphs. This PageRank characterization of a coevolutionary digraph measures and ranks the performance of individual solutions.

Our theoretical support involves interdisciplinary studies in large-scale coevolutionary systems, Markov models of PageRank and digraph theory. We provide guarantees of the existence of PageRank for any coevolutionary system. We prove the PageRank vector to be a redistribution of the stationary vector associated with coevolutionary Markov chains (CMCs) operating on coevolutionary digraphs. This is a result of introducing restarts in the coevolutionary process. Subsequent changes in the PageRank authorities due to different probability α can be quantified precisely. We obtain loose theoretical bounds that cover coevolutionary digraphs of any cycle structure. However, there are cases where we exploit qualitative knowledge of digraph structures to obtain sharp bounds. We consider a restricted class of population-one coevolutionary systems, which covers other learning algorithms involving self play. The advantage is the coevolutionary digraph captures all underlying structures induced by the pairwise preferences over solutions

for the problem under consideration. Specific reducible digraphs would cover evolutionary cases as in recent studies that apply PageRank to evolutionary systems [43].

Although the main motivation of our study is to address the fundamental challenge arising from performing quantitative analysis on coevolutionary systems with little prior qualitative knowledge of the problem structures, our technical contributions are general and can be applied to other problem areas whereby the model one adopts is a random walk on semicomplete digraphs (an edge can be bioriented) that include the more specific case of complete oriented graphs. The resulting finite-state Markov chains are non-reversible. Most classical results for such models focus on irreducible Markov chains (via the Perron-Frobenius Theorem). Our technical work has used recent results from random walks on digraphs and matrix analysis to characterize changes to the behavior of the random walk on semicomplete digraphs (through its stationary distribution) as the parameter that controls the rate of restart is changed, qualitatively and quantitatively. Furthermore, we empirically study (and argue from a leakage perspective) the case when the underlying digraph structure is reducible.

Coevolutionary systems are notoriously difficult to study. One consequence is that different aspects of these systems are typically, though not always, studied in isolation using a variety of common frameworks. Even within a single framework, one could apply different methodologies given the interplay between coevolutionary systems’ design, problem structures, and dynamics. For example, studies on coevolutionary dynamics in an evolutionary game theoretic setting from a continuous dynamical systems framework focus on population-level analysis with respect to the constituents or mixtures of pure strategies. [9] provided quantitative characterizations of these dynamics to different regimes (e.g., from simple attractive to periodic and complex chaotic dynamics) based on numerically generated trajectories as a result of different selection mechanisms. We [10] introduced the means by which qualitative determination of shadowing property in coevolutionary systems can be made based on the notion of structural stability from the dynamical systems theory. This is of main interest in complex coevolutionary dynamics studies: If one can demonstrate that the underlying dynamics is characterized by coexistence of both unstable and stable features (one can have divergence of a noise-affected pseudo-trajectory from the true trajectory, but still the corrupted trajectory is shadowed by another nearby true trajectory), it would thus make it possible to use numerically generated pseudo-trajectories as faithful representations of the complex dynamics. In addition, such theory can provide links between infinite and finite population models [10].

Another example is the various studies within a pareto coevolution framework. Here, the common aspect taken is the evaluation of individual coevolving solution using a set of test cases, usually described from the perspective of pareto dominance in a multi-objective optimization setting. However, unlike the evolutionary setting, in pareto coevolution each test case is an objective that has to be optimized. In a typical problem domain such as games, there could arise situations where there are no obvious dominant subset of solutions and that coevolutionary search would cycle. [44] introduced a problem generation methodology whereby specific attributes (e.g., intransitivity) in the test objectives giving rise to complex coevolutionary dynamics (e.g. cyclic) can be introduced in a controlled manner. [45] developed coevolutionary algorithms that could detect and exploit ‘gradients’ (pareto covering order) between individual layers or subsets of non-dominated solutions. [46] comprehensively develop theoretical underpinnings via category and group theory to show how functional specification for the evaluation of solutions via test cases can be formalized, among others, to impose a pareto covering order on the solution set, and to study the emergence of geometric organization on the test set that can be exploited for more informative pareto coevolutionary search (comparison) of solutions.

There are other frameworks (e.g., based on machine learning methodologies [47, 48, 49]) but one can immediately appreciate challenges associated with complete understanding of coevolutionary systems given the breadth and depth of available frameworks for study. Are there obvious connections between these frameworks, for example, that of pareto coevolution with the framework of digraph representation of coevolutionary problems and random walks for coevolutionary processes we introduced earlier in [12]? One close connection is that the formal methodology to uncover the structure of the pairwise comparison space in [46] and the qualitative characterization of the underlying structures in coevolutionary digraphs in [12] are both crucial for the design and analysis of effective pareto coevolutionary search. For any competitive coevolutionary problem, qualitative knowledge of the problem is crucial towards obtaining guarantees that it can be

solved because there exist a dominant subset of solutions. Its underlying reducible coevolutionary digraph would admit a decomposition over the solution set into strong components having an acyclic ordering. When one by design uses the solution set itself for evaluations in pareto coevolution, the induced pareto covering order on the solution set (search space) suggests a structure that can be exploited for coevolutionary search between those pareto layers and eventually the single dominant subset of solutions.

As a further illustration of the complementary nature of these two frameworks, one can setup an inductive argument for a program that can perform pseudo-embedding of coevolved solutions:

1. Take a transitive tournament of $n \geq 4$ vertices labelled $\{v_i\}_1^n$ according to its score sequence with an ordering $s_1 < s_2 < s_3 < \dots < s_n$.
2. Perform a single arc reversal on $v_1 v_n$ to $v_n v_1$ to obtain a pancyclic (maximal transitive subtournament) tournament.
3. The pancyclic tournament is pseudo-embedded on \mathbb{N}^2 with the linear realiser $L = \{(\cdot)_X, (\cdot)_Y\} = \{([v_1], [v_2], [v_3], \dots, [v_n]), ([v_n], [v_2], [v_3], \dots, [v_1])\}$.

We use the notation $L = \{(\cdot)_X, (\cdot)_Y\}$ to indicate that the pseudo-embedding can be visualised as a \mathbb{N}^2 -space spanned along the x-axis by $(\cdot)_X$ and along the y-axis by $(\cdot)_Y$. The specific pancyclic structure whereby the subtournament with $n - 2$ vertices $v_2, v_3, v_4, \dots, v_{n-1}$ is always transitive allows one to setup an inductive argument and use the above program to do the pseudo-embedding for tournaments of $n \geq 4$ vertices. The inductive step can be visualized as moving the embedded line of points specified by the two ends from $\{(v_1, v_n), (v_n, v_1)\}$ to $\{(v_1, v_{n+1}), (v_{n+1}, v_1)\}$ – in the latter one adds an additional point corresponding to the vertex that forms the transitive subtournament $v_2, v_3, v_4, \dots, v_n$. It would be of interest in future studies to examine pseudo-embedding of other strong tournaments, for example, beyond \mathbb{N}^2 -space.

Although we could construct quantitative measures for analysis of coevolutionary processes from [12], there remains the issue that these measures require prior qualitative knowledge about the structure of the digraph. Instead, one could take on the perspective of coevolution on what it views as important (how often it searches) a solution in the space. The quantity of interest is the stationary distribution of the CMC. However, coevolution on reducible digraphs corresponds to an absorbing CMC – the visitation probabilities will be concentrated entirely on the dominant subset. The other remaining vertices would have zero probabilities, and in this case, we would have no knowledge about the structures underlying them (whether they are reducible or irreducible). Even for irreducible CMC, one needs some prior knowledge about the structure of the digraph to interpret those quantities. PageRank addresses this issue by incorporating in its formalism information of the network (digraph) structure that we show explicitly in Section 2.3, which we further demonstrate via controlled experiments in Section 3.3. Unlike CMC without restart, PageRank authorities are able to distinguish common structures associated with reducible and irreducible coevolutionary tournaments of various degree of complexity. Further characterization would require some additional prior knowledge of the digraph structure, for example, as in the case of characterizing pancyclic (maximal transitive subtournaments) tournaments with the knowledge of the two vertices with the most and least number of incoming arcs. Our empirical results also corroborate with our understanding of random walks on irreducible tournaments with prominent transitive structures (detailed in full in Corollary 8 and its subsequent notes in the Appendix section). The prominent transitive structures themselves force most of the transfer in authorities to be localized to a small subset of vertices when one PageRank these tournaments so that the loss of information (that we measure as perturbations of PageRanks) is reduced.

This study is focused on laying down the foundations so that relevant quantitative analysis can be made although there are real challenges associated with large, real-world coevolutionary systems. On the one hand, PageRank can be used as a quantitative analysis tool for which new methods to discover and exploit digraph structures (locally and globally) would be needed to obtain the relevant characterizations for large-scale and complex systems. Unlike other problem domains with sparse \mathbf{P} [14] for which there exists methods to speed up computation [23], there are at least half of nonzero entries in \mathbf{P} for coevolutionary systems by definition. On the other hand, PageRank’s dual nature means it can be interpreted as a CMC with restart. One has algorithmic implementation of the random walk but very little is known about \mathbf{P} (e.g., there is a search space induced by the choice of player representation and genetic operators, but one has no direct

access to the solution space). In practice, relatively short runs are taken so that only some small regions of the search space are visited. More studies on how one can in principle aggregate these runs to build a relevant picture of the search would be needed.

