PROOF OF THE HAMILTONICITY - TRACE CONJECTURE FOR SINGULARLY PERTURBED MARKOV CHAINS[*]

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Abstract. We prove the conjecture formulated in [12], namely, that the trace of the fundamental matrix of a singularly perturbed Markov chain is minimized at policies corresponding to Hamiltonian cycles, over the set of all stochastic policies feasible for a given graph.

Key words. Stochastic matrices, Hamiltonian Cycles, Perturbed Markov chains

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1. Preliminaries and Notation. Let Γ be a connected graph of size N, $\mathbf{P}$ be an $N \times N$ probability transition matrix corresponding to a feasible policy on Γ, which means that $p_{ij} = 0$ whenever (i, j) is not an edge on Γ, and $\mathbf{J}$ be an $N \times N$ matrix where every element is unity. Consider the following singular perturbation of $\mathbf{P}$

$$\mathbf{P}(\varepsilon) := (1 - \varepsilon)\mathbf{P} + \frac{\varepsilon}{N}\mathbf{J}, \tag{1.1}$$

which we call the linear symmetric perturbation of $\mathbf{P}$ and denote $\mathbf{P}(\varepsilon)$ as $\mathbf{P}^{\varepsilon}$.

An important recent application of symmetric linear perturbation matrices is ranking in complex networks. Specifically, this sort of matrix is used in the Google PageRank algorithm that determines popularity of Web pages. The PageRank is defined as the stationary distribution of a Markov chain on the set of Web pages. This Markov chain serves as the following elementary model of a surfing process. At each step, with probability $(1-\varepsilon)$, a surfer follows a randomly chosen out-going hyperlink of a current page, and with probability ε, the surfer is bored and picks a new page on the Web at random. A jump to a random page with probability ε corresponds to the symmetric linear perturbation of a random walk on the Web graph, and the PageRank vector $\mathbf{r}$ is the stationary probability vector of $\mathbf{P}^{\varepsilon}$, that is, $\mathbf{r}\mathbf{P}^{\varepsilon} = \mathbf{r}$, where all components of $\mathbf{r}$ are non-negative and sum up to unity. The parameter ε, originally set equal to 0.15, is commonly called a 'damping factor'. Choosing $\varepsilon > 0$ ensures that there exists a unique PageRank vector $\mathbf{r}$. Furthermore, this parameter is responsible for the fast convergence of the power iteration procedure [11], for the robustness of the algorithm [1, 3], and for fair distribution of the PageRank mass among Web components [2]. After the introduction of the PageRank by Brin and Page [4], a great deal of work has been done on the PageRank computation and analysis. We refer to [11] for an excellent survey of this research. Throughout the paper we will explain the relation of our results to the analysis of PageRank.

Let $\mathbf{P}^*(\mathbf{P}, \varepsilon)$ be the stationary distribution matrix of $\mathbf{P}^{\varepsilon}$, namely,

$$\mathbf{P}^*(\mathbf{P}, \varepsilon) := \lim_{t \to \infty} (\mathbf{P}^{\varepsilon})^t.$$

Let $\mathbf{G}(\mathbf{P}, \varepsilon)$ be the fundamental matrix of the Markov chain with transition matrix $\mathbf{P}^{\varepsilon}$, which is defined as $\mathbf{G}(\mathbf{P}, \varepsilon) := (\mathbf{I} - \mathbf{P}^{\varepsilon} + \mathbf{P}^*(\mathbf{P}, \varepsilon))^{-1}$. Write $\mathbf{I} - \mathbf{P}^{\varepsilon} + \mathbf{P}^*(\mathbf{P}, \varepsilon)$ as $\mathbf{A}_*(\mathbf{P}, \varepsilon)$, and $\mathbf{I} - \mathbf{P}^{\varepsilon} + \frac{1}{N}\mathbf{J}$ as $\mathbf{A}(\mathbf{P}, \varepsilon)$.

For the sake of completeness, we are listing a few recent results on $\mathbf{G}(\mathbf{P}, \varepsilon)$, $\mathbf{A}(\mathbf{P}, \varepsilon)$ and the Hamiltonicity of Γ.

THEOREM 1.1. ([5], [6]) *For $\varepsilon \in [0,1)$ and any stochastic policy* $\mathbf{P}$ *feasible on a given Hamiltonian graph,*

$$\max_{\mathbf{P}^{\varepsilon}} \det \mathbf{A}(\mathbf{P}, \varepsilon) = \det \mathbf{A}(\mathbf{P}_{\mathrm{HC}}, \varepsilon).$$

In particular,

$$\det \mathbf{A}(\mathbf{P}_{\mathrm{HC}}, \varepsilon) = \begin{cases} N, & \text{for } \varepsilon = 0, \\ \dfrac{1 - (1-\varepsilon)^N}{\varepsilon}, & \text{for } \varepsilon \in (0,1), \end{cases}$$

for any $\mathbf{P}_{\mathrm{HC}}$ *corresponding to a Hamiltonian Cycle.*

In [12], it was proved that for $\varepsilon \in [0,1)$ the minimizers of $\mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$ over the set of all doubly stochastic policies correspond to Hamiltonian Cycles. It was also shown that this result holds over the set of all stochastic policies for $\varepsilon = 0$, that is, without any perturbation, namely

THEOREM 1.2. ([12]) *For $\varepsilon = 0$ and for any stochastic policy* $\mathbf{P}$ *feasible on a given Hamiltonian graph,*

$$\min_{\mathbf{P}} \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = \mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)],$$

for any $\mathbf{P}_{\mathrm{HC}}$ *corresponding to a Hamiltonian Cycle.*

The paper [12] also includes a conjecture that the result holds for $\varepsilon \in [0,1)$, as follows

CONJECTURE 1.1. ([12]) *For any $\varepsilon \in [0,1)$ and any stochastic policy* $\mathbf{P}$ *feasible on a given Hamiltonian graph,*

$$\min_{\mathbf{P}} \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = \mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)],$$

for any $\mathbf{P}_{\mathrm{HC}}$ *corresponding to a Hamiltonian Cycle.*

In this paper, we present a proof of the above statement, which we call the Hamiltonicity-Trace conjecture.

