Completion problems and sparsity for Kemeny's constant

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Abstract. For a partially specified stochastic matrix, we consider the problem of completing it so as to minimize Kemeny's constant. We prove that for any partially specified stochastic matrix for which the problem is well defined, there is a minimizing completion that is as sparse as possible. We also find the minimum value of Kemeny's constant in two special cases: when the diagonal has been specified and when all specified entries lie in a common row.

1 Introduction and motivation

We live in a world of incomplete information. Consequently, we face the challenge: based only on partial information, can we achieve some desirable objective, and if so how?

That question is at the core of many matrix completion problems. Recall that a *partial matrix* is one in which only some of the entries are specified, while a matrix that arises by assigning values to each of the unspecified entries is known as a *completion* of the partial matrix. There is a wealth of literature on matrix completion problems, often focusing on completions that possess some desirable property (e.g., positive definiteness or total nonnegativity) or that optimize some scalar function (e.g., rank or determinant). See, for example, [2, 5] for overviews of the literature on matrix completion problems.

In this paper, we adopt the perspective of completion problems on the topic of stochastic matrices. Recall that a square matrix is *stochastic* if it is entrywise nonnegative, and each row sum is equal to 1. Any stochastic matrix has 1 as an eigenvalue, with **1**, the all-ones vector of the appropriate order, as a corresponding eigenvector. Stochastic matrices are central to the study of Markov chains, a rich and widely applied class of stochastic processes. Each partial matrix P that we will consider satisfies the following properties:

(i) P is square; (ii) all specified entries of P are nonnegative; (iii) in each row of P, the sum of the specified entries is bounded above by 1, and is equal to 1 for any fully specified row; (iv) any row of P for which the sum of the specified entries is equal to 1 is in fact fully specified; and (v) any row of P that is not fully specified contains at least two unspecified entries.

We say that a partial matrix P satisfying (i)–(v) is a *partial stochastic matrix*. Evidently, any partial stochastic matrix has a completion to a stochastic matrix. We note that conditions (iv) and (v) above are imposed largely to avoid uninteresting cases. If there is a row of P for which the sum of the specified entries is equal to 1, then any stochastic completion necessarily assigns the value 0 to the unspecified entries in that row (so those positions of P are specified de facto). Similarly, if the jth row of P has just one unspecified entry, say in the kth position, then any stochastic completion assigns the value $1 - \sum_{\ell \neq k} p_{j,\ell}$ to the (j, k) position (so that the entire jth row of P is specified de facto).

Next, we briefly discuss Kemeny's constant (which first appeared in [6]), the scalar function that will be minimized in this paper. Given an irreducible $n \times n$ stochastic matrix T and indices $j, k = 1, \ldots, n$, the entry $t_{j,k}$ is the probability that the Markov chain transitions from state j to state k in one time step. Recall that there is a unique positive left eigenvector $w^\top$ whose entries sum to 1 such that $w^\top T = w^\top$; that vector is known as the *stationary vector* for the corresponding Markov chain. For each pair of indices $j, k = 1, \ldots, n$, the *mean first passage time from j to k*, $m_{j,k}$ is the expected number of steps for the Markov chain to enter state k for the first time, given that it began in state j (we note in passing that $m_{j,j} = \frac{1}{w_j}$ for each such j). *Kemeny's constant*, denoted $\mathcal{K}(T)$, is then given by $\sum_{k \neq j} m_{j,k} w_k$. It turns out that $\mathcal{K}(T)$ does not depend on the choice of j, and $\mathcal{K}(T)$ can be interpreted in terms of the expected number of steps required for the Markov chain to reach a randomly chosen state, starting from state j. Since $\sum_{j=1}^n w_j = 1$, we find that $\mathcal{K}(T) = \sum_{k,j,k \neq j} w_j m_{j,k} w_k$. Hence, $\mathcal{K}(T)$ also reflects the expected number of steps required to transition from a randomly chosen initial state to a randomly chosen destination state, and so measures the overall ease of movement from state to state. For this reason, Kemeny's constant has been proposed as an indicator of the average travel time in a Markov chain model for vehicle traffic networks [1].