Our technical approach extends the rich area in the study of random walks generalized to digraphs. In particular, [26] has introduced a symmetric form of digraph Laplacian to examine links between PageRank and other frameworks associated with random walks and electrical networks. This is generalized by [30] that examines the impact of asymmetry in the digraph Laplacian on random walks operating on a digraph, in addition to the derivation of quantities such as hitting times associated with it. In comparison, our study here considers non-reversible CMCs operating on both irreducible and reducible digraphs, in particular, the class of semicomplete digraph for which an edge of its underlying complete graph can be bioriented (having two parallel arcs with opposing directions), and the specific limiting case in the form of a complete oriented graph for which there is only one arc (a single oriented edge) between each pair of vertices. Our approach is motivated by insights from digraph and specifically tournament theory for which we can develop a more natural formalism to study coevolution as random walks on specific digraphs that represent problem structures that are common to the problem domain (modelled as two-player strategic games). There has been recent works, for example in [50] that has developed a full electrical network behind non-reversible Markov chains by replacing the single resistor with a non-symmetric component. The study does not consider electrical networks with totally asymmetric components in the form of oriented graphs. [51] derive formulas for expected hitting times of random walks on graphs in terms of voltages. However, as in our approach, the underlying core building block in such approaches is the notion of Markov chain. For future studies, it would be of interests to consider these alternative frameworks for coevolutionary problems taking on the form of two-player strategic games whereby the outcomes are probabilistic.

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Appendix A. Complete Proofs for Theoretical Results Listed in Main Texts

Lemma 1. *Let $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be a coevolutionary digraph. Let \mathbf{P} be the probability transition matrix associated with a CMC operating on $D_C(V_{S(n)})$ and $\mathbf{Z} = (\mathbf{I} + \mathbf{P})/2$ its lazy version. The row vector \mathbf{s} is the probability distribution over the set vertices $V_{S(n)}$. Given $\alpha \in (0, 1)$ and $\beta = \frac{2\alpha}{1-\alpha}$, the personalized PageRank vector is the unique solution to the linear system defined as*

$$\psi_\alpha(\mathbf{s}) = \alpha \mathbf{s} + (1 - \alpha) \psi_\alpha(\mathbf{s}) \mathbf{Z} \quad (\text{A.1})$$

and can be computed as

$$\psi_\alpha(\mathbf{s}) = \beta \mathbf{s} (\beta \mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1}. \quad (\text{A.2})$$

Proof: We can rewrite Equation A.1 as follows

$$\begin{aligned} \psi_\alpha(\mathbf{s}) &= \alpha \mathbf{s} + (1 - \alpha) \psi_\alpha(\mathbf{s}) \mathbf{Z} \\ \psi_\alpha(\mathbf{s}) (\alpha \mathbf{I} + (1 - \alpha) \mathbf{I} - (1 - \alpha) \mathbf{Z}) &= \alpha \mathbf{s} \\ \psi_\alpha(\mathbf{s}) (\mathbf{I} + \frac{(1 - \alpha)}{2\alpha} (\mathbf{I} - \mathbf{P})) &= \mathbf{s} \\ \psi_\alpha(\mathbf{s}) (\mathbf{I} + \frac{(1 - \alpha)}{2\alpha} (\mathbf{I} - \mathbf{P})) &= \mathbf{s} \end{aligned}$$

so that now it can be expressed in the usual matrix form for linear systems

$$\psi_\alpha(\mathbf{s}) (\beta \mathbf{I} + (\mathbf{I} - \mathbf{P})) = \beta \mathbf{s} \quad (\text{A.3})$$

where $\beta = \frac{2\alpha}{1-\alpha} > 0$.

$\beta\mathbf{I} + (\mathbf{I} - \mathbf{P})$ is a *strictly dominant diagonal matrix* and so is nonsingular (invertible) [27]. This can be proven as follows. Let $\mathbf{W} = \beta\mathbf{I} + (\mathbf{I} - \mathbf{P}) = (1 + \beta)\mathbf{I} - \mathbf{P}$. Since \mathbf{P} is a row stochastic matrix, then for each row i , $\sum_{j \neq i} |w_{ij}| \leq 1$. But $|w_{ii}| = 1 + \beta > \sum_{j \neq i} |w_{ij}|$ for $\beta > 0$. \square

Lemma 2. Let $\psi_\alpha(\mathbf{s})(\beta\mathbf{I} + (\mathbf{I} - \mathbf{P})) = \beta\mathbf{s}$ be the formulation of the PageRank problem as a linear system. The coefficient matrix $\mathbf{W} = \beta\mathbf{I} + (\mathbf{I} - \mathbf{P})$ has the following properties:

1. \mathbf{W} is an M-matrix.
2. \mathbf{W} is nonsingular.
3. The row sums of \mathbf{W} are β .
4. $\|\mathbf{W}\|_\infty = 2 + \beta$.
5. $\mathbf{W}^{-1} \geq \mathbf{0}$.
6. The row sums of \mathbf{W}^{-1} are $\frac{1}{\beta}$.
7. $\|\mathbf{W}^{-1}\|_\infty = \frac{1}{\beta}$.
8. $\kappa_\infty(\mathbf{W}) = \frac{2+\beta}{\beta} = \frac{1}{\alpha}$.

Proof: The properties of \mathbf{W} and their proofs follow a similar exposition in [23]. Let $\mathbf{R}^{n \times n}$ be the set of real, square $n \times n$ matrices. $\mathbf{A} \in \mathbf{R}^{n \times n}$ is an M-matrix if it can be written in the form $\mathbf{A} = c\mathbf{I} - \mathbf{B}$, where $\mathbf{B} \geq \mathbf{0}$ (i.e., $\mathbf{B} = (b_{ij} \geq 0 : 1 \leq i, j \leq n)$) and $c \geq \rho(\mathbf{B})$ with $\rho(\cdot)$ denoting the spectral radius (Chapter 6, [28]). Then, we have the following.

1. \mathbf{W} is an M-matrix: $\mathbf{W} = \beta\mathbf{I} + (\mathbf{I} - \mathbf{P}) = c\mathbf{I} - \mathbf{B}$ where $c = 1 + \beta$ and $\mathbf{B} = \mathbf{P}$. Applying the Perron-Frobenius Theorem to the stochastic matrix \mathbf{P} , $\rho(\mathbf{P}) = \|\mathbf{P}\|_\infty = 1$ (Chapter 8, [19]). Obviously, $c = 1 + \beta > \rho(\mathbf{P}) = 1$ for $\beta > 0$. As such, \mathbf{W} is an M-matrix.
2. \mathbf{W} is nonsingular: This was shown earlier in the proof for Lemma 1.
3. The row sums of \mathbf{W} are β : Note that for each row i , $w_{ii} - \sum_{j \neq i} w_{ij} = (1 + \beta) - 1 = \beta$. So, $\mathbf{W}\mathbf{e}^T = \beta\mathbf{e}^T$ where \mathbf{e}^T is the column vector of ones.
4. $\|\mathbf{W}\|_\infty = 2 + \beta$: Applying the definition of ∞ -norm [19], $\|\mathbf{W}\|_\infty = \max_i \sum_j |w_{ij}| = 2 + \beta$.
5. Since \mathbf{W} is an M-matrix, then $\mathbf{W}^{-1} \geq \mathbf{0}$: This is simply a direct application of Theorem 2.3 in Chapter 6 of [28]. Since \mathbf{W} is a nonsingular M-matrix, it is *inverse-positive*, i.e., \mathbf{W}^{-1} exists and $\mathbf{W}^{-1} \geq \mathbf{0}$.
6. The row sums of \mathbf{W}^{-1} are $\frac{1}{\beta}$: We note

$$\begin{aligned} \mathbf{W}\mathbf{e}^T &= \beta\mathbf{e}^T \\ \frac{1}{\beta}\mathbf{e}^T &= \mathbf{W}^{-1}\mathbf{e}^T. \end{aligned}$$

7. $\|\mathbf{W}^{-1}\|_\infty = \frac{1}{\beta}$: Since $\mathbf{W}^{-1} \geq \mathbf{0}$ and $\mathbf{W}^{-1}\mathbf{e}^T = \frac{1}{\beta}\mathbf{e}^T$, then $\|\mathbf{W}^{-1}\|_\infty = \frac{1}{\beta}$.
8. $\kappa_\infty(\mathbf{W}) = \frac{2+\beta}{\beta} = \frac{1}{\alpha}$: The condition number κ for a nonsingular \mathbf{A} is $\|\mathbf{A}\| \|\mathbf{A}^{-1}\|$ [19]. Applying results in (4) and (7) with $\beta = \frac{2\alpha}{1-\alpha}$, we have

$$\begin{aligned} \kappa_\infty(\mathbf{W}) &= \|\mathbf{W}\|_\infty \|\mathbf{W}^{-1}\|_\infty \\ &= \frac{2 + \beta}{\beta} \\ &= \frac{1}{\alpha}. \end{aligned}$$

\square

Theorem 3. Let $\boldsymbol{\pi}$ be the stationary vector associated with a CMC operating on an irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$. The personalized PageRank vector is given by

$$\psi_\alpha(\mathbf{s}) = \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}}). \quad (\text{A.4})$$

Furthermore,

$$\lim_{\beta \rightarrow 0} \tilde{\mathcal{L}}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} = \tilde{\mathcal{L}}(\tilde{\mathcal{L}})^+ = \tilde{\mathcal{L}}\tilde{\mathcal{Z}}$$

where $\beta = \frac{2\alpha}{1-\alpha}$ and $\tilde{\mathcal{Z}} = \tilde{\mathcal{L}}^+$ is the Moore-Penrose pseudoinverse of $\tilde{\mathcal{L}}$. For small values of α (subsequently, small values of β), the PageRank vector is approximated by the stationary vector, i.e., $\psi_\alpha(\mathbf{s}) \approx \boldsymbol{\pi}$ with equality ($\psi_0(\mathbf{s}) = \boldsymbol{\pi}$) for any \mathbf{s} .