2. Main Result.

THEOREM 2.1. *For any $\varepsilon \in (0,1)$ and for any stochastic policy* $\mathbf{P}$ *feasible on a given Hamiltonian graph,*

$$\min_{\mathbf{P}} \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = \mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)] = 1 + \frac{\varepsilon N - (1 - (1-\varepsilon)^N)}{\varepsilon(1 - (1-\varepsilon)^N)},$$

for any $\mathbf{P}_{HC}$ *corresponding to a Hamiltonian Cycle.*

The structure for the proof of Theorem 2.1 is as follows: In Lemma 3.1, we derive relationships between eigenvalues and eigenvectors of various relevant matrices, which lead to the derivation of alternative formulae for the trace function in Lemma 3.2. In Lemma 4.1, we prove that the value of the trace of $\mathbf{G}(\mathbf{P}, \varepsilon)$ when $\varepsilon \in (0,1)$ for any randomized policy is bounded above by that of some deterministic policy, and bounded below by that of some other deterministic policy. This enables us to reduce our proof from the set of all stochastic policies to the set of all deterministic policies only. We derive the exact formulae for four exhaustive, mutually exclusive types of deterministic policies in Lemmata 4.2-4.5. Finally, we show that among these, Hamiltonian cycles are minimizers for the objective function.

3. Properties of the trace of the fundamental matrix for perturbed Markov chains. Let η_i be the eigenvalues of $\mathbf{P}^{\varepsilon}$, for $i = 1, \ldots, N$.

LEMMA 3.1. *For any $\varepsilon \in (0,1)$ and any stochastic matrix* $\mathbf{P}$, *the following properties hold:*
   (i) *Any right eigenvector of* $\mathbf{P}^{\varepsilon}$ *corresponding to an eigenvalue $\eta_i < 1$ is a right eigenvector of* $\mathbf{P}^*(\mathbf{P}, \varepsilon)$ *corresponding to eigenvalue 0 and hence is a right eigenvector of* $\mathbf{A}_*(\mathbf{P}, \varepsilon)$ *corresponding to the eigenvalue $1 - \eta_i$. The right eigenvector $\boldsymbol{e} = (1, \ldots, 1)^T$ of* $\mathbf{P}^{\varepsilon}$ *corresponding to the unique eigenvalue $\eta_N = 1$ is a right eigenvector of* $\mathbf{P}^*(\mathbf{P}, \varepsilon)$ *corresponding to eigenvalue 1 and hence it is a right eigenvector of* $\mathbf{A}_*(\mathbf{P}, \varepsilon)$ *corresponding to eigenvalue 1.*

(ii) $\mathbf{A}_*(\mathbf{P},\varepsilon)$ *and* $\mathbf{A}(\mathbf{P},\varepsilon)$ *share the set of eigenvalues* $\{\mu_i = 1 - \eta_i,\ \text{for } i = 1, \ldots, N-1, \mu_N = 1\}.$

(iii) $\det \mathbf{A}_*(\mathbf{P},\varepsilon) = \det \mathbf{A}(\mathbf{P},\varepsilon) = \displaystyle\prod_{i=1}^{N-1} (1 - \eta_i).$

Proof.

(i) Let $\mathbf{u}_1, \ldots, \mathbf{u}_N$ be the left eigenvectors of $\mathbf{P}^\varepsilon$ with $\mathbf{u}_N$ corresponding to the eigenvalue one, which makes it the stationary distribution of the Markov chain with transition matrix $\mathbf{P}^\varepsilon$. As $\mathbf{P}^\varepsilon$ is irreducible and aperiodic, any right eigenvector $\mathbf{y}_i$ of $\mathbf{P}^\varepsilon$ corresponding an eigenvalue $\eta_i < 1$ is orthogonal to $\mathbf{u}_N$, so $\mathbf{P}^*(\mathbf{P},\varepsilon)\mathbf{y}_i = \mathbf{v}_N \mathbf{u}_N \mathbf{y}_i = \mathbf{0}$. This gives us $\mathbf{A}_*(\mathbf{P},\varepsilon)\mathbf{y} = (1 - \eta_i)\mathbf{y}_i$.

(ii) For $\mathbf{A}_*(\mathbf{P},\varepsilon)$: We observe that $\mathbf{e}$ is an eigenvector of both $\mathbf{P}^\varepsilon$ and $\mathbf{A}_*(\mathbf{P},\varepsilon)$ with eigenvalue 1. As $\mathbf{u}_1, \ldots, \mathbf{u}_{N-1}$ span $\ker(\mathbf{P}^*(\mathbf{P},\varepsilon))$, then the remaining eigenvalues of $\mathbf{A}_*(\mathbf{P},\varepsilon)$ are $1-\eta_i$, for $i = 1, \ldots, N-1$.

For $\mathbf{A}(\mathbf{P},\varepsilon)$: It is straightforward to see that $\mathbf{e}$ is also an eigenvector of $\mathbf{A}(\mathbf{P},\varepsilon)$ with eigenvalue 1. Let $\mathbf{w} \neq \mathbf{e}$ be an eigenvector of $\mathbf{P}^\varepsilon - \frac{1}{N}\mathbf{J}$, with eigenvalue $\gamma \neq 0$, then $\mathbf{w} = \mathbf{t} + \alpha\mathbf{e}$ for some α and some $\mathbf{t} \in \ker(\mathbf{J})$. Now we will show that there exists a corresponding vector $\mathbf{s} = \mathbf{t} + \beta\mathbf{e}$ such that $\mathbf{P}^\varepsilon\mathbf{s} = \gamma\mathbf{s}$. Indeed, taking $\beta = -\alpha\gamma/(\gamma - 1)$, we see that

$$
\begin{aligned}
\mathbf{P}^\varepsilon\mathbf{s} &= \mathbf{P}^\varepsilon(\mathbf{t} + \beta\mathbf{e}) \\
&= \left(\mathbf{P}^\varepsilon - \frac{1}{N}\mathbf{J} + \frac{1}{N}\mathbf{J}\right)(\mathbf{t} + \alpha\mathbf{e} - \alpha\mathbf{e} + \beta\mathbf{e}) = \left(\mathbf{P}^\varepsilon - \frac{1}{N}\mathbf{J} + \frac{1}{N}\mathbf{J}\right)(\mathbf{t} + \alpha\mathbf{e} - \alpha\mathbf{e}) + \beta\mathbf{e} \\
&= \gamma\mathbf{w} + \left(\frac{1}{N}\mathbf{0} + \alpha\mathbf{e}\right) - \alpha\mathbf{e} + \beta\mathbf{e} = \gamma(\mathbf{t} + \alpha\mathbf{e}) + \beta\mathbf{e} = \gamma\mathbf{t} + \alpha\gamma\mathbf{e} - \frac{\alpha\gamma}{\gamma - 1}\mathbf{e} = \gamma\mathbf{t} + \gamma\beta\mathbf{e} = \gamma\mathbf{s}.
\end{aligned}
$$

Thus, the set of eigenvalues γ_i of $\mathbf{P}^\varepsilon - \frac{1}{N}\mathbf{J}$, $i = 1, \ldots, N-1$, $\gamma_i \neq 0$ is also the set of eigenvalues η_i of $\mathbf{P}^\varepsilon$, $i = 1, \ldots, N-1$, $\eta_i \neq 1$, and vice versa. Consequently, with one eigenvalue of $\mathbf{A}_*(\mathbf{P},\varepsilon)$ being unity, the remaining eigenvalues of $\mathbf{A}_*(\mathbf{P},\varepsilon)$ are $1 - \eta_i$, for $i = 1, \ldots, N-1$.