There are several different formulas for Kemeny's constant, and each has proven itself to be useful depending on the context. Setting $Q = I - T$, we find that Q is singular, and when T is irreducible, Q has 0 as an eigenvalue of algebraic multiplicity one. Hence, while Q is not invertible, it has a group inverse, $Q^{\#}$, and it transpires that $\mathcal{K}(T) = \text{trace}(Q^{\#})$ (see [10] for background on the group inverse and its use in the analysis of Markov chains). From this, we find readily that if T has eigenvalues $1 = \lambda_1, \lambda_2, \ldots, \lambda_n$ (including multiplicities), then $\mathcal{K}(T) = \sum_{j=2}^n \frac{1}{1-\lambda_j}$ [11] and that if $Q = XY$ is a full rank factorization of Q, then since $Q^{\#} = (X(YX)^{-2}Y$, we have $\mathcal{K}(T) = \text{trace}(X(YX)^{-2}Y) = \text{trace}((YX)^{-1})$. We note that while Kemeny's constant was originally defined for the case that T is irreducible (so that all of the mean first passage times are well defined), the definition can be extended to cover the case that T has 1 as an algebraically simple eigenvalue. In that setting, we may use any of $\text{trace}(Q^{\#})$, $\text{trace}((YX)^{-1})$, and $\sum_{j=2}^n \frac{1}{1-\lambda_j}$ as the definition for $\mathcal{K}(T)$.

For any stochastic matrix T, the multiplicity of 1 as an eigenvalue can be understood from a combinatorial viewpoint. Recall that a state j of an n-state Markov chain is *essential* if it has the property that, for any vertex k in the directed graph of T, if there is a walk from j to k, then necessarily there is a walk back from k to j. The essential states can thus be partitioned into *essential classes*, that is, subsets of states

such that (a) within each class, any state can be reached from any other state in the class and (b) no state from outside the class can be reached from any state inside the class. (See, for example, [12] for further details.) It is well known that the algebraic multiplicity of 1 as an eigenvalue of the corresponding transition matrix coincides with the number of essential classes. Hence, 1 is an algebraically simple eigenvalue of a stochastic matrix T if and only if there is a single essential class of states in the Markov chain associated with T. When that is the case, then either T is irreducible, or it is permutationally similar to a stochastic matrix of the form $\begin{bmatrix} T_1 & 0 \\ X & T_2 \end{bmatrix}$, where T_1 is irreducible and stochastic, and the spectral radius of T_2 is less than 1; observe that since the spectral radius of T_2 is less than 1, necessarily $X \neq 0$.

In view of the interpretation of Kemeny's constant as a measure of the ease of movement between states, there is interest in identifying stochastic matrices for which the corresponding value of Kemeny's constant is small. In [4], it is shown that for any irreducible stochastic matrix of order n, Kemeny's constant is bounded below by $\frac{n-1}{2}$; [7] proves that the adjacency matrix of a directed n-cycle is the unique irreducible stochastic matrix of order n with $\frac{n-1}{2}$ as the value for Kemeny's constant. In a related vein, [7] identifies the stochastic matrix T whose directed graph is subordinate to a given directed graph and has the smallest value for $\mathcal{K}(T)$, while [8] identifies the stochastic matrices with prescribed stationary distribution that minimize Kemeny's constant.

In each of [4], [7], and [8], the minimizing matrices are *sparse*, that is, the ratio of zero entries to nonzero entries is high. At least part of our agenda in the present work is to develop a better understanding of how the sparsity of a stochastic matrix affects the value of Kemeny's constant. The following observation goes in that direction.