Proof: Since $\tilde{\mathcal{L}} = \boldsymbol{\Pi}^{\frac{1}{2}}(\mathbf{I} - \mathbf{P})\boldsymbol{\Pi}^{-\frac{1}{2}}$ can be rewritten as $(\mathbf{I} - \mathbf{P}) = \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\boldsymbol{\Pi}^{\frac{1}{2}}$,

$$\begin{aligned} (\beta \mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1} &= (\beta \mathbf{I} + \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\boldsymbol{\Pi}^{\frac{1}{2}})^{-1} \\ &= (\beta \mathbf{I})^{-1} - (\beta \mathbf{I})^{-1}\boldsymbol{\Pi}^{-\frac{1}{2}}(\mathbf{I} + \tilde{\mathcal{L}}\boldsymbol{\Pi}^{\frac{1}{2}}(\beta \mathbf{I})^{-1}\boldsymbol{\Pi}^{-\frac{1}{2}})^{-1}\tilde{\mathcal{L}}\boldsymbol{\Pi}^{\frac{1}{2}}(\beta \mathbf{I})^{-1} \\ &= (\beta \mathbf{I})^{-1} - (\beta \mathbf{I})^{-1}\boldsymbol{\Pi}^{-\frac{1}{2}}(\mathbf{I} + \tilde{\mathcal{L}}(\beta \mathbf{I})^{-1})^{-1}\tilde{\mathcal{L}}(\beta \mathbf{I})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}} \\ &= (\beta \mathbf{I})^{-1} - (\beta \mathbf{I})^{-1}\boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta \mathbf{I})^{-1}(\mathbf{I} + \tilde{\mathcal{L}}(\beta \mathbf{I})^{-1})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}} \\ &= \frac{1}{\beta}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}}). \end{aligned}$$

On the second line, we used the generalized identity for the inverse of a sum of matrices $(\mathbf{A} + \mathbf{UBV})^{-1} = \mathbf{A}^{-1} - \mathbf{A}^{-1}\mathbf{U}(\mathbf{I} + \mathbf{BVA}^{-1}\mathbf{U})^{-1}\mathbf{BVA}^{-1}$ where \mathbf{A} is nonsingular and \mathbf{U} , \mathbf{B} , and \mathbf{V} are square matrices in our case. On the fourth line, we used the identity $(\mathbf{I} + \mathbf{C})^{-1}\mathbf{C} = \mathbf{C}(\mathbf{I} + \mathbf{C})^{-1}$ where for any \mathbf{C} , $(\mathbf{I} + \mathbf{C})^{-1}$ is nonsingular [31].

The personalized PageRank for coevolutionary digraphs is calculated as

$$\psi_\alpha(\mathbf{s}) = \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}})$$

since $(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}$ is nonsingular (by Theorem 1.2.17 in page 54, [27]). What happens when $\beta \rightarrow 0$? We know the linear system should reduce to the case whereby the solution is the stationary vector $\boldsymbol{\pi}$ if we assume that the coevolutionary digraph is irreducible.

Since $\tilde{\mathcal{Z}} = \tilde{\mathcal{L}}^+$ is the Moore-Penrose pseudoinverse of $\tilde{\mathcal{L}}$,

$$\begin{aligned} \tilde{\mathcal{L}} &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}}\tilde{\mathcal{L}} \\ \tilde{\mathcal{L}} + \boldsymbol{\varepsilon} &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\beta \mathbf{I} + \tilde{\mathcal{L}}) \\ \boldsymbol{\varepsilon} &= \beta \tilde{\mathcal{L}}\tilde{\mathcal{Z}}. \end{aligned}$$

Then,

$$\begin{aligned} \tilde{\mathcal{L}} + \boldsymbol{\varepsilon} &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\beta \mathbf{I} + \tilde{\mathcal{L}}) \\ (\tilde{\mathcal{L}} + \boldsymbol{\varepsilon})(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}} \\ \tilde{\mathcal{L}}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}} - \boldsymbol{\varepsilon}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} \\ &= \tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\mathbf{I} - \beta(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}). \end{aligned}$$

We rewrite the personalized PageRank for coevolutionary digraphs as follows

$$\begin{aligned} \psi_\alpha(\mathbf{s}) &= \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\mathbf{I} - \beta(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1})\boldsymbol{\Pi}^{\frac{1}{2}}) \\ &= \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}} + \beta\boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}}\boldsymbol{\Pi}^{-\frac{1}{2}}(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}\boldsymbol{\Pi}^{\frac{1}{2}}) \\ &= \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}} + \beta\boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}}(\beta\boldsymbol{\Pi}^{-\frac{1}{2}}\boldsymbol{\Pi}^{\frac{1}{2}} + \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\boldsymbol{\Pi}^{\frac{1}{2}})^{-1}) \\ &= \mathbf{s}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}}) + \beta\mathbf{s}(\boldsymbol{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\boldsymbol{\Pi}^{\frac{1}{2}}(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}) \end{aligned}$$

$$\begin{aligned}
&= \mathbf{s}(\mathbf{I} - \mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}) + \beta \mathbf{s}(\mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}) \\
&= \boldsymbol{\pi} + \beta(\mathbf{s} - \boldsymbol{\pi})(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}
\end{aligned}$$

where $\tilde{\mathcal{L}}\tilde{\mathcal{Z}} = (\mathbf{I} - \tilde{\mathcal{J}})$. We need to show that $\mathbf{s}(\mathbf{I} - \mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}) = \boldsymbol{\pi}$ and $\mathbf{s}(\mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}) = \mathbf{s} - \boldsymbol{\pi}$.

First, we obtain by direct calculation that

$$\mathbf{I} - \mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}} = \begin{pmatrix} \pi_1 & \pi_2 & \pi_3 & \cdots & \pi_n \\ \pi_1 & \pi_2 & \pi_3 & \cdots & \pi_n \\ \pi_1 & \pi_2 & \pi_3 & \cdots & \pi_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \pi_1 & \pi_2 & \pi_3 & \cdots & \pi_n \end{pmatrix}$$

where $\tilde{\mathcal{J}} = (\boldsymbol{\pi}^{1/2})^T \boldsymbol{\pi}^{1/2}$. Since $\mathbf{s} = (s_i)_{i=1}^n$ with $\sum_i s_i = 1$, we can calculate $\mathbf{s}(\mathbf{I} - \mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}) = (\sum_i \pi_j s_i)_{j=1}^n = (\pi_j \sum_i s_i)_{j=1}^n = (\pi_j)_{j=1}^n = \boldsymbol{\pi}$.

Second, let $\mathbf{s} = (s_1, s_2, s_3, \dots, s_n)$ and $\boldsymbol{\pi} = (\pi_1, \pi_2, \pi_3, \dots, \pi_n)$. Direct calculation shows that $\mathbf{s}(\mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}) = (s_1 - \pi_1, s_2 - \pi_2, s_3 - \pi_3, \dots, s_n - \pi_n) = \mathbf{s} - \boldsymbol{\pi}$. Note that the product of the row vector \mathbf{s} with the first column of the matrix $\mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}$ is

$$\begin{aligned}
&(s_1, s_2, s_3, \dots, s_n)(1 - \pi_1, -\pi_1, -\pi_1, \dots, -\pi_1)^T \\
&= s_1(1 - \pi_1) + s_2(-\pi_1) + s_3(-\pi_1) + \cdots + s_n(-\pi_1) \\
&= s_1 - \pi_1
\end{aligned}$$

whereby the product of \mathbf{s} with the i th-column of $\mathbf{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\mathbf{\Pi}^{\frac{1}{2}}$ is $s_i - \pi_i$.

We have calculated that

$$\boldsymbol{\psi}_\alpha(\mathbf{s}) = \boldsymbol{\pi} + \beta(\mathbf{s} - \boldsymbol{\pi})(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}. \tag{A.5}$$

Since $\beta \mathbf{I} + \mathbf{I} - \mathbf{P}$ is nonsingular, then

$$\boldsymbol{\psi}_\alpha(\mathbf{s})(\beta \mathbf{I} + \mathbf{I} - \mathbf{P}) = \boldsymbol{\pi}(\beta \mathbf{I} + \mathbf{I} - \mathbf{P}) + \beta(\mathbf{s} - \boldsymbol{\pi}).$$

Note that when we let $\alpha \rightarrow 0 \Rightarrow \beta \rightarrow 0$, we obtain

$$\begin{aligned}
\boldsymbol{\psi}_0(\mathbf{s})(\mathbf{I} - \mathbf{P}) &= \boldsymbol{\pi}(\mathbf{I} - \mathbf{P}) + \tilde{\mathbf{0}} \\
&= \boldsymbol{\pi}(\mathbf{I} - \mathbf{P})
\end{aligned}$$

520 where $\tilde{\mathbf{0}}$ is the zero row vector. As such, $\boldsymbol{\psi}_0(\mathbf{s}) = \boldsymbol{\pi}$ for any \mathbf{s} .