(iii) This result follows immediately from part (ii) above. □

LEMMA 3.2. *For any* $\varepsilon \in (0,1)$ *and any stochastic matrix* $\mathbf{P}$,

(i) *The set of eigenvalues of* $\mathbf{G}(\mathbf{P},\varepsilon)$ *is* $\{1, \frac{1}{1-\eta_i}, i = 1, \ldots, N-1\}.$

(ii) $\text{Tr}[\mathbf{G}(\mathbf{P},\varepsilon)] = 1 + \displaystyle\sum_{i=1}^{N-1} \frac{1}{1 - \eta_i},$

(iii) $\text{Tr}[\mathbf{G}(\mathbf{P},\varepsilon)] = \text{Tr}[\mathbf{A}^{-1}(\mathbf{P},\varepsilon))].$

Proof. Part (i) follows directly from the fact that for any $\varepsilon \in (0,1)$ and for any stochastic $\mathbf{P}$, the matrix $\mathbf{A}(\mathbf{P},\varepsilon)$ is invertible, as the minimum value of $\det \mathbf{A}(\mathbf{P},\varepsilon)$ is strictly greater than zero (see [6]); consequently, $\mathbf{A}_*(\mathbf{P},\varepsilon)$ is also invertible. Part (ii) follows from part (i), and part (iii) follows directly from part (ii) and Lemma 3.1. □

The result of Lemma 3.2 is quite puzzling. It turns out that if we replace $\mathbf{P}^*(\mathbf{P},\varepsilon)$ by $(\frac{1}{N})\mathbf{J}$ in the fundamental matrix $\mathbf{G}(\mathbf{P},\varepsilon) = \mathbf{A}_*^{-1}(\mathbf{P},\varepsilon)$, then the trace remains invariant. This interesting observation can also be explained using a probabilistic argument. To this end, we first need to perform some simple calculations.

Let $\mathbf{W}$ be a rank-one stochastic matrix. Such matrix consists of identical rows, each row representing a probability distribution on $1, \ldots, N$. Formally, $\mathbf{W} = \mathbf{e}^\mathrm{T}\mathbf{w}$, where $\mathbf{w}$ is a vector of length N and the ith coordinate of $\mathbf{w}$ stands for the probability of value i. It is easy to verify that $\mathbf{PW} = \mathbf{W}$ for *any* stochastic matrix $\mathbf{P}$. Now, assume that $\mathbf{P}$ is irreducible, and consider the matrix $\mathbf{A}_\mathrm{w}(\mathbf{P}) = \mathbf{I} - \mathbf{P} + \mathbf{W}$. The inverse $\mathbf{A}_\mathrm{w}^{-1}(\mathbf{P})$ exists and can be viewed as a generalization of a fundamental matrix. Moreover, using the argument as in the proof Lemma 3.1(ii), one can show that if $\eta_1, \ldots, \eta_{N-1}, \eta_N = 1$ are the eigenvalues of $\mathbf{P}$ then $\eta_1, \ldots, \eta_{N-1}, 0$ are the eigenvalues of $\mathbf{P} - \mathbf{W}$. Hence, the spectral radius of $\mathbf{P} - \mathbf{W}$

is smaller than 1, and expending $\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P})$ in a power series, we get

$$\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P}) = \mathbf{I} + \sum_{n=1}^{\infty}[\mathbf{P} - \mathbf{W}]^n = \mathbf{I} + [\mathbf{P} - \mathbf{W}] + \sum_{n=1}^{\infty}[\mathbf{P} - \mathbf{W}]^{n+1}. \tag{3.1}$$

Since for $n \geq 1$

$$\begin{aligned} [\mathbf{P} - \mathbf{W}]^{n+1} &= [\mathbf{P} - \mathbf{W}]^n\mathbf{P} - [\mathbf{P} - \mathbf{W}]^n\mathbf{W} \\ &= [\mathbf{P} - \mathbf{W}]^n\mathbf{P} - [\mathbf{P} - \mathbf{W}]^{n-1}[\mathbf{W} - \mathbf{W}] \\ &= [\mathbf{P} - \mathbf{W}]^n\mathbf{P} = \cdots = [\mathbf{P} - \mathbf{W}]\mathbf{P}^n, \end{aligned} \tag{3.2}$$

equation (3.1) reduces to

$$\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P}) = \mathbf{I} + \sum_{n=0}^{\infty}[\mathbf{P} - \mathbf{W}]\mathbf{P}^n = \lim_{t\to\infty}\left\{\sum_{n=0}^{t}\mathbf{P}^n - \sum_{n=0}^{t-1}\mathbf{W}\mathbf{P}^n\right\}, \tag{3.3}$$

where the second equality is obtained by expanding $\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P})$ in (3.1) up to $[\mathbf{P} - \mathbf{W}]^t$ and then letting $t \to \infty$. Now consider a Markov chain governed by $\mathbf{P}$. Then the element (i, j) of the matrix inside the curly braces in the last expression of (3.3) equals to the difference between two values: (i) the average number of visits to j on $[0, t]$ of the chain started at i, and (ii) the average number of visits to j on $[0, t-1]$ of the chain started from the distribution given by $\mathbf{w}$, the row of $\mathbf{W}$. Thus, indicating the initial distribution as a lower index of the expectation, from (3.3) we derive

$$\begin{aligned} \mathrm{Tr}[\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P})] &= \sum_i \left[\mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P})\right]_{ii} = \lim_{t\to\infty}\sum_i \{\mathbb{E}_i[\# \text{ visits to } i \text{ on } [0, t]] - \mathbb{E}_{\mathbf{w}}[\# \text{ visits to } i \text{ on } [0, t-1]]\} \\ &= \lim_{t\to\infty}\left\{\sum_i \mathbb{E}_i[\# \text{ visits to } i \text{ on } [0, t]] - (t-1)\right\}, \end{aligned}$$

which is finite and, surprisingly, does not depend on $\mathbf{W}$. Coming back to Lemma 3.2, we see that for all $\varepsilon \in (0, 1)$ the matrix $\mathbf{P}^{\varepsilon}$ is an irreducible stochastic matrix. Thus, the trace of $[\mathbf{I} - \mathbf{P}^{\varepsilon} + \mathbf{W}]^{-1}$ is the same for any rank-one stochastic matrix $\mathbf{W}$. This generalizes Part (ii) of Lemma 3.2, which can be now obtained by setting $\mathbf{W} = \mathbf{P}^*(\mathbf{P}, \varepsilon)$ or $\mathbf{W} = \frac{1}{N}\mathbf{J}$.