Observation 1.1 *Suppose that we have an irreducible stochastic matrix T of order n, with corresponding mean first passage matrix M and stationary vector $w^\top$. In [9], the following quantity, known as an accessibility index, is defined for each $k = 1, \ldots, n$: $\alpha_k = w^\top M e_k - 1$. Observe that $\mathcal{K}(T) = \sum_{k=1}^n w_k \alpha_k$.*

For each $k = 1, \ldots, n$, let R_k denote the random variable that is the time of the first return to state k. Denote the expectation operator by $E(\cdot)$. It is well known that $w_k = \frac{1}{E(R_k)}$, and in [9] it is shown that $\alpha_k = \frac{1}{2}\left(\frac{E(R_k^2)}{E(R_k)} - 1\right)$, $k = 1, \ldots, n$. Hence, $w_k \alpha_k = \frac{1}{2}\left(\frac{E(R_k^2)}{(E(R_k))^2} - w_k\right) = \frac{1}{2}\left(\frac{E(R_k^2) - (E(R_k))^2}{(E(R_k))^2}\right) + \frac{1-w_k}{2} = \frac{w_k^2}{2} Var(R_k) + \frac{1-w_k}{2}$, and we deduce that

$$(1.1) \qquad \mathcal{K}(T) = \frac{1}{2} \sum_{k=1}^n w_k^2 Var(R_k) + \frac{n-1}{2}.$$

The presence of $Var(R_k)$ in (1.1) provides some intuition as to how sparsity plays a role, as zeros in the transition matrix T may serve to decrease the variances of the first return times. Indeed, in the extreme case that $\mathcal{K}(T) = \frac{n-1}{2}$, T has just one nonzero entry in each row and $Var(R_k) = 0$, $k = 1, \ldots, n$.

In this paper, we consider the following class of questions. Given a partial stochastic matrix P, over all stochastic completions of P, what is the minimum value of Kemeny's

constant, and which completions yield that minimum? In Section 2, we show that, provided that P admits a completion for which Kemeny's constant is well defined, there is a completion that minimizes Kemeny's constant and has the property that in each row, at most one of the unspecified entries is assigned a positive value. In particular, such a minimizing completion is as sparse as possible. In the remaining sections, we solve two specific completion problems; Theorem 3.11 of Section 3 addresses the completion problem for the case that the partial stochastic matrix has its specified entries on the diagonal, while Corollary 4.10 in Section 4 covers the case that the partial stochastic matrix has its specified entries in a common row. The solutions to both completion problems correspond to sparse transition matrices, as anticipated by the results of Section 2. Both completion problems help to explain how local information (probability of transition back to the same state, and probabilities of transitions out of a single state, respectively) influences the global behavior of the Markov chain as measured by Kemeny's constant.

We note that the techniques introduced in [7] inform much of our approach. Indeed, some of the results in Section 2 are modest adaptations of the results in that paper. This is not so surprising, as the main problem in [7] is to minimize Kemeny's constant over all stochastic matrices whose directed graph is a subgraph of a given directed graph D. This in turn can be rephrased as a completion problem: the relevant partial matrix has a prescribed entry 0 in position (j, k) for each pair of indices j, k such that the arc $j \to k$ is not present in D. Evidently, the completions of that partial matrix correspond to stochastic matrices with directed graphs subordinate to D.

Throughout, we rely on a mix of combinatorial and matrix analytic techniques. We also employ basic results and terminology from nonnegative matrix theory and the study of Markov chains. The reader is referred to [6, 12] for the necessary background.

2 Preliminaries

Our interest in this paper is Kemeny's constant, which is only well defined for a stochastic matrix having a single essential class of indices. For this reason, we first identify the partial stochastic matrices for which at least one completion has a single essential class of indices. Here we use the notation that for a matrix A and nonempty subsets X, Y of its row and column indices, respectively, $A[X, Y]$ denotes the submatrix of A on rows indexed by X and columns indexed by Y.

Proposition 2.1   *Suppose that P is a partial stochastic matrix of order n. There is a completion of P having a single essential class of indices if and only if for each nonempty $X \subset \{1, \ldots, n\}$, one of $P[X, X^c]$ and $P[X^c, X]$ contains either a positive entry or an unspecified entry.*

Proof   We first note that a stochastic matrix T has a single essential class if and only if it cannot be written as a direct sum of stochastic matrices of smaller order. This in turn is equivalent to the property that for each nonempty proper subset X of the index set, either $T[X, X^c]$ or $T[X^c, X]$ has a positive entry.