Can we calculate $\boldsymbol{\psi}_\alpha(\mathbf{s}) = \mathbf{s}(\mathbf{I} - \mathbf{\Pi}^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}(\mathbf{I} - \beta(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1})\mathbf{\Pi}^{\frac{1}{2}})$ directly? We need to be able to calculate $\boldsymbol{\psi}_0(\mathbf{s})$ also. Let $\mathbf{N}_\beta = \beta(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}$. This means calculating \mathbf{N}_0 also. \mathbf{N}_β is nonsingular. Then,

$$\begin{aligned}
\mathbf{N}_\beta &= \beta(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} \\
\beta \mathbf{I} \mathbf{N}_\beta + \mathbf{N}_\beta \tilde{\mathcal{L}} &= \beta \mathbf{I}.
\end{aligned}$$

Assume \mathbf{N}_0 is nonsingular. As $\beta \rightarrow 0$, we have

$$\begin{aligned}
\mathbf{0} \mathbf{N}_0 + \mathbf{N}_0 \tilde{\mathcal{L}} &= \mathbf{0} \\
\mathbf{N}_0 \tilde{\mathcal{L}} &= \mathbf{0}.
\end{aligned}$$

We know $\tilde{\mathcal{L}}$ is singular. But for the last equality $\mathbf{N}_0 \tilde{\mathcal{L}} = \mathbf{0}$, the original statement that \mathbf{N}_0 is nonsingular would be a contradiction. \mathbf{N}_0 must be singular.

We can apply the theoretical result involving several identities relating to the normalized digraph Laplacian [30] and obtain the solution for $\mathbf{N}_0 \tilde{\mathcal{L}} = \mathbf{0}$ as $\mathbf{N}_0 = \tilde{\mathcal{J}}^k = \tilde{\mathcal{J}}$, $k = 1, 2, 3, \dots$ (by repeatedly applying the identity $\tilde{\mathcal{J}}^2 = \tilde{\mathcal{J}}$) or $\mathbf{N}_0 = \mathbf{0}$ (the zero matrix). Here, $\tilde{\mathcal{J}} \tilde{\mathcal{L}} = \mathbf{0}$ (by Lemma 1 in [30]) and $\mathbf{0} \tilde{\mathcal{L}} = \mathbf{0}$. We furnish a direct calculation for $\tilde{\mathcal{J}} \tilde{\mathcal{L}}$ here since it is sketched only in [30]. Let \mathbf{J} be the square matrix of ones and \mathbf{e} the row vector of ones. Then,

$$\begin{aligned} \tilde{\mathcal{J}} \tilde{\mathcal{L}} &= (\Pi^{\frac{1}{2}} \mathbf{J} \Pi^{\frac{1}{2}}) (\Pi^{\frac{1}{2}} (\mathbf{I} - \mathbf{P}) \Pi^{-\frac{1}{2}}) \\ &= \Pi^{\frac{1}{2}} \mathbf{J} \Pi (\mathbf{I} - \mathbf{P}) \Pi^{-\frac{1}{2}} \\ &= \Pi^{\frac{1}{2}} \mathbf{e}^T \boldsymbol{\pi} (\mathbf{I} - \mathbf{P}) \Pi^{-\frac{1}{2}} \\ &= \mathbf{0} \end{aligned}$$

since $\boldsymbol{\pi} (\mathbf{I} - \mathbf{P}) = \boldsymbol{\pi} - \boldsymbol{\pi} \mathbf{P} = \boldsymbol{\pi} - \boldsymbol{\pi} = \tilde{\mathbf{0}}$ and $\mathbf{e}^T \tilde{\mathbf{0}} = \mathbf{0}$ where $\tilde{\mathbf{0}}$ is the zero row vector and $\mathbf{0}$ is the zero matrix.

However, we can establish what \mathbf{N}_0 is, directly. First we rewrite the expression $(\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}$ as follows

$$\begin{aligned} (\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} &= (\beta \mathbf{I} + (\tilde{\mathcal{L}} + \tilde{\mathcal{J}}) - \tilde{\mathcal{J}})^{-1} \\ &= \left((\tilde{\mathcal{L}} + \tilde{\mathcal{J}}) (\mathbf{I} + (\tilde{\mathcal{L}} + \tilde{\mathcal{J}})^{-1} (\beta \mathbf{I} - \tilde{\mathcal{J}})) \right)^{-1} \\ &= (\tilde{\mathcal{L}} + \tilde{\mathcal{J}})^{-1} (\mathbf{I} + (\tilde{\mathcal{L}} + \tilde{\mathcal{J}})^{-1} (\beta \mathbf{I} - \tilde{\mathcal{J}}))^{-1} \\ &= (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) (\mathbf{I} + (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) (\beta \mathbf{I} - \tilde{\mathcal{J}}))^{-1} \\ &= (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) (\mathbf{I} + \beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) - \tilde{\mathcal{Z}} \tilde{\mathcal{J}} - \tilde{\mathcal{J}} \tilde{\mathcal{J}})^{-1} \\ &= (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) (\beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) + (\mathbf{I} - \tilde{\mathcal{J}}))^{-1}, \end{aligned}$$

using identities $(\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) = (\tilde{\mathcal{L}} + \tilde{\mathcal{J}})^{-1}$ on the fourth line (by Theorem 1 in [30]), $\tilde{\mathcal{Z}} \tilde{\mathcal{J}} = \mathbf{0}$ and $\tilde{\mathcal{J}} \tilde{\mathcal{J}} = \tilde{\mathcal{J}}$ on the last line (by Lemma 1 in [30]).

Since $\mathbf{N}_\beta = \beta (\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1}$ is nonsingular, then

$$\begin{aligned} \mathbf{N}_\beta &= \beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) (\beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) + (\mathbf{I} - \tilde{\mathcal{J}}))^{-1} \\ \mathbf{N}_\beta (\beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}) + (\mathbf{I} - \tilde{\mathcal{J}})) &= \beta (\tilde{\mathcal{Z}} + \tilde{\mathcal{J}}). \end{aligned}$$

As $\beta \rightarrow 0$, we have

$$\begin{aligned} \mathbf{N}_0 (\mathbf{0} + (\mathbf{I} - \tilde{\mathcal{J}})) &= \mathbf{0} \\ \mathbf{N}_0 &= \mathbf{N}_0 \tilde{\mathcal{J}}. \end{aligned}$$

Given that $\tilde{\mathcal{J}}$ is singular, the solutions to the equality $\mathbf{N}_0 = \mathbf{N}_0 \tilde{\mathcal{J}}$ are $\mathbf{N}_0 = \mathbf{0}$ and $\mathbf{N}_0 = \tilde{\mathcal{J}}^k = \tilde{\mathcal{J}}$, $k = 1, 2, 3, \dots$

As $\alpha \rightarrow 0 \Rightarrow \beta \rightarrow 0$, we can then reduce the equation $\tilde{\mathcal{L}} (\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} = \tilde{\mathcal{L}} \tilde{\mathcal{Z}} (\mathbf{I} - \beta (\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1})$ as follows

$$\begin{aligned} \tilde{\mathcal{L}} (\tilde{\mathcal{L}})^+ &= \tilde{\mathcal{L}} \tilde{\mathcal{Z}} (\mathbf{I} - \mathbf{N}_0) \\ &= \tilde{\mathcal{L}} \tilde{\mathcal{Z}} (\mathbf{I} - \tilde{\mathcal{J}}) \\ &= \tilde{\mathcal{L}} \tilde{\mathcal{Z}}, \end{aligned}$$

given that $\tilde{\mathcal{L}} \tilde{\mathcal{Z}} = \mathbf{I} - \tilde{\mathcal{J}}$ and $\tilde{\mathcal{L}} \tilde{\mathcal{Z}} \tilde{\mathcal{L}} = \tilde{\mathcal{L}}$. The conclusion is the same if we consider $\mathbf{N}_0 = \mathbf{0}$. This implies that

$$\begin{aligned} \lim_{\beta \rightarrow 0} \tilde{\mathcal{L}} (\beta \mathbf{I} + \tilde{\mathcal{L}})^{-1} &= \tilde{\mathcal{L}} (\tilde{\mathcal{L}})^+ \\ &= \tilde{\mathcal{L}} \tilde{\mathcal{Z}}. \end{aligned}$$

For small values of α (subsequently small values of β), we can use this approximation

$$\tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} \approx \tilde{\mathcal{L}}\tilde{\mathcal{Z}} = \mathbf{I} - \tilde{\mathcal{J}},$$

with equality when $\beta = 0$. We can approximate the personalized PageRank for irreducible coevolutionary digraphs as

$$\psi_\alpha(\mathbf{s}) \approx \mathbf{s}(\mathbf{I} - \Pi^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\Pi^{\frac{1}{2}}) = \pi$$

with equality, i.e., $\psi_0(\mathbf{s}) = \pi$, for any \mathbf{s} . □

Lemma 4. *Let a CMC operating on irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be associated with a probability transition matrix \mathbf{P} , stationary distribution π , and the fundamental matrix Z . Correspondingly, the personalized PageRank on $D_C(V_{S(n)})$ is a CMC with probability transition matrix \mathbf{P}_{PR} and stationary distribution $\psi_\alpha(\mathbf{s})$. Then*

$$\begin{aligned} \pi - \psi_\alpha(\mathbf{s}) &= -\psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})Z \\ &= \beta(\pi - \mathbf{s})(\beta\mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1}. \end{aligned}$$

Proof: The following makes use of results of Perturbation theory applied to finite Markov chains in [32]. Let $\pi_A = \pi$, $\mathbf{P}_A = \mathbf{P}$, $\pi_B = \psi_\alpha(\mathbf{s})$, and $\mathbf{P}_B = \mathbf{P}_{PR}$. The distance between \mathbf{P} and \mathbf{P}_{PR} is defined as

$$\mathbf{U}_{AB} = (\mathbf{P}_{PR} - \mathbf{P})Z$$

with the fundamental matrix $Z = Z_A$. Applying two theoretical results in [32] (Theorems 1 and 2), we obtain

$$\begin{aligned} \psi_\alpha(\mathbf{s}) &= \pi(\mathbf{I} - \mathbf{U}_{AB})^{-1} \\ \psi_\alpha(\mathbf{s}) - \psi_\alpha(\mathbf{s})\mathbf{U}_{AB} &= \pi \\ \pi - \psi_\alpha(\mathbf{s}) &= -\psi_\alpha(\mathbf{s})\mathbf{U}_{AB} \\ &= \psi_\alpha(\mathbf{s})(\mathbf{P} - \mathbf{P}_{PR})Z \\ &= -\psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})Z, \end{aligned}$$

where we use $\psi_\alpha(\mathbf{s})\mathbf{P}_{PR} = \psi_\alpha(\mathbf{s})$.