We can now derive a convenient expression for our quantity of interest, $\mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$. Let $\mathbf{Q}$ be another rank-one stochastic matrix, and consider generalized versions of $\mathbf{P}^{\varepsilon}$ and $\mathbf{A}_{\mathrm{w}}(\mathbf{P}, \varepsilon)$ defined as

$$\mathbf{P}(\mathbf{Q}, \varepsilon) = (1 - \varepsilon)\mathbf{P} + \varepsilon\mathbf{Q}, \quad \mathbf{A}_{\mathrm{w}}(\mathbf{P}, \mathbf{Q}, \varepsilon) = \mathbf{I} - \mathbf{P}(\mathbf{Q}, \varepsilon) + \mathbf{W}.$$

Then we have

$$\mathbf{A}_{\mathrm{w}}(\mathbf{P}, \mathbf{Q}, \varepsilon) = \mathbf{I} - (1 - \varepsilon)\mathbf{P} + [\mathbf{W} - \varepsilon\mathbf{Q}] = \mathbf{I} - (1 - \varepsilon)\mathbf{P} + (1 - \varepsilon)\mathbf{W}',$$

where $\mathbf{W}' = [\mathbf{W} - \varepsilon\mathbf{Q}]/(1 - \varepsilon)$ is a matrix with identical rows $\mathbf{w}'$ such that each row sums up to unity but some elements might be negative. Nevertheless, the spectral radius of $[\mathbf{P} - \mathbf{W}']$ is still smaller than 1, and the expression $\mathbf{P}\mathbf{W}' = \mathbf{W}'$ still holds in this case. Hence, we can apply the argument from (3.2) to deduce that for $n \geq 1$,

$$[\mathbf{P} - \mathbf{W}']^{n+1} = [\mathbf{P} - \mathbf{W}']\mathbf{P}^n,$$

and expanding $\mathbf{G}_{\mathrm{w}}(\mathbf{P}, \mathbf{Q}, \varepsilon) = \mathbf{A}_{\mathrm{w}}^{-1}(\mathbf{P}, \mathbf{Q}, \varepsilon)$ in a power series, we obtain

$$\begin{aligned} \mathbf{G}_{\mathrm{w}}(\mathbf{P}, \mathbf{Q}, \varepsilon) &= \sum_{n=0}^{\infty}(1 - \varepsilon)^n[\mathbf{P} - \mathbf{W}']^n \\ &= \sum_{n=0}^{\infty}(1 - \varepsilon)^n\mathbf{P}^n - \sum_{n=1}^{\infty}(1 - \varepsilon)^n\mathbf{W}'\mathbf{P}^{n-1} \\ &= [\mathbf{I} - (1 - \varepsilon)\mathbf{P}]^{-1} - (1 - \varepsilon)\mathbf{W}'[1 - (1 - \varepsilon)\mathbf{P}]^{-1}. \end{aligned} \tag{3.4}$$

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The first matrix in the last equation has a simple probabilistic meaning. Consider a random walk similar to the one in the PageRank definition but with a stop instead of a random jump. With probability $(1-\varepsilon)$, such Markov random walk makes a step according to the transition matrix $\mathbf{P}$, and with probability ε the random walk terminates. In other words, we have a Markov chain with transition matrix $\mathbf{P}$ and a stopping time $T(\varepsilon)$, which is distributed geometrically with parameter ε. Then the element (i,i) of

$$[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1} = \sum_{n=0}^{\infty}(1-\varepsilon)^n\mathbf{P}^n \tag{3.5}$$

is nothing else but the average number of visits to node i on the interval $[0, T(\varepsilon)]$, provided that the random walk started at i. Furthermore, the element (i,i) of $\mathbf{W}'[1 - (1-\varepsilon)\mathbf{P}]^{-1}$ equals

$$\sum_j \mathbf{W}'_{ij}\mathbb{E}_j[\# \text{ visits to } i \text{ on } [0, T(\varepsilon)]].$$

Note that for all i, the element $\mathbf{W}'_{ij}$ is simply the jth coordinate of $\mathbf{w}'$. Thus, summing over i, and using the fact that the stopping time $T(\varepsilon)$ is independent of the random walk, we obtain

$$\text{Tr}[\mathbf{W}'[1 - (1-\varepsilon)\mathbf{P}]^{-1}] = \sum_j [j\text{th coordinate of } \mathbf{w}'] \sum_i \mathbb{E}_j[\# \text{ visits to } i \text{ on } [0, T(\varepsilon)]]$$

$$= \sum_j [j\text{th coordinate of } \mathbf{w}']\mathbb{E}_j[T(\varepsilon)]$$

$$= \sum_j [j\text{th coordinate of } \mathbf{w}'](1/\varepsilon) = 1/\varepsilon. \tag{3.6}$$

Substituting (3.6) in the trace of (3.4) we get

$$\text{Tr}[\mathbf{G}_{\text{w}}(\mathbf{P}, \mathbf{Q}, \varepsilon)] = \text{Tr}[[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}] - \frac{1-\varepsilon}{\varepsilon}, \tag{3.7}$$

for any rank-one stochastic perturbation $\mathbf{Q}$ and any rank-one stochastic matrix $\mathbf{W}$. This result generalizes Part (iii) of Lemma 3.2, which can be obtained from (3.7) when $\mathbf{Q} = \frac{1}{N}\mathbf{J}$ and $\mathbf{W} = \mathbf{P}^*(\mathbf{P}, \varepsilon)$.

We would like to remark that in the recent literature, the matrix $\mathbf{P}(\mathbf{Q}, \varepsilon)$ is often used instead of $\mathbf{P}^\varepsilon$ in the PageRank definition. This modified model is commonly referred to as a *personalized* or *topic-sensitive* PageRank [9]. In this model, after a random jump, a surfer picks a page according to some probability distribution $\mathbf{q}$, which is not necessarily uniform. The probability vector $\mathbf{q}$ may reflect personal or thematic preferences. Also, this model is used for spam detection by giving higher preference to trusted pages [8]. In [10], partial results on eigenvalues and eigenvectors of $\mathbf{P}(\mathbf{Q}, \varepsilon)$ were obtained, using the arguments of a similar kind as in the proof of Lemma 3.1.