Let P be a partial stochastic matrix and suppose that T is a completion with a single essential class of indices. Fix a nonempty subset $X \subset \{1, \ldots, n\}$. Then one of $T[X, X^c]$

and $T[X^c, X]$ has a positive entry, from which we conclude that one of $P[X, X^c]$ and $P[X^c, X]$ contains either a positive entry or an unspecified entry.

Conversely, suppose that for each nonempty $X \subset \{1, \ldots, n\}$, one of $P[X, X^c]$ and $P[X^c, X]$ contains either a positive entry or an unspecified entry. Let T be a completion of P having the largest number of positive entries; from properties (i)–(v), we find that T assigns a positive number to each unspecified entry in P. It now follows readily that T has a single essential class of indices. ∎

For a partial stochastic matrix P, let $SC(P) = \{T | T$ is a stochastic completion of $P\}$, and in the case that there is a stochastic completion of P with a single essential class, we define $m(P) = \inf\{\mathcal{K}(T) | T \in SC(P)$ and has a single essential class$\}$. In this section, we establish some technical lemmas, and prove a general result (Proposition 2.3 below) regarding completions that realize $m(P)$.

The proof of the next result is basically the same as that of Lemma 2.4 in [7]. Its proof uses the fact (established by adapting the proof of Lemma 2.3 in [7]) that for an $n \times n$ stochastic matrix T with 1 as an algebraically simple eigenvalue, if $\lambda \neq 1$ is an eigenvalue of T, then $|1 - \lambda| \geq \frac{1 - \cos(\frac{2\pi}{n})}{\mathcal{K}(T)}$.

Lemma 2.2 *Let P be a partial stochastic matrix for which there is a stochastic completion having a single essential class of indices. There is a $T \in SC(P)$ having a single essential class such that $\mathcal{K}(T) = m(P)$.*

The following result is a slight extension of Lemma 2.5 in [7]. We include a short proof in order to illustrate a key technique.

Proposition 2.3 *Let P be a partial stochastic matrix for which there is a stochastic completion having a single essential class of indices. There is a $T \in SC(P)$ such that*

(i) *T has a single essential class,*

(ii) *$\mathcal{K}(T) = m(P)$, and*

(iii) *for each $j = 1, \ldots, n$, there is at most one k such that $p_{j,k}$ is unspecified and $t_{j,k} > 0$.*

Proof From Lemma 2.2, there is a $T \in SC(P)$ satisfying (i) and (ii). If T also satisfies (iii), we are done, so suppose that for some indices j, k_1, k_2, the $(j, k_1), (j, k_2)$ entries of P are unspecified and $t_{j,k_1}, t_{j,k_2} > 0$. Our goal is to construct a matrix $\hat{T}$ satisfying (i) and (ii) such that $\hat{T}$ has fewer positive entries than T does. The conclusion will then follow by an induction step on the number of positive entries.

For each $x \in [-t_{j,k_1}, t_{j,k_2}]$, let $E_x = x e_j (e_{k_1} - e_{k_2})^\top$, and observe that $T + E_x \in SC(P)$ for all such x. Arguing as in the proof of Lemma 2.5 of [7], we find that for each x such that $x(e_{k_1} - e_{k_2})^\top (I - T)^\# e_j \neq 1, \mathcal{K}(T + E_x) = \mathcal{K}(T) + \frac{x}{1 - x(e_{k_1} - e_{k_2})^\top (I-T)^\# e_j}(e_{k_1} - e_{k_2})^\top ((I - T)^\#)^2 e_j$; in particular, this holds whenever $|x|$ is sufficiently small. Further, when $|x|$ is sufficiently small, it is also the case that $T + E_x$ has a single essential class. Since $\mathcal{K}(T)$ is a minimum, it must be the case that $(e_{k_1} - e_{k_2})^\top ((I - T)^\#)^2 e_j = 0$. Hence, $\mathcal{K}(T) = \mathcal{K}(T + E_x)$ for any $x \in [-t_{j,k_1}, t_{j,k_2}]$ such that $x(e_{k_1} - e_{k_2})^\top (I - T)^\# e_j \neq 1$. Further, since $\mathcal{K}(T + E_x)$ is a minimum, it must be the case that $T + E_x$ has a single essential class for any

such x. If $(e_{k_1} - e_{k_2})^\top (I - T)^\# e_j \leq 0$, we find that $T + E_{t_{j,k_2}}$ satisfies (i) and (ii) and has fewer positive entries than T does, while if $(e_{k_1} - e_{k_2})^\top (I - T)^\# e_j > 0$, $T + E_{-t_{j,k_1}}$ satisfies (i) and (ii) and has fewer positive entries than T does. ∎