We show that the vector $\pi - \psi_\alpha(\mathbf{s})$ is invariant under multiplication of the matrix $(\mathbf{I} - \mathbf{P})Z$, i.e., $(\pi - \psi_\alpha(\mathbf{s}))(\mathbf{I} - \mathbf{P})Z = \pi - \psi_\alpha(\mathbf{s})$. Furthermore, $((\mathbf{I} - \mathbf{P})Z)^k = (\mathbf{I} - \mathbf{P})Z$, $k = 1, 2, 3, \dots$. First,

$$\begin{aligned} (\pi - \psi_\alpha(\mathbf{s}))(\mathbf{I} - \mathbf{P})Z &= \pi(\mathbf{I} - \mathbf{P})Z - \psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})Z \\ &= \tilde{\mathbf{0}} - \psi_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})Z \\ &= \pi - \psi_\alpha(\mathbf{s}), \end{aligned}$$

where $\tilde{\mathbf{0}}$ is the zero row vector. Second, using identities $\tilde{\mathcal{L}} = \Pi^{\frac{1}{2}}(\mathbf{I} - \mathbf{P})\Pi^{-\frac{1}{2}}$ and $\tilde{\mathcal{Z}} = \Pi^{\frac{1}{2}}Z\Pi^{-\frac{1}{2}}$ [30], we obtain $(\mathbf{I} - \mathbf{P})Z = \Pi^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\Pi^{\frac{1}{2}}$. Then,

$$\begin{aligned} ((\mathbf{I} - \mathbf{P})Z)((\mathbf{I} - \mathbf{P})Z) &= (\Pi^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\Pi^{\frac{1}{2}})(\Pi^{-\frac{1}{2}}\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\Pi^{\frac{1}{2}}) \\ &= (\mathbf{I} - \mathbf{P})Z, \end{aligned}$$

530 where we use $\tilde{\mathcal{L}}\tilde{\mathcal{Z}}\tilde{\mathcal{L}} = \tilde{\mathcal{L}}$. We obtain $((\mathbf{I} - \mathbf{P})Z)^k = (\mathbf{I} - \mathbf{P})Z$, $k = 1, 2, 3, \dots$ by applying the equality above repeatedly.

Applying Equation A.5 from the proof section of Theorem 3, we obtain

$$\pi - \psi_\alpha(\mathbf{s}) = \beta(\pi - \mathbf{s})(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}.$$

Multiplying $(\mathbf{I} - \mathbf{P})Z$ on both sides of the equality

$$\begin{aligned} (\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s}))(\mathbf{I} - \mathbf{P})Z &= \beta(\boldsymbol{\pi} - \mathbf{s})(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}(\mathbf{I} - \mathbf{P})Z \\ \boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s}) &= \beta\boldsymbol{\pi}(\mathbf{I} - \mathbf{P})Z - \beta\mathbf{s}(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}(\mathbf{I} - \mathbf{P})Z \\ &= \tilde{\mathbf{0}} - \beta\mathbf{s}(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}(\mathbf{I} - \mathbf{P})Z \\ &= -\boldsymbol{\psi}_\alpha(\mathbf{s})(\mathbf{I} - \mathbf{P})Z, \end{aligned}$$

where we use Equation A.2 from Lemma 1, which completes the proof. \square

Corollary 5. For $\boldsymbol{\pi}$ and $\boldsymbol{\psi}_\alpha(\mathbf{s})$ associated with CMC on an irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$, the following inequality is given for restart probabilities $\alpha_1 \leq \alpha_2$

$$\|\boldsymbol{\pi} - \boldsymbol{\psi}_{\alpha_1}(\mathbf{s})\| \leq \|\boldsymbol{\pi} - \boldsymbol{\psi}_{\alpha_2}(\mathbf{s})\| \quad (\text{A.6})$$

where $\alpha_1, \alpha_2 \in (0, 1)$.

Proof: First, we rewrite the equation as follows

$$\begin{aligned} \boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s}) &= \beta(\boldsymbol{\pi} - \mathbf{s})(\beta\mathbf{I} + \mathbf{I} - \mathbf{P})^{-1} \\ \mathbf{y} &= (\boldsymbol{\pi} - \mathbf{s})\mathbf{A}^{-1} \end{aligned}$$

where $\mathbf{y} = \boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})$ and $\mathbf{A} = \mathbf{I} + \frac{1}{\beta}(\mathbf{I} - \mathbf{P})$. \mathbf{A}^{-1} is by definition a nonsingular M-matrix and as such is inverse-positive $\mathbf{A}^{-1} \geq \mathbf{0}$ (Theorem 2.3, Chapter 6, [28]) with positive $\|\star\|$. Furthermore, since each row sum of \mathbf{A} is equal to one, then \mathbf{A} is a uniformly strictly diagonally dominant M-matrix and that \mathbf{A}^{-1} is a row stochastic matrix (Corollary 2 in [52]). We have three cases when: (a) $\alpha = 0$, (b) $\alpha = 1$, and (c) $\alpha \in (0, 1)$. We evaluate these cases individually using several results in the proof of Theorem 3.

For (a), Theorem 3 implies that as $\alpha \rightarrow 0 \Rightarrow \beta \rightarrow 0$, we have $\lim_{\beta \rightarrow 0} \|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\| = 0$. We can show this directly here. We rewrite \mathbf{A}^{-1} as

$$\begin{aligned} \mathbf{A}^{-1} &= \left(\mathbf{I} + \frac{1}{\beta}(\mathbf{I} - \mathbf{P})\right)^{-1} \\ &= \mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}} \tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} \boldsymbol{\Pi}^{\frac{1}{2}} \end{aligned}$$

since $(\beta\mathbf{I} + (\mathbf{I} - \mathbf{P}))^{-1} = \frac{1}{\beta}(\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}} \tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} \boldsymbol{\Pi}^{\frac{1}{2}})$.

Let $\mathbf{y}(0) = \lim_{\beta \rightarrow 0} (\boldsymbol{\pi} - \mathbf{s})\mathbf{A}^{-1}$. As $\alpha \rightarrow 0 \Rightarrow \beta \rightarrow 0$, we obtain

$$\begin{aligned} \mathbf{y}(0) &= \lim_{\beta \rightarrow 0} (\boldsymbol{\pi} - \mathbf{s})\mathbf{A}^{-1} \\ &= (\boldsymbol{\pi} - \mathbf{s}) \lim_{\beta \rightarrow 0} (\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}} \tilde{\mathcal{L}}(\beta\mathbf{I} + \tilde{\mathcal{L}})^{-1} \boldsymbol{\Pi}^{\frac{1}{2}}) \\ &= (\boldsymbol{\pi} - \mathbf{s})\mathbf{e}^T \boldsymbol{\pi} \\ &= \tilde{\mathbf{0}} \end{aligned}$$

where we use $\mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}} \tilde{\mathcal{L}} \tilde{\mathcal{Z}} \boldsymbol{\Pi}^{\frac{1}{2}} = \mathbf{I} - \boldsymbol{\Pi}^{-\frac{1}{2}}(\mathbf{I} - \tilde{\mathcal{J}})\boldsymbol{\Pi}^{\frac{1}{2}} = \mathbf{e}^T \boldsymbol{\pi}$. So, $\|\mathbf{y}(0)\| = 0$.

For (b), as $\alpha \rightarrow 1 \Rightarrow \beta \rightarrow \infty$, we have $\lim_{\beta \rightarrow \infty} \|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\| = \|\boldsymbol{\pi} - \mathbf{s}\|$ since $\boldsymbol{\psi}_1(\mathbf{s}) = \mathbf{s}$, given that $\lim_{\beta \rightarrow \infty} \mathbf{A}^{-1} = \mathbf{I}^{-1} = \mathbf{I}$ and $\boldsymbol{\psi}_\alpha(\mathbf{s}) = \mathbf{s}\mathbf{A}^{-1}$. We can show this directly as follows. Let $\mathbf{y}(1) = \lim_{\beta \rightarrow \infty} (\boldsymbol{\pi} - \mathbf{s})\mathbf{A}^{-1}$. Then,

$$\begin{aligned} \mathbf{y}(1) &= \lim_{\beta \rightarrow \infty} (\boldsymbol{\pi} - \mathbf{s})\mathbf{A}^{-1} \\ &= (\boldsymbol{\pi} - \mathbf{s}) \lim_{\beta \rightarrow \infty} \mathbf{A}^{-1} \end{aligned}$$

$$= \boldsymbol{\pi} - \mathbf{s}.$$

So, $\|\mathbf{y}(1)\| = \|\boldsymbol{\pi} - \mathbf{s}\|$.