Let $\mathbf{r}(\mathbf{Q}, \varepsilon)$ be the personalized PageRank vector with perturbation matrix $\mathbf{Q}$, which consists of identical rows $\mathbf{q}$. By definition, $\mathbf{r}(\mathbf{Q}, \varepsilon)$ is a stationary vector of $\mathbf{P}(\mathbf{Q}, \varepsilon)$:

$$\mathbf{r}(\mathbf{Q}, \varepsilon) = \mathbf{r}(\mathbf{Q}, \varepsilon)[(1-\varepsilon)\mathbf{P} + \varepsilon\mathbf{Q}].$$

Then since $\mathbf{r}(\mathbf{Q}, \varepsilon)\mathbf{Q} = \mathbf{q}$, we immediately obtain

$$\mathbf{r}(\mathbf{Q}, \varepsilon) = \mathbf{q}[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}.$$

This formula highlights the role of the matrix $[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}$ in the PageRank analysis. Although the matrix inversion is not practical from computational point of view, the formula can be used to derive many interesting properties of the PageRank. For instance, the PageRank of page i can be written as a product of three terms, where one of the terms is the element (i,i) of $[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}$, and it is the only component that depends on outgoing links of i and thus can be influenced by this page itself [1].

4. Optimality of the Hamiltonian cycle. The following lemma shows that the trace of the fundamental matrix can be maximized or minimized only on deterministic policies.

LEMMA 4.1. *For any $\varepsilon \in (0,1)$ and for every randomized policy $\mathbf{P}$, there exist some deterministic policies $\mathbf{D}_1$ and $\mathbf{D}_2$ such that*

$$\mathrm{Tr}[\mathbf{G}(\mathbf{D}_1, \varepsilon)] \leq \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] \leq \mathrm{Tr}[\mathbf{G}(\mathbf{D}_2, \varepsilon)]. \tag{4.1}$$

Proof. Let $\mathbf{P}$ be a randomized policy. We consider the randomization at each row i of $\mathbf{P}$ separately. Suppose a particular row i is of the following structure:

$$[\ldots a \ldots b \ldots c \ldots], \quad a, b \in (0,1).$$

Consider a policy $\mathbf{P}_\lambda$ that coincides with $\mathbf{P}$ in all rows except row i, where it is replaced by

$$\left[\ldots \lambda \ldots \frac{(1-\lambda)}{1-a} b \ldots \frac{(1-\lambda)}{1-a} c \ldots\right], \quad \lambda \in [0,1].$$

Note that for $\lambda = a$, $\mathbf{P}_\lambda$ reduces to $\mathbf{P}$. By Lemma 3.2 part (iii) and writing the inverse in terms of the adjoint,

$$\mathrm{Tr}\left[\mathbf{G}(\mathbf{P}_\lambda, \varepsilon)\right] = \mathrm{Tr}\left[\mathbf{A}^{-1}(\mathbf{P}_\lambda, \varepsilon)\right] = \sum_{i=1}^{N} \frac{|\mathbf{A}_{ii}(\mathbf{P}_\lambda, \varepsilon)|}{|\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)|},$$

where $\mathbf{A}(\mathbf{P}_\lambda, \varepsilon) = \mathbf{I} - \mathbf{P}_\lambda^\epsilon + \frac{1}{N}\mathbf{J}$ and $\mathbf{A}_{ii}(\mathbf{P}_\lambda, \varepsilon)$ is $\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)$ with the i-th row and the i-th column removed. Both $|\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)|$ and $|\mathbf{A}_{ii}(\mathbf{P}_\lambda, \varepsilon)|$ are linear functions of λ for all $i = 1, \ldots, N$. Therefore,

$$\mathrm{Tr}\left[\mathbf{G}(\mathbf{P}_\lambda, \varepsilon)\right] = \frac{C_1 |\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)| + C_2}{|\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)|} = C_1 + \frac{C_2}{|\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)|},$$

for some C_1, C_2 constant, $C_1 \neq 0$. Differentiating the objective function with respect to λ gives us

$$\frac{d}{d\lambda} \mathrm{Tr}\left[\mathbf{G}(\mathbf{P}_\lambda, \varepsilon)\right] = -\frac{C_2}{|\mathbf{A}(\mathbf{P}_\lambda, \varepsilon)|^2},$$

which is either zero for all $\lambda \in (0,1)$, if $C_2 = 0$, or never zero for all $\lambda \in (0,1)$, if $C_2 \neq 0$. In both cases, this implies that $\mathrm{Tr}[\mathbf{G}(\mathbf{P}_\lambda, \varepsilon)]$ is a monotone function over $\lambda \in [0,1]$, and is maximized or minimized at either extreme of the interval. As the i-th row in $\mathbf{P}_{\lambda=0}$ or $\mathbf{P}_{\lambda=1}$ has at least one more row than the i-th row in $\mathbf{P}$, $\mathbf{P}_{\lambda=0}$ or $\mathbf{P}_{\lambda=1}$ has at least one more zero than $\mathbf{P}$, and:
 (1) either $\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\lambda=0}, \varepsilon)]$ or $\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\lambda=1}, \varepsilon)] \geq \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, and
 (2) either $\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\lambda=1}, \varepsilon)]$ or $\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\lambda=0}, \varepsilon)] \leq \mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, respectively.

Applying this process of increasing the number of zeros (and consequently reducing the number of randomizations), we can find $\mathbf{D}_1$ and $\mathbf{D}_2$ that satisfy the inequalities in (4.1).   □

LEMMA 4.2. *For any $\varepsilon \in (0,1)$ and any $\mathbf{P}_{HC}$ that corresponds to a Hamiltonian Cycle, that is, a policy with a single ergodic class and no transient states,*

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{HC}, \varepsilon)] = 1 + \frac{\varepsilon N - (1 - (1-\varepsilon)^N)}{\varepsilon(1 - (1-\varepsilon)^N)}.$$

Proof. As $\mathbf{P}_{HC}^\varepsilon$ is doubly stochastic and irreducible, $\mathbf{P}^*(\mathbf{P}, \varepsilon)$ reduces to $\frac{1}{N}\mathbf{J}$ and consequently the fundamental matrix $\mathbf{G}(\mathbf{P}_{HC}, \varepsilon)$ reduces to $(\mathbf{I} - \mathbf{P}_{HC}^\varepsilon + \frac{1}{N}\mathbf{J})^{-1} = \mathbf{A}^{-1}(\mathbf{P}_{HC}, \varepsilon)$.