3 *P* with all specified entries on the diagonal

In this section, we consider the problem of finding $m(P)$ for the case that the specified entries of the partial stochastic matrix P are all on the diagonal. The following technical result will be useful in the subsequent discussion. Recall that a square matrix is *substochastic* if it is entrywise nonnegative and each row sum is at most 1.

Lemma 3.1 *Let T be an $n \times n$ substochastic matrix whose spectral radius is strictly less than 1. We have* $\operatorname{trace}((I - T)^{-1}) \geq \sum_{k=1}^n \frac{1}{1 - t_{k,k}}$.

Proof We proceed by induction on n, and note that the case $n = 1$ is readily established. Suppose now that $n \geq 2$ and that the statement holds for matrices of order $n - 1$. Write $I - T$ in a partitioned form as $I - T = \left[\begin{array}{c|c} I - \hat{T} & -x \\ \hline -y^\top & 1 - t_{n,n} \end{array} \right]$, where $\hat{T}$ is of order $n - 1$ and $x, y \geq 0$. From the partitioned form of the inverse [3], we find that

$$\operatorname{trace}((I - T)^{-1}) = \operatorname{trace}\left(\left(I - \hat{T} - \frac{1}{1 - t_{n,n}} x y^\top \right)^{-1} \right) + \frac{1}{1 - t_{n,n} - y^\top (I - \hat{T})^{-1} x}.$$

Hence,

$$\operatorname{trace}((I - T)^{-1})) =$$
$$\operatorname{trace}\left((I - \hat{T})^{-1} + \frac{1}{1 - t_{n,n} - y^\top (I - \hat{T})^{-1} x} (I - \hat{T})^{-1} x y^\top (I - \hat{T})^{-1} \right)$$
$$+ \frac{1}{1 - t_{n,n} - y^\top (I - \hat{T})^{-1} x}.$$

We deduce that $\operatorname{trace}((I - T)^{-1})) \geq \operatorname{trace}((I - \hat{T})^{-1})) + \frac{1}{1 - t_{n,n}}$, and applying the induction hypothesis now yields the desired inequality. ∎

Lemma 3.2 *Suppose that T is a stochastic matrix of order n with a single essential class. Suppose that $T = \left[\begin{array}{c|c} S & 1 - S\mathbf{1} \\ \hline u^\top & 1 - \mathbf{1}^\top u \end{array} \right]$, where the spectral radius of S is less than 1. Then*

$$\mathcal{K}(T) = \operatorname{trace}((I - S)^{-1}) - \frac{1}{1 + u^\top (I - S)^{-1} \mathbf{1}} \operatorname{trace}((I - S)^{-1} \mathbf{1} u^\top (I - S)^{-1}).$$

Proof Write $X = \left[\begin{array}{c} I - S \\ \hline -u^\top \end{array} \right]$, $Y = \left[\begin{array}{c|c} I & -\mathbf{1} \end{array} \right]$, so that $I - T = XY$ is a full rank factorization of $I - T$. As noted in Section 1, $\mathcal{K}(T) = \operatorname{trace}((YX)^{-1})$. Since $YX = I - S + \mathbf{1}u^\top$, the conclusion follows from the Sherman–Morrison formula [3]. ∎