For (c), note that \mathbf{y} and \mathbf{A} consist of entries that are differentiable functions of a real variable β [19] whereby

$$\begin{aligned} \frac{d\mathbf{y}}{d\beta} &= (\boldsymbol{\pi} - \mathbf{s}) \frac{d}{d\beta} \mathbf{A}^{-1} \\ &= \frac{1}{\beta^2} (\boldsymbol{\pi} - \mathbf{s}) \mathbf{A}^{-1} (\mathbf{I} - \mathbf{P}) \mathbf{A}^{-1} \end{aligned}$$

since

$$\begin{aligned} \frac{d}{d\beta} \mathbf{A} &= \frac{d}{d\beta} \left(\mathbf{I} + \frac{1}{\beta} (\mathbf{I} - \mathbf{P}) \right) \\ &= -\frac{1}{\beta^2} (\mathbf{I} - \mathbf{P}) \end{aligned}$$

and

$$\begin{aligned} \frac{d}{d\beta} \mathbf{A}^{-1} &= -\mathbf{A}^{-1} \left(\frac{d}{d\beta} \mathbf{A} \right) \mathbf{A}^{-1} \\ &= \frac{1}{\beta^2} \mathbf{A}^{-1} (\mathbf{I} - \mathbf{P}) \mathbf{A}^{-1}. \end{aligned}$$

We note that

$$\begin{aligned} (\boldsymbol{\pi} - \mathbf{s}) \mathbf{A}^{-1} (\mathbf{I} - \mathbf{P}) \mathbf{A}^{-1} &= (\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})) (\mathbf{I} - \mathbf{P}) \mathbf{A}^{-1} \\ &= (\boldsymbol{\psi}_\alpha(\mathbf{s}) \mathbf{P} - \boldsymbol{\psi}_\alpha(\mathbf{s})) \mathbf{A}^{-1}. \end{aligned}$$

Given that $\lim_{\beta \rightarrow \infty} \mathbf{A}^{-1} = \mathbf{I}$, we obtain

$$\begin{aligned} \lim_{\beta \rightarrow \infty} (\boldsymbol{\pi} - \mathbf{s}) \mathbf{A}^{-1} (\mathbf{I} - \mathbf{P}) \mathbf{A}^{-1} &= (\boldsymbol{\pi} - \mathbf{s}) (\mathbf{I} - \mathbf{P}) \\ &= \mathbf{sP} - \mathbf{s}. \end{aligned}$$

As $\alpha \rightarrow 1 \Rightarrow \beta \rightarrow \infty$, $\lim_{\beta \rightarrow \infty} \left\| \frac{d\mathbf{y}}{d\beta} \right\| = \lim_{\beta \rightarrow \infty} \frac{1}{\beta^2} \|\mathbf{sP} - \mathbf{s}\| = 0$.

$\left\| \frac{d\mathbf{y}}{d\beta} \right\|$ is positive for $\alpha \in (0, 1)$ and goes to zero as $\alpha \rightarrow 1$. Furthermore, we know that $\mathbf{y}(\alpha)$ is bounded entrywise with $\|\mathbf{y}(0)\| = 0$ and $\|\mathbf{y}(1)\| = \|\boldsymbol{\pi} - \mathbf{s}\|$. Since $\|\mathbf{y}(\alpha)\|$ is monotonically increasing in the interval of α for $(0, 1)$, it follows that $\|\boldsymbol{\pi} - \boldsymbol{\psi}_{\alpha_1}(\mathbf{s})\| \leq \|\boldsymbol{\pi} - \boldsymbol{\psi}_{\alpha_2}(\mathbf{s})\|$ for $\alpha_1 \leq \alpha_2$ where $\alpha_1, \alpha_2 \in (0, 1)$. \square

Corollary 6. *Associated to each irreducible $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ is CMC with stationary distribution $\boldsymbol{\psi}_\alpha(\mathbf{s})$ for $\alpha \in (0, 1)$ and $\boldsymbol{\pi}$ with the following perturbation bound*

$$\|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_\infty \leq \|\boldsymbol{\pi} - \mathbf{s}\|_\infty \quad (\text{A.7})$$

with equality when $\alpha = 1$.

Proof: Since $\|(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}\|_\infty = \frac{1}{\beta}$ from Lemma 2 and from the property of induced matrix norm [19], we obtain

$$\begin{aligned} \|\boldsymbol{\pi} - \boldsymbol{\psi}_\alpha(\mathbf{s})\|_\infty &= \|\beta(\boldsymbol{\pi} - \mathbf{s})(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}\|_\infty \\ &\leq \beta \|\boldsymbol{\pi} - \mathbf{s}\|_\infty \|(\beta \mathbf{I} + \mathbf{I} - \mathbf{P})^{-1}\|_\infty \\ &= \|\boldsymbol{\pi} - \mathbf{s}\|_\infty. \end{aligned}$$

Equality is obtained as $\alpha = 1$ since $\psi_1(\mathbf{s}) = \mathbf{s}$. \square

Note: Lemma 4 expresses the difference between stationary and PageRank vectors of a CMC explicitly, which is followed by Corollary 5 that shows for a given vector norms, $\|\pi - \psi_\alpha(\mathbf{s})\|$ is directly proportional to the restart probability α . This can be seen from the expression $\pi - \psi_\alpha(\mathbf{s}) = (\pi - \mathbf{s})\mathbf{A}^{-1}$ where $\mathbf{A}^{-1} = (\mathbf{I} + \frac{1}{\beta}(\mathbf{I} - \mathbf{P}))^{-1}$. \mathbf{A}^{-1} is a row stochastic matrix that changes from $\mathbf{e}^T \pi$ (as $\alpha \rightarrow 0$) to \mathbf{I} (as $\alpha \rightarrow 1$). Although it is not possible to find a general expression of \mathbf{A}^{-1} for $\alpha \in (0, 1)$, given that \mathbf{A} is a nonsingular M-matrix that is diagonally dominant, \mathbf{A}^{-1} is diagonally dominant of its column entries (i.e., for $\mathbf{B} = \mathbf{A}^{-1}$, $|b_{ii}| > |b_{ij}|$, $j \neq i$, $i = 1, 2, 3, \dots, n$) [53]. Furthermore, $\pi \mathbf{A}^{-1} = \pi$ from Equation A.5. One can observe that $\|(\pi - \mathbf{s})\mathbf{A}^{-1}\| = \|\pi - \mathbf{s}\mathbf{A}^{-1}\|$ monotonically increases as $\alpha \rightarrow 1$. For example, $\|(\pi - \mathbf{s})\mathbf{A}^{-1}\|_1 = \sum_{i=1}^n |\pi_i - s_i|$ since $s_i(\alpha)$ changes from $s_i(0) = \pi_i$ to $s_i(1) = s_i$. For $\|(\pi - \mathbf{s})\mathbf{A}^{-1}\|_\infty$, in the case where $|\pi_1 - s_1| \geq |\pi_i - s_i|$, $i = 2, 3, 4, \dots, n$ and assuming uniform \mathbf{s} , monotonicity can be observed from changes in $\mathbf{s}\mathbf{A}^{-1}$ from $\mathbf{s}\mathbf{e}^T \pi = \pi$ to $\mathbf{s}\mathbf{I} = \mathbf{s}$.

Appendix B. Theoretical Bounds for One Norm $\|\pi - \psi_\alpha(\mathbf{s})\|_1$

Appendix B.1. General Bound for Coevolutionary Digraphs

General bounds can be obtained for any (reducible and irreducible) coevolutionary digraph. A simple argument would be to take the maximum one norm for probability vectors $(0, 0, 0, \dots, 1)$ and $(1, 0, 0, \dots, 0)$ as 2 [23]. However, we can improve the bound by considering random walks on labelled or isomorphic tournaments [33, 34]. A probability vector $(a_1, a_2, a_3, \dots, a_n)$ associated for a tournament with vertices consistently indexed according to their score sequences will have for its unilateral and directional dual (vertices indexed in the reversed order of their score sequences), $(a_n, a_{n-1}, a_{n-2}, \dots, a_1)$ [17, 35].

A straightforward digraph-theoretic argument would be to take the one norm between stationary vectors associated with transitive ($\pi_{\text{tran}} = (0, 0, 0, \dots, 1)$) and regular ($\pi_{\text{reg}} = (\frac{1}{n}, \frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n})$) tournaments

$$\begin{aligned} \max \|\star\|_1 &= \|\pi_{\text{tran}} - \pi_{\text{reg}}\|_1 \\ &= (n-1)\frac{1}{n} + \left(1 - \frac{1}{n}\right) \\ &= 2\left(1 - \frac{1}{n}\right) \end{aligned}$$

as the upper bound, that is, for the one norm of probability vectors associated with CMCs operating on tournaments π_1 and π_2

$$\|\pi_1 - \pi_2\|_1 \leq 2\left(1 - \frac{1}{n}\right). \quad (\text{A.8})$$

Appendix B.2. Bounds based on Digraph-Theoretic and Coupling Arguments

The bound given by the inequality in Equation A.8 also reflects the difference for a PageRank random walker operating on a transitive tournament between two opposite cases: (1) For $\alpha = 0$, all the probability mass is concentrated at a single absorbing vertex. (2) For $\alpha = 1$ (i.e. restarts all the time with a uniform teleportation vector), the mass is now uniformly distributed over all vertices. What happens when α is varied in $(0, 1)$? In general, one would obtain loose bounds. In [36], a coupling argument is introduced to provide the relevant bounds, which we improve here.

Let μ and ν be the probability distributions of the random variables X and Y , respectively. Both X and Y take on values in the state space \mathcal{V} . Let (X, Y) be the pair of the two random variables. Let q be the joint distribution of (X, Y) on $\mathcal{V} \times \mathcal{V}$, i.e., $q(x, y) = \mathbb{P}(X = x, Y = y)$, such that $\sum_{y \in \mathcal{V}} q(x, y) = \mathbb{P}(X = x) = \mu_x$ and $\sum_{x \in \mathcal{V}} q(x, y) = \mathbb{P}(Y = y) = \nu_y$. A coupling of μ and ν refers to the pair (X, Y) defined on a single probability space whereby its marginal distributions of X and Y are μ and ν , respectively, i.e., satisfying $\mathbb{P}(X = x) = \mu_x$ and $\mathbb{P}(Y = y) = \nu_y$ for all $x, y \in \mathcal{V}$ [54].