From [6], for $i = 1, \ldots, N-1$, the eigenvalues λ_i of $\mathbf{P}_{HC}$ are the N-th roots of unity, and $\lambda_N = 1$; for $i = 1, \ldots, N-1$, the eigenvalues μ_i of $\mathbf{A}(\mathbf{P}_{HC}, \varepsilon)$ are $1 - (1-\varepsilon)\lambda_i$, and $\mu_N = 1$. By Lemma 3.2 part

(ii),

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}},\varepsilon)] = 1 + \sum_{i=1}^{N-1} \frac{1}{1-(1-\varepsilon)\lambda_i} = 1 + \frac{d}{\prod_{i=1}^{N-1}(1-(1-\varepsilon)\lambda_i)}$$

$$= 1 + \frac{d}{\dfrac{1-(1-\varepsilon)^N}{\varepsilon}}, \tag{4.2}$$

where

$$d = (N-1) - (1-\varepsilon)(N-2)\sum_{i=1}^{N-1}\lambda_i + (1-\varepsilon)^2(N-3)\sum_{\substack{i>j \\ i,j=1}}^{N-1}\lambda_i\lambda_j$$

$$- \cdots + (-1)^{N-2}(1-\varepsilon)^{N-2}(N-(N-1))\sum_{\substack{i_1>i_2>\ldots>i_{N-2} \\ i_1,i_2,\ldots,i_{N-2}=1}}^{N-1}\lambda_{i_1}\lambda_{i_2}\ldots\lambda_{i_{N-2}}$$

$$= (N-1) - (1-\varepsilon)(N-2)q_1(\lambda) + (1-\varepsilon)^2(N-3)q_2(\lambda) - \cdots + (-1)^{N-2}(1-\varepsilon)^{N-2}(N-(N-1))q_{N-2}(\lambda),$$

and the last equality in (4.2) follows from Lemma 3.3 in [6]. From the proof of Proposition 1 in [5], the values of the elementary symmetric polynomials $q_i(\lambda_i)$ are: $q_1(\lambda_i) = -1, q_2(\lambda_i) = 1, \ldots, q_{N-2}(\lambda_i) = (-1)^{N-2}$. Hence, d simplifies to

$$d = (N-1) + (1-\varepsilon)(N-2) + (1-\varepsilon)^2(N-3) + \cdots + (1-\varepsilon)^{N-2}(N-(N-1)).$$

Let $r := 1 - \varepsilon$,

$$d = (N-1)r^0 + (N-2)r^1 + (N-3)r^2 + \cdots + (N-(N-1))r^{N-2}$$

$$= N\sum_{i=0}^{N-2}r^i - \sum_{i=0}^{N-2}(i+1)r^i = N\sum_{i=0}^{N-2}r^i - \sum_{i=1}^{N-1}ir^{i-1} = N\sum_{i=0}^{N-2}r^i - \sum_{i=0}^{N-1}ir^{i-1}$$

$$= N\frac{1-r^{N-1}}{1-r} - \left(\frac{1-r^N}{(1-r)^2} - \frac{Nr^{N-1}}{1-r}\right) = \frac{N(1-r)-(1-r^N)}{(1-r)^2}. \tag{4.3}$$

Substituting the right-hand side of (4.3) into (4.2):

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}},\varepsilon)] = 1 + \frac{N(1-r)-(1-r^N)}{(1-r)^2}\frac{1-r}{1-r^N} = 1 + \frac{N(1-r)-(1-r^N)}{(1-r)(1-r^N)} = 1 + \frac{\varepsilon N - (1-(1-\varepsilon)^N)}{\varepsilon(1-(1-\varepsilon)^N)}.$$

□

Alternative proof. It follows from (3.7) that it is sufficient to compute the element (i,i) of $[\mathbf{I}-(1-\varepsilon)\mathbf{P}]^{-1}$ for each $i = 1, \ldots, N$. Consider a Markov walk that starts at i and is governed by $\mathbf{P}$. Then the required diagonal element equals to the expected number of visits to i on $[0, T(\varepsilon)]$, where $T(\varepsilon)$ is a random variable that has a geometric distribution with parameter ε (see also formula (3.5) and its explanation). In other words, the Markov chain may terminate at each step with probability ε, and we are interested in the number of visits to i before termination. Now assume that $\mathbf{P} = \mathbf{P}_{\mathrm{HC}}$. Then the random walk proceeds in cycles of length N, and thus, starting from i, the probability that it returns to i is $(1-\varepsilon)^N$, implying that the expected number of returns is $(1-(1-\varepsilon)^N)^{-1}$. Furthermore, this holds for any $i = 1, \ldots, N$. Hence, from (3.7) we obtain

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}},\varepsilon)] = \frac{N}{1-(1-\varepsilon)^N} - \frac{1-\varepsilon}{\varepsilon} = 1 + \frac{\varepsilon N - (1-(1-\varepsilon)^N)}{\varepsilon(1-(1-\varepsilon)^N)}.$$

□

LEMMA 4.3. *For $\varepsilon \in (0,1)$ and for any $\mathbf{P}$ that corresponds to a policy with $l > 1$ ergodic classes and no transient states,*

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = 1 + \frac{l-1}{\varepsilon} + \sum_{i=1}^{l} \left[\frac{m_i \varepsilon - (1 - (1-\varepsilon)^{m_i})}{\varepsilon(1 - (1-\varepsilon)^{m_i})} \right],$$

where m_i is the size of the i-th ergodic class in $\mathbf{P}$.

Proof. The proof follows the same reasoning as that of Lemma 4.2. The matrix $\mathbf{P}_{\mathrm{HC}}^{\varepsilon}$ is doubly stochastic and irreducible, so $\mathbf{P}^*(\mathbf{P}, \varepsilon)$ reduces to $\frac{1}{N}\mathbf{J}$ and consequently the fundamental matrix $\mathbf{G}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)$ reduces to $(\mathbf{I} - \mathbf{P}_{\mathrm{HC}}^{\varepsilon} + \frac{1}{N}\mathbf{J})^{-1} = \mathbf{A}^{-1}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)$.

Without loss of generality, let $l = 2$, and $m_1, m_2 > 0$ be the size of the two ergodic classes in $\mathbf{P}$, $m_1 + m_2 = N$. Let $\mathbf{P}_{\mathrm{HC},k}$ denote a Hamiltonian Cycle for a graph of size k. From the proof of Lemma 3.5 in [6], for $i = 1, \ldots, m_1 - 1$, the eigenvalues λ_i of $\mathbf{P}$ coincide with the eigenvalues of $\mathbf{P}_{\mathrm{HC},m_1}$, excluding $\lambda_{m_1} = 1$, and for $i = m_1 + 1, \ldots, m_1 + m_2 - 1$, eigenvalues λ_i of $\mathbf{P}$ coincide with the eigenvalues of $\mathbf{P}_{\mathrm{HC},m_2}$, excluding $\lambda_{m_1+m_2} = \lambda_N = 1$.