Example 3.3 Suppose that for our partial stochastic matrix P of order n, the specified entries are on the diagonal, with $p_{j,j} = d_j, j = 1, \ldots, n$. As a warm-up exercise, we first consider the case that some diagonal entry of P is 1. Without loss of generality, we assume that $d_1 = 1$ and $d_j < 1, j = 2, \ldots, n$. For any stochastic completion T of P having just one essential class, T is of the form

$$T = \left[\begin{array}{c|c} 1 & 0^\top \\ \hline \mathbf{1} - \hat{T}\mathbf{1} & \hat{T} \end{array} \right],$$

where the spectral radius of $\hat{T}$ is less than 1, and $t_{j,j} = d_j, j = 2, \ldots, n$. Then $\mathcal{K}(T) = \text{trace}((I - \hat{T})^{-1}) \geq \sum_{j=2}^n \frac{1}{1-d_j}$, the inequality following from Lemma 3.1. Evidently, equality in the lower bound can be attained by letting $\hat{T}$ be the diagonal matrix with diagonal entries $d_2, \ldots, d_n$. Hence, $m(P) = \sum_{j=2}^n \frac{1}{1-d_j}$.

In the remainder of this section, we assume that $d_j < 1, j = 1, \ldots, n$.

Theorem 3.4 Suppose that $d_j \in [0, 1), j = 1, \ldots, n$. Let C be the adjacency matrix for a directed n-cycle, and define $D = \text{diag}(d_1, \ldots, d_n)$, $T = D + (I - D)C$. Then

$$\mathcal{K}(T) = \frac{1}{2\sum_{j=1}^n \frac{1}{1-d_j}} \left(\left(\sum_{j=1}^n \frac{1}{1 - d_j} \right)^2 - \sum_{j=1}^n \frac{1}{(1 - d_j)^2} \right).$$

Proof Without loss of generality, we assume that C corresponds to the cycle $1 \to 2 \to \cdots \to n \to 1$. We apply Lemma 3.2 and note that in the notation of that lemma, the submatrix of T consisting of its first $n - 1$ columns can be written as $\left[\begin{array}{c} \hat{D} + (I - \hat{D})N \\ \hline (1 - d_n)e_1^\top \end{array} \right]$, where N is the matrix of order $n - 1$ whose first superdiagonal consists of ones, and where all other entries are zero, and where $\hat{D}$ is the leading $(n - 1) \times (n - 1)$ principal submatrix of D. It now follows that $\mathcal{K}(T)$ is the trace of the matrix

$$(I - N)^{-1}(I - \hat{D})^{-1} - \left(\frac{1 - d_n}{1 + (1 - d_n)e_1^\top(I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}} \right) \times$$
$$(I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}e_1^\top(I - N)^{-1}(I - \hat{D})^{-1}.$$

Observe that $(I - N)^{-1}$ is the upper triangular matrix of order $n - 1$ whose entries on and above the diagonal are ones. From that observation, we find the following: (a) $\text{trace}((I - N)^{-1}(I - \hat{D})^{-1}) = \sum_{j=1}^{n-1} \frac{1}{1-d_j}$; (b) $\frac{1-d_n}{1+(1-d_n)e_1^\top(I-N)^{-1}(I-\hat{D})^{-1}\mathbf{1}} = \frac{1}{\sum_{j=1}^n \frac{1}{1-d_j}}$. Recalling that for vectors $u, v \in \mathbb{R}^{n-1}, \text{trace}(uv^\top) = v^\top u$, we find that $\text{trace}((I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}e_1^\top(I - N)^{-1}(I - \hat{D})^{-1}) = \sum_{j=1}^{n-1} \frac{1}{1-d_j} \sum_{\ell=j}^{n-1} \frac{1}{1-d_\ell}$.

Next, we note that $\sum_{j=1}^{n-1} \frac{1}{1-d_j} \sum_{\ell=j}^{n-1} \frac{1}{1-d_\ell}$ can be written as $\frac{1}{2}((\sum_{j=1}^{n-1} \frac{1}{1-d_j})^2 + \sum_{j=1}^{n-1} \frac{1}{(1-d_j)^2})$. Assembling these observations, we find that

$$\mathcal{K}(T) = \sum_{j=1}^{n-1} \frac{1}{1-d_j} - \frac{(\sum_{j=1}^{n-1} \frac{1}{1-d_j})^2 + \sum_{j=1}^{n-1} \frac{1}{(1-d_j)^2}}{2(\sum_{j=1}^{n} \frac{1}{1-d_j})}.$$