The following result show how to bound the distance between stationary $\mu = \pi$ and PageRank $\nu = \psi_\alpha(\mathbf{s})$ distributions of the coupled CMCs $\{(X_t, Y_t) : t \in \mathbb{N}_0\}$, where $\{X_t : t \in \mathbb{N}_0\}$ is without restart and

$\{Y_t : t \in \mathbb{N}_0\}$ is with restart. Our proof uses a combination of digraph-theoretic and coupling arguments. We exploit specific structures in irreducible coevolutionary digraphs $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ to construct a specific coupling of the two CMCs. Then, we use the equivalent characterizations of variation distance between the marginal distributions of the coupling ($\|\pi - \psi_\alpha(\mathbf{s})\|_{\text{TV}} = \frac{1}{2}\|\pi - \psi_\alpha(\mathbf{s})\|_1 = \min \mathbb{P}(X \neq Y)$) [55] and subsequently bound $\|\pi - \psi_\alpha(\mathbf{s})\|_1$ with an asymptotic upper-bound of $\mathbb{P}(X_\infty \neq Y_\infty)$.

Lemma 7. *Let $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be an irreducible coevolutionary digraph. Let $\{(X_t, Y_t) : t \in \mathbb{N}_0\}$ be a coupling of the two CMCs. Associated with CMC $\{X_t : t \in \mathbb{N}_0\}$ is the probability transition matrix \mathbf{P} and stationary distribution π . Associated with CMC $\{Y_t : t \in \mathbb{N}_0\}$ is the perturbed probability transition matrix \mathbf{P}_{PR} and stationary distribution $\psi_\alpha(\mathbf{s})$. The lazy random walk versions are considered for both CMCs. The two stationary distributions satisfy the relation:*

$$\begin{aligned} \|\pi - \psi_\alpha(\mathbf{s})\|_1 &\leq \frac{2}{1-\alpha} \mathbb{P}(X_\infty \neq Y_\infty) \\ &\leq \frac{2}{1-\alpha} d_\alpha \\ &\leq \frac{2}{1-\alpha} \end{aligned}$$

where $d_\alpha = \max \mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t = Y_t \mid \text{restart at } t+1)$.

For $\{\tilde{Y}_t : t \in \mathbb{N}_0\}$ with no restart ($\alpha = 0$), there is an optimal coupling $\{(X_t, \tilde{Y}_t) : t \in \mathbb{N}_0\}$ such that $\|\pi - \psi_0(\mathbf{s})\|_1 = 0$, which implies $\psi_0(\mathbf{s}) = \pi$.

Proof: Let $\{(X_t, Y_t) : t \in \mathbb{N}_0\}$ be a coupling of the two CMCs with the following construction.

- (i) $X_0 = Y_0$ is drawn randomly from π .
- (ii) The state transitions are as follows: At time step $t+1$, decide with probability $1-\alpha$ not to restart or with probability α to restart.
 - a. If there is no restart, then $X_{t+1} = Y_{t+1}$ always. If $X_t = Y_t$, then $X_{t+1} = Y_{t+1}$ (i.e., both chains jump to the same vertex) that is chosen randomly according to \mathbf{P} . If $X_t \neq Y_t$, then X_{t+1} and Y_{t+1} are chosen such that $X_{t+1} = Y_{t+1}$.
 - b. If there is restart, then $X_{t+1} \neq Y_{t+1}$ always if $X_t \neq Y_t$. Otherwise, if $X_t = Y_t$, then X_{t+1} is chosen randomly according to \mathbf{P} and Y_{t+1} is chosen uniformly at random such that $X_{t+1} \neq Y_{t+1}$.

For the coupling of the two CMCs, we first show that when there is no restart, $X_{t+1} = Y_{t+1}$ regardless of the state of the coupled CMCs at time t . Applying Moon's Theorem [33], an irreducible coevolutionary digraph $D_C(V_{S(n)}, A) \in \mathcal{D}_C(V_{S(n)})$ is vertex-pancyclic. In particular, any three distinct vertices $x, y, z \in V_{S(n)}$ forms a 3-cycle, i.e., cycle of length three. We use the simplified notation $xyzx$ to indicate $x \rightarrow y \rightarrow z \rightarrow x$. Let $X_t = x$ and $Y_t = y$. For lazy random walks, if the 3-cycle is $xzyx$, then arbitrarily set $X_{t+1} = X_t = x$ and $Y_{t+1} = x$. Similarly, if the 3-cycle is $yzxy$, then arbitrarily set $Y_{t+1} = Y_t = y$ and $X_{t+1} = y$. If X_t and Y_t are at the same vertex y , depending on the 3-cycle configuration, then both chains either jump to the same vertex z , i.e., $X_{t+1} = Y_{t+1} = z$ (if the 3-cycle is $xyzx$) or stay at vertex y (if the 3-cycle is $yxzy$). Similar arguments can be made for the case of $X_t = Y_t = x$.

When there is restart and if $X_t = Y_t$, we choose X_{t+1} randomly according to \mathbf{P} and then choose Y_{t+1} uniformly at random such that $X_{t+1} \neq Y_{t+1}$. By construction, $X_{t+1} \neq Y_{t+1}$ always when $X_t \neq Y_t$. Although the two transitions are correlated, each of the two CMCs are still using their state transitions independently. As such, we have a coupled CMCs $\{(X_t, Y_t) : t \in \mathbb{N}_0\}$ such that their marginal distributions are π and $\psi_\alpha(\mathbf{s})$.

We now use the coupling argument introduced in [36] (Theorem 3) for our coupling construction. Let $d_t = \mathbb{P}(X_t \neq Y_t)$. Since $X_0 = Y_0$, $\mathbb{P}(X_0 \neq Y_0) = 0$. Then,

$$\begin{aligned} d_{t+1} &= \mathbb{P}(X_{t+1} \neq Y_{t+1}) \\ &= \mathbb{P}(X_{t+1} \neq Y_{t+1} \mid \text{no restart at } t+1) \mathbb{P}(\text{no restart}) \\ &\quad + \mathbb{P}(X_{t+1} \neq Y_{t+1} \mid \text{restart at } t+1) \mathbb{P}(\text{restart}) \end{aligned}$$

$$\begin{aligned}
&= (0)(1 - \alpha) + \alpha(\mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t \neq Y_t \mid \text{restart at } t+1)) \\
&\quad + \alpha(\mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t = Y_t \mid \text{restart at } t+1)) \\
&\leq \alpha(\mathbb{P}(X_t \neq Y_t) + \mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t = Y_t \mid \text{restart at } t+1)) \\
&= \alpha(d_t + \mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t = Y_t \mid \text{restart at } t+1)).
\end{aligned}$$

Since we start with $d_0 = 0$ and taking $d_\alpha = \max \mathbb{P}(X_{t+1} \neq Y_{t+1}, X_t = Y_t \mid \text{restart at } t+1)$ with a slight abuse of notation, as we iterate the bound on $d_{t+1} \leq \alpha(d_t + d_\alpha)$, we obtain $d_1 = (\alpha)d_\alpha$, $d_2 = (\alpha + \alpha^2)d_\alpha$, $d_3 = (\alpha + \alpha^2 + \alpha^3)d_\alpha, \dots$, which follows a geometric progression. We can asymptotically bound $d_\infty \leq \frac{1}{1-\alpha}d_\alpha$. Furthermore, since (X_∞, Y_∞) is drawn from the stationary distribution of the correlated chains, the marginal distributions of X_∞ and Y_∞ are π and $\psi_\alpha(\mathbf{s})$, respectively. As such, $\mathbb{P}(X_\infty \neq Y_\infty) = d_\infty \leq \frac{1}{1-\alpha}d_\alpha$.

We apply the *Coupling Lemma* (Lemma 2.19 in [55]) to obtain the variation distance between the two marginal distributions

$$\begin{aligned}
\|\pi - \psi_\alpha(\mathbf{s})\|_{\text{TV}} &= \frac{1}{2} \|\pi - \psi_\alpha(\mathbf{s})\|_1 \\
&= \min \mathbb{P}(X \neq Y)
\end{aligned}$$

to obtain the bound $\|\pi - \psi_\alpha(\mathbf{s})\|_1 \leq 2\mathbb{P}(X_\infty \neq Y_\infty) = 2d_\infty \leq \frac{2}{1-\alpha}d_\alpha \leq \frac{2}{1-\alpha}$.