In other words, for $i = 1, \ldots, m_1 - 1$, λ_i are the m_1-th roots of unity, excluding one eigenvalue of unity, and for $i = m_1 + 1, \ldots, m_1 + m_2 - 1$, λ_i are the m_2-th roots of unity, excluding one eigenvalue of unity. From the proof of Lemma 4.2,

$$\sum_{i=1}^{m_1-1} \frac{1}{1 - (1-\varepsilon)\lambda_i} + \sum_{i=m_1+1}^{m_1+m_2-1} \frac{1}{1 - (1-\varepsilon)\lambda_i} = \left[\frac{m_1(1-r) - (1 - r^{m_1})}{(1-r)(1 - r^{m_1})} \right] + \left[\frac{m_2(1-r) - (1 - r^{m_2})}{(1-r)(1 - r^{m_2})} \right].$$

For $i = m_1$, the eigenvalue $\lambda_{m_1} = 1$ of $\mathbf{P}$ corresponds to an eigenvector $\mathbf{v}_{m_1}$. It is straightforward that $\mathbf{v}_{m_1}$ is also an eigenvector of $\mathbf{A}(\mathbf{P}, \varepsilon)$, corresponding to $\mu_{m_1} = 1$. For $i = m_1 + m_2 = N$, the eigenvalue $\lambda_N = 1$ corresponds to another eigenvector $\mathbf{v}_N = \underline{e}$, which is also an eigenvector of $\mathbf{A}(\mathbf{P}, \varepsilon)$, this time corresponding to $\mu_N = \varepsilon$. It is worth reminding the reader that this difference is caused by $\mathbf{P}^*(\mathbf{P}, \varepsilon) = \frac{1}{N}\mathbf{J}$ having one eigenvalue of unity of multiplicity 1, and one eigenvalue of zero of multiplicity $N - 1$. Therefore,

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = 1 + \frac{1}{\varepsilon} + \sum_{i=1}^{2} \left[\frac{m_i(1-r) - (1 - r^{m_i})}{(1-r)(1 - r^{m_i})} \right].$$

It is a straightforward to generalize to the case of arbitrary $1 < l \leq \frac{N}{2}$ and $\sum_{i=1}^{l} m_l = N$. $\square$

Alternative proof. Consider again a diagonal element of $[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}$. If there are l ergodic classes then the Markov chain given by $\mathbf{P}$ splits in separate cycles of lengths $m_1, \ldots, m_l$. For each of the cycles, we can apply the argument from the alternative proof of Lemma 4.2. Then a diagonal element that corresponds to a state in ergodic class i, equals $1/(1 - (1-\varepsilon)^{m_i})$. Summing over all diagonal elements and using (3.7) we derive

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}_{\mathrm{HC}}, \varepsilon)] = \sum_{i=1}^{l} \frac{m_i}{1 - (1-\varepsilon)^{m_i}} - \frac{1-\varepsilon}{\varepsilon} = 1 + \frac{l-1}{\varepsilon} + \sum_{i=1}^{l} \left[\frac{m_i \varepsilon - (1 - (1-\varepsilon)^{m_i})}{\varepsilon(1 - (1-\varepsilon)^{m_i})} \right].$$

To get the last equation, it is sufficient to subtract and add $(l-1)(1-\varepsilon)/\varepsilon$ in the second expression and then use the result of Lemma 4.2. $\square$

LEMMA 4.4. *For any $\varepsilon \in (0,1)$ and any $\mathbf{P}$ that corresponds to a policy with a single ergodic class and one or more transient states,*

$$\mathrm{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = (N - m + 1) + \frac{m\varepsilon - (1 - (1-\varepsilon)^m)}{\varepsilon(1 - (1-\varepsilon)^m)},$$

where $m < N$ is the size of the single ergodic class.

Proof. From the proof of Lemma 3.4, for $i = 1, \ldots, m-1$, λ_i coincide with the eigenvalues of $\mathbf{P}_{\text{HC},m}$, $\lambda_m = 1$ and for $i = m+1, \ldots, N$, $\lambda_i = 0$. Correspondingly, we can determine the eigenvalues of $\mathbf{P}^{\varepsilon} = (1-\varepsilon)\mathbf{P} + \frac{\varepsilon}{N}\mathbf{J}$ as follows:

$$
\eta_i = \begin{cases}
(1-\varepsilon)\lambda_i + 0 = (1-\varepsilon)\lambda + i, & i = 1, \ldots, m-1, \\
(1-\varepsilon)\lambda_i + \varepsilon = 1, & i = m, \\
(1-\varepsilon)\lambda_i + 0 = 0, & i = m+1, \ldots, N.
\end{cases}
$$

Consequently, the eigenvalues of $\mathbf{A}(\mathbf{P}, \varepsilon) = \mathbf{I} - \mathbf{P}^{\varepsilon} + \mathbf{P}^{*}(\mathbf{P}, \varepsilon)$ are

$$
\mu_i = \begin{cases}
1 - (1-\varepsilon)\lambda_i + 0 & = & 1 - (1-\varepsilon)\lambda_i, & i = 1, \ldots, m-1, \\
1 - 1 + 1 & = & 1, & i = m, \\
1 - 0 + 0 & = & 1, & i = m+1, \ldots, N.
\end{cases}
$$

Hence,

$$
\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = (N - m + 1) + \sum_{i=1}^{m-1} \frac{1}{1 - (1-\varepsilon)\lambda_i} = (N - m + 1) + \frac{m\varepsilon - (1 - (1-\varepsilon)^m)}{\varepsilon(1 - (1-\varepsilon)^m)},
$$

the first equality follows from Lemma 3.2 part (ii) and the second from the proof of Lemma 4.2. □

Alternative proof. Consider a diagonal element (i, i) of $[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}$ where i is a transient state. Since $\mathbf{P}$ is deterministic, a Markov random walk with transition matrix $\mathbf{P}$ started in i can never return to i. Recalling that the diagonal element of $[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}$ is the average number of visits to i starting from i, we conclude that each transient state contributes one to $\text{Tr}\left[[\mathbf{I} - (1-\varepsilon)\mathbf{P}]^{-1}\right]$. On the other hand, ergodic states form a cycle of length m, and we can compute the contribution of these states by applying the argument as in the alternative proof of Lemma 4.2 with $N = m$. Summing the contributions of transient and ergodic states and applying (3.7) we get the result of the lemma. □

LEMMA 4.5. *For any $\varepsilon \in (0, 1)$ and for any $\mathbf{P}$ corresponds to a policy with multiple ergodic classes and one or more transient states,*

$$
\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = \left(N - \sum_{i=1}^{l} m_i + 1\right) + \frac{l-1}{\varepsilon} + \sum_{i=1}^{l}\left[\frac{m_i\varepsilon - (1 - (1-\varepsilon)^{m_i})}{\varepsilon(1 - (1-\varepsilon)^{m_i})}\right],
$$

where m_i is the size of the i-th ergodic class in $\mathbf{P}$.