Simplifying that expression now yields

$$\mathcal{K}(T) = \frac{1}{2(\sum_{j=1}^{n} \frac{1}{1-d_j})} \left(\left(\sum_{j=1}^{n-1} \frac{1}{1-d_j} \right)^2 + \frac{2}{1-d_n} \sum_{j=1}^{n-1} \frac{1}{1-d_j} - \sum_{j=1}^{n-1} \frac{1}{(1-d_j)^2} \right)$$

$$= \frac{1}{2 \sum_{j=1}^{n} \frac{1}{1-d_j}} \left(\left(\sum_{j=1}^{n} \frac{1}{1-d_j} \right)^2 - \sum_{j=1}^{n} \frac{1}{(1-d_j)^2} \right). \qquad \blacksquare$$

Lemma 3.5 *Suppose that $n \geq 2$ and $x_j > 0$, $j = 1, \ldots, n$, and let*

$$s_k = \frac{(\sum_{j=1}^{k} x_j)^2 - \sum_{j=1}^{k} x_j^2}{2 \sum_{j=1}^{k} x_j} + \sum_{j=k+1}^{n} x_j.$$

We have $s_1 > s_2 > \cdots > s_n$.

Proof Suppose that $1 \leq k \leq n-1$. Observe that

$$s_k - s_{k+1} = -\frac{1}{2}x_{k+1} + x_{k+1} + \frac{\sum_{j=1}^{k+1} x_j^2}{2 \sum_{j=1}^{k+1} x_j} - \frac{\sum_{j=1}^{k} x_j^2}{2 \sum_{j=1}^{k} x_j}$$

$$= \frac{1}{2} \left(x_{k+1} + \frac{\sum_{j=1}^{k} x_j \sum_{j=1}^{k+1} x_j^2 - \sum_{j=1}^{k+1} x_j \sum_{j=1}^{k} x_j^2}{\sum_{j=1}^{k} x_j \sum_{j=1}^{k+1} x_j} \right)$$

$$= \frac{1}{2 \sum_{j=1}^{k} x_j \sum_{j=1}^{k+1} x_j} \left(x_{k+1}^2 \sum_{j=1}^{k} x_j + x_{k+1} \sum_{j=1}^{k} x_j \sum_{j=1}^{k+1} x_j - x_{k+1} \sum_{j=1}^{k} x_j^2 \right).$$

Since $\sum_{j=1}^{k} x_j \sum_{j=1}^{k+1} x_j > \sum_{j=1}^{k} x_j^2$, we deduce that $s_k > s_{k+1}$. $\qquad \blacksquare$

Theorem 3.6 *Suppose that $d_j \in [0, 1)$, $j = 1, \ldots, n$, and that P is an $n \times n$ partial stochastic matrix with $p_{j,j} = d_j$, $j = 1, \ldots, n$ and all other entries unspecified. Then*

$$m(P) = \frac{1}{2 \sum_{j=1}^{n} \frac{1}{1-d_j}} \left(\left(\sum_{j=1}^{n} \frac{1}{1-d_j} \right)^2 - \sum_{j=1}^{n} \frac{1}{(1-d_j)^2} \right).$$

Proof Suppose that T is a completion of P such that $\mathcal{K}(T) = m(P)$. By Proposition 2.3, we may assume, without loss of generality, that T has precisely one nonzero off-diagonal entry in each row, and a single essential class of indices. In the directed graph of T, for each vertex j, there is precisely one vertex $\ell \neq j$ such that $j \to \ell$. Hence, this directed graph has at least one cycle of length greater than 1, and if it were to have more

than one such cycle, then there would be more than one essential class. We deduce that the directed graph of T has precisely one cycle, of length k say, and without loss of generality, it is on vertices $1, \ldots, k$.