Where there is no restart, the CMC is a copy of $\{X_t : t \in \mathbb{N}_0\}$. Let $\{\tilde{Y}_t : t \in \mathbb{N}_0\}$ denote such a CMC. Starting with $X_0 = \tilde{Y}_0$ that is drawn randomly from π , there is an optimal coupling $\{(X_t, \tilde{Y}_t) : t \in \mathbb{N}_0\}$ whereby $X_{t+1} = \tilde{Y}_{t+1}$ always. In this case, $X_0 = \tilde{Y}_0, X_1 = \tilde{Y}_1, X_2 = \tilde{Y}_2, \dots$ whereby $\|\pi - \psi_0(\mathbf{s})\|_{\text{TV}} = \min \mathbb{P}(X_\infty, Y_\infty) = 0$, which implies that $\psi_0(\mathbf{s}) = \pi$. \square

Corollary 8. Let $\mathcal{D}_C(V_{S(n)})$ be the set of irreducible coevolutionary digraphs. Let any $D_C(V_{S(n)}) \in \mathcal{D}_C(V_{S(n)})$ be an irreducible coevolutionary digraph so that the vertices $v_1, v_2, v_3, \dots, v_n$ are ordered according to the score sequence $d_T^-(v_1) \leq d_T^-(v_2) \leq d_T^-(v_3) \leq \dots \leq d_T^-(v_n)$, where $d_T^-(v_i)$ is the in-degree of vertex v_i . Assume the digraph having the following structure:

1. The set of vertices $V_{S(n)}$ can be partitioned into three disjoint subsets with $\{v_1\} \cup V_{S(n-2)} \cup \{v_n\} = V_{S(n)}$, where $V_{S(n-2)} = V_{S(n)} \setminus \{v_1, v_n\}$, $\{v_1\} \cap V_{S(n-2)} = \emptyset$, and $\{v_n\} \cap V_{S(n-2)} = \emptyset$.
2. $\{v_1\} \mapsto V_{S(n-2)} \mapsto \{v_n\}$. That is, $v_1 \rightarrow v_i$ for all $v_i \in V_{S(n-2)}$ and that $v_i \rightarrow v_n$ for all $v_i \in V_{S(n-2)}$.
3. $v_1 \rightarrow v_i \rightarrow v_n \rightarrow v_1$ forms a 3-cycle for all $v_i \in V_{S(n-2)}$.

For a coupled CMCs $\{(X_t, Y_t) : t \in \mathbb{N}_0\}$ operating on $D_C(V_{S(n)})$, there is the following bound in distance

$$\|\pi - \psi_\alpha(\mathbf{s})\|_1 \leq \frac{2}{1-\alpha} \left(1 - \left(\pi_{v_n} - \frac{1}{n} \right) \right).$$

Proof: Since $X_0 = Y_0$ is drawn randomly from π and that (X_∞, Y_∞) is drawn from the stationary distribution of the correlated chains, we can bound d_∞ as follows

$$\begin{aligned}
d_\infty &\leq \frac{1}{1-\alpha} \mathbb{P}(X_\infty \neq Y_\infty) \\
&\leq \frac{1}{1-\alpha} (1 - \mathbb{P}(X_\infty = Y_\infty)) \\
&\leq \frac{1}{1-\alpha} \left(1 - \sum_{v_i \in V_{S(n)}} \mathbb{P}((X_\infty = v_i) \wedge (Y_\infty = v_i)) \right) \\
&\leq \frac{1}{1-\alpha} \left(1 - \sum_{v_i \in V_{S(n)}} \min\{\mathbb{P}(X_\infty = v_i), \mathbb{P}(Y_\infty = v_i)\} \right) \\
&\leq \frac{1}{1-\alpha} \left(1 - \min\{\mathbb{P}(X_\infty = v_n), \mathbb{P}(Y_\infty = v_n)\} \right)
\end{aligned}$$

$$\leq \frac{1}{1-\alpha} \left(1 - \left(\pi_{v_n} - \frac{1}{n} \right) \right).$$

Our argument proceeds as follows. By construction, $(X_\infty = Y_\infty)$ occurs when there is no restart. (X_∞, Y_∞) is drawn from the stationary distribution of the correlated chains with the marginal distributions of X_∞ and Y_∞ are π and $\psi_\alpha(\mathbf{s})$, respectively. We can use the bound $\mathbb{P}((X_\infty = v_i) \wedge (Y_\infty = v_i)) \leq \min\{\mathbb{P}(X_\infty = v_i), \mathbb{P}(Y_\infty = v_i)\}$ for the third inequality [54]. In this manner, $\mathbb{P}(X_\infty = v_i) = \pi_{v_i}$ and $\mathbb{P}(Y_\infty = v_i) = \psi_{v_i}$ for all $v_i \in V_{S(n)}$. For the fifth inequality, given that probabilities range in $[0, 1]$, we could choose the vertex that the CMC would most often jump to (i.e., v_n) as the upper bound. For the sixth inequality, $\min\{\pi_{v_n}, \psi_{v_n}\} = \psi_{v_n}$ but we can bound the term $1 - \min\{\pi_{v_n}, \psi_{v_n}\}$ by noting that $\pi_{v_n} - \frac{1}{n} \leq \psi_{v_n} \leq \pi_{v_n}$.

Since X_∞ is drawn from the stationary distribution π , we need to show that $\pi_{v_i} \leq \pi_{v_1} \leq \pi_{v_n}$ for all $v_i \in V_{S(n-2)}$. We use a digraph-theoretic argument. We can assume that the subdigraph $D_C(V_{S(n-2)})$ induced by $V_{S(n-2)}$ is transitive. We apply the *Canonical Decomposition of quasi-transitive digraphs* (Theorem 4.8.5 [17]) on $D_C(V_{S(n)}, A)$ and obtain a strong semicomplete digraph (in this case, a digraph of 3-cycle) $u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_1$ whereby $u_1 = v_1$, $u_3 = v_n$, and u_2 is the contraction of $V_{S(n-2)}$. We can then view the CMC as a random walk that is jumping clockwise along the direction of $u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_1$.

Given that the score sequence $d_T^-(v_1) \leq d_T^-(v_2) \leq d_T^-(v_3) \leq \dots \leq d_T^-(v_n)$ of $D_C(V_{S(n)})$ orders the vertices according to its in-degrees, a random walk on this digraph will spend most of the fraction of its time at v_n . Note that although $d_T^-(v_n) = d_T^-(v_{n-1})$ in the case $D_C(V_{S(n-2)})$ is transitive, v_{n-1} is oriented towards v_n . Furthermore, although for any $v_i \in V_{S(n-2)} \setminus \{v_{n-1}\}$, there could be equal probability (for a *standard* random walk) of jumping towards v_{n-1} and v_n , the relation $v_{n-1} \rightarrow v_n$ ensures that any time the random walk jumps to v_{n-1} it must then jump to v_n . At other times, the random walk could jump directly to v_n so that on average the random walk spends more fraction of its time in v_n . We also note that since v_n is oriented towards v_1 only, every time the random walk jumps to v_n it will then jump to v_1 , in which case $\pi_{v_1} = \pi_{v_n}$. As such, $\pi_{v_i} \leq \pi_{v_1} = \pi_{v_n}$ for all $v_i \in V_{S(n-2)}$. \square

Note: For an irreducible coevolutionary digraph $D_C(V_{S(n)})$ having structures described in Corollary 8, it is possible to compute π_{v_n} directly without having to compute the full π . When $D_C(V_{S(n)})$ is pancyclic with the least number of 3-cycles, we can calculate $\pi_{v_n} = \pi_{v_1} = \frac{1}{2}(1 - \sum_{i=2}^{n-1} \pi_i)$ using only hitting times. Note $D_C(V_{S(n-2)})$ is transitive. We calculate $1 - \sum_{i=2}^{n-1} \pi_i$ as the fraction of time on average the random walk spends jumping along the subdigraph $D_C(V_{S(n-2)})$ as it cycles along $u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_1$. More precisely, it is the average of the expected hitting time to v_n over starting vertices $v_i \in V_{S(n-2)}$.

The subdigraph induced by $V_{S(n-2)} \cup \{v_n\}$ is transitive and that $\{v_1\} \mapsto V_{S(n-2)}$. So, we can treat the random walk on the subdigraph as an absorbing CMC with transient states $v_i \in V_{S(n-2)}$ and a single absorbing state v_n . Let $\mathbb{E}_{v_i}(\tau_{v_n})$ be the expected hitting time starting from v_i to v_n . We relabel the vertices as x_m , $m = n - i$, $i = 1, 2, 3, \dots, n - 2$ (e.g., vertex v_{n-1} is now x_1). It can be shown that $\mathbb{E}_{v_i}(\tau_{v_n}) = \mathbb{E}_{x_m}(\tau_{v_n}) = \sum_{j=1}^m \frac{1}{j}$. In this case, we have

$$\begin{aligned} \mathbb{E}_{v_{n-1}}(\tau_{v_n}) &= \mathbb{E}_{x_1}(\tau_{v_n}) = 1 \\ \mathbb{E}_{v_{n-2}}(\tau_{v_n}) &= \mathbb{E}_{x_2}(\tau_{v_n}) = 1 + \frac{1}{2} \\ &\vdots \\ \mathbb{E}_{v_2}(\tau_{v_n}) &= \mathbb{E}_{x_{n-2}}(\tau_{v_n}) = 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n-2}. \end{aligned}$$

Let $\mathbb{E}(\eta_{V_{S(n-2)}}) = \frac{1}{n-2} \sum_{m=1}^{n-2} \mathbb{E}_{x_m}(\tau_{v_n})$ be the fraction of time on average the random walk spends in $V_{S(n-2)}$ as it cycles through $u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_1$. $\mathbb{E}(\eta_{v_1}) = 1$ and $\mathbb{E}(\eta_{v_n}) = 1$. So the total average time would be $2 + \mathbb{E}(\eta_{V_{S(n-2)}})$. We can calculate $1 - \sum_{i=2}^{n-1} \pi_i$ using these fraction of times as the random walk cycles through $u_1 \rightarrow u_2 \rightarrow u_3 \rightarrow u_1$ as follows

$$\pi_{v_n} = \pi_{v_1} = \frac{1}{2} \left(1 - \frac{\mathbb{E}(\eta_{V_{S(n-2)}})}{2 + \mathbb{E}(\eta_{V_{S(n-2)}})} \right). \quad (\text{A.9})$$

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