Proof. Let $m_1, \ldots, m_l$ be the size of l ergodic classes, $\sum_{i=1}^{l} m_i < N$. Using analogous arguments to the proofs of Lemmata 4.3 and 4.4, we can show that:

$$
\mu_i = \begin{cases}
1 - (1-\varepsilon)\lambda_i & , \text{for } i = 1, \ldots, m_1 - 1, & (\lambda_i : m_1\text{-th roots of unity, excl. 1}) \\
1 - (1-\varepsilon)\lambda_i & , \text{for } i = m_1 + 1, \ldots, m_1 + m_2 - 1, & (\lambda_i : m_2\text{-th roots of unity, excl. 1}) \\
\vdots & & \\
1 & , \text{for } i = m_1, & \\
\varepsilon & , \text{for } i = m_2, m_3, \ldots, m_l, & \\
1 & , \text{for } i = 1 + \sum_{i=1}^{l} m_i, \ldots, N.
\end{cases}
$$

Consequently,

$$
\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)] = \left(N - \sum_{i=1}^{l} m_i + 1\right) + \frac{l-1}{\varepsilon} + \sum_{i=1}^{l}\left[\frac{m_i\varepsilon - (1 - (1-\varepsilon)^{m_i})}{\varepsilon(1 - (1-\varepsilon)^{m_i})}\right].
$$

□

Alternative proof. The proof follows by combining the arguments in alternative proofs of Lemmata 4.3 and 4.4. □

9

Proof of Theorem 2.1. We need to show that for any $\varepsilon \in (0, 1)$ and for any stochastic policy $\mathbf{P}$ feasible on a given Hamiltonian graph, Hamiltonian cycles are indeed the minimizers.

As the result of Lemma 4.1 enables us to reduce the proof for the set of stochastic policies to the proof for the set of deterministic policies, by Lemmata 4.2, 4.3, 4.4, and 4.5, all we need to show now is that, for $l > 1$ and $m, m_i < N$,

$$1 + \frac{\varepsilon N - (1 - (1 - \varepsilon)^N)}{\varepsilon (1 - (1 - \varepsilon)^N)} \leq 1 + \frac{l - 1}{\varepsilon} + \sum_{i=1}^{l} \left[\frac{m_i \varepsilon - (1 - (1 - \varepsilon)^{m_i})}{\varepsilon (1 - (1 - \varepsilon)^{m_i})} \right], \tag{4.4}$$

$$1 + \frac{\varepsilon N - (1 - (1 - \varepsilon)^N)}{\varepsilon (1 - (1 - \varepsilon)^N)} \leq (N - m + 1) + \frac{m \varepsilon - (1 - (1 - \varepsilon)^m)}{\varepsilon (1 - (1 - \varepsilon)^m)}, \tag{4.5}$$

$$1 + \frac{\varepsilon N - (1 - (1 - \varepsilon)^N)}{\varepsilon (1 - (1 - \varepsilon)^N)} \leq \left(N - \sum_{i=1}^{l} m_i + 1 \right) + \frac{l - 1}{\varepsilon} + \sum_{i=1}^{l} \left[\frac{m_i \varepsilon - (1 - (1 - \varepsilon)^{m_i})}{\varepsilon (1 - (1 - \varepsilon)^{m_i})} \right]. \tag{4.6}$$

From Lemmata 4.2–4.5 we know that in the above inequalities, the left-hand side is equal to $\text{Tr}[\mathbf{G}(\mathbf{P}_{\text{HC}}, \varepsilon)]$, and the right-hand side is equal to $\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, where $\mathbf{P}$ is some other deterministic policy. Thus, the proof follows from (3.7) by comparing the contribution of each state into $\text{Tr}\left[[\mathbf{I} - (1 - \varepsilon)\mathbf{P}]^{-1} \right]$.

Let us start with (4.4). In the right-hand side, we have $\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, where $\mathbf{P}$ consists of l ergodic classes as in Lemma 4.3. From the alternative proofs of Lemmata 4.2 and 4.3 we see that the contribution of each state into $\text{Tr}\left[[\mathbf{I} - (1 - \varepsilon)\mathbf{P}]^{-1} \right]$ in the left-hand side of (4.4) is $1/(1 - (1 - \varepsilon)^N)$. This is clearly smaller than $1/(1 - (1 - \varepsilon)^{m_i})$, the contribution of a state from ergodic class i on the right-hand side. Since this holds for every state in $\{1, \ldots, N\}$, the inequality (4.4) follows immediately from (3.7).

Now consider (4.5). In the right-hand side, we have $\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, where $\mathbf{P}$ consists of one ergodic class of m states and $N - m$ transient states, as in Lemma 4.4. From the alternative proof of Lemma 4.4 we know that each transient state contributes a unity into $\text{Tr}\left[[\mathbf{I} - (1 - \varepsilon)\mathbf{P}]^{-1} \right]$, while each ergodic state contributes $1/(1 - (1 - \varepsilon)^m)$. Thus, we have to compare

$$\frac{N}{1 - (1 - \varepsilon)^N} = N + \frac{N(1 - \varepsilon)^N}{1 - (1 - \varepsilon)^N} \text{ and } N - m + \frac{m}{1 - (1 - \varepsilon)^m} = N + \frac{m(1 - \varepsilon)^m}{1 - (1 - \varepsilon)^m}.$$

Consider the function

$$g(x) = \frac{x a^x}{1 - a^x}, \quad x \geq 0, \ 0 < a < 1.$$

Differentiation gives

$$g'(x) = \frac{a^x (1 - a^x + x \ln(x))}{(1 - a^x)^2}.$$

Clearly, the denominator is positive for all $x > 0$. Considering the numerator, denote $h(x) = 1 - a^x + x \ln(a)$ and observe that $h(0) = 0$ and $h'(x) = -a^x \ln(a) + \ln(a) = \ln(a)(1 - a^x) < 0$ for $x > 0$. Thus, we have $h(x) < 0$ for $x > 0$, which implies that $g'(x) < 0$ and thus $g(x)$ is decreasing with x. Setting $a = 1 - \varepsilon$ we obtain the desired result.

Finally, in the right-hand side of (4.6), we have $\text{Tr}[\mathbf{G}(\mathbf{P}, \varepsilon)]$, where $\mathbf{P}$ consists of l ergodic classes and transient states. The proof is a straightforward combination of the proofs of (4.4) and (4.5). $\square$

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