If $k < n$, then $\mathcal{K}(T) = \dfrac{(\sum_{j=1}^{k} \frac{1}{1-d_j})^2 - \sum_{j=1}^{k} \frac{1}{(1-d_j)^2}}{2\sum_{j=1}^{k} \frac{1}{1-d_j}} + \sum_{j=k+1}^{n} \frac{1}{1-d_j}$. Appealing to Lemma 3.5 (with $x_j = \frac{1}{1-d_j}$), we see that T cannot minimize Kemeny's constant over $SC(P)$. Hence, $k = n$, and the conclusion now follows from Theorem 3.4. ∎

Remark 3.7   Fix an index $j_0 = 1, \ldots, n$, and consider the expression

$$f \equiv \frac{1}{\sum_{j=1}^{n} \frac{1}{1-d_j}} \left(\left(\sum_{j=1}^{n} \frac{1}{1-d_j} \right)^2 - \sum_{j=1}^{n} \frac{1}{(1-d_j)^2} \right)$$

as a function of d_{j_0}. A straightforward computation shows that $\frac{\partial f}{\partial d_{j_0}}$ has the same sign as $\left(\sum_{j \neq j_0} \frac{1}{1-d_j} \right)^2 + \sum_{j \neq j_0} \frac{1}{(1-d_j)^2}$. In particular, f is increasing in each d_j.

Corollary 3.8   *Suppose that $d_j \in [0,1), j = 1, \ldots, k$. Suppose that P is a partial stochastic matrix of order $n > k$ with $p_{j,j} = d_j, j = 1, \ldots, k$, and all other entries unspecified. Then $m(P) =$*

$$\frac{1}{2(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k)} \left(\left(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k \right)^2 - \sum_{j=1}^{k} \frac{1}{(1-d_j)^2} - (n-k) \right).$$

Proof   Set $d_{k+1}, \ldots, d_n$ all equal to 0. From Theorem 3.6 and Remark 3.7, we find that for any stochastic matrix T such that $t_{j,j} = d_j, j = 1, \ldots, k$, $\mathcal{K}(T) \geq \frac{1}{2(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k)} \left(\left(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k \right)^2 - \sum_{j=1}^{k} \frac{1}{(1-d_j)^2} - (n-k) \right)$. Let C denote a cyclic permutation matrix of order n. Setting $D = \mathrm{diag}(d_1, \ldots, d_n)$ and $T_0 = D + (I - D)C$, we find from Theorem 3.4 that $\mathcal{K}(T_0) =$

$$\frac{1}{2(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k)} \left(\left(\sum_{j=1}^{k} \frac{1}{1-d_j} + n - k \right)^2 - \sum_{j=1}^{k} \frac{1}{(1-d_j)^2} - (n-k) \right). \quad ∎$$

Our next goal is to characterize the matrices yielding the minimum value $m(P)$ in Theorem 3.6. We first establish some technical results that will assist in that characterization. The following formula appears in the proof of Lemma 2.5 in [7].

Lemma 3.9   *Suppose that T is a stochastic matrix with one essential class, and for each $x \in [-t_{i,p}, t_{i,q}]$, set $S_x = T + x e_i (e_p - e_q)^\top$. Then, for any $x \in [-t_{i,p}, t_{i,q}]$ such that $1 - x(e_p - e_q)^\top (I - T)^\# e_i \neq 0$, $\mathcal{K}(S_x) = \mathcal{K}(T) + \frac{x}{1 - x(e_p - e_q)^\top (I-T)^\# e_i} (e_p - e_q)^\top ((I - T)^\#)^2 e_i$.*

Lemma 3.10   *Suppose that $d_j \in [0,1), j = 1, \ldots, n$, let $D = \mathrm{diag}(d_1, \ldots, d_n)$ and let C be the permutation matrix corresponding to the cyclic permutation $1 \to 2 \to \cdots \to n -$*

$1 \to n \to 1$. *Let* $T = D + (I - D)C$. *Fix an index* $k = 2, \ldots, n-1$, *and for each* $x \in [0, 1 - d_n]$, *let* $T_x = T + x e_n (e_k - e_1)^\top$. *Then* $\mathcal{K}(T_x) > \mathcal{K}(T)$ *for all* $x \in (0, 1 - d_n]$.

Proof   Here we employ the notation of Theorem 3.4. Let $X = \begin{bmatrix} (I - \hat{D})(I - N) \\ -(1 - d_n)e_1^\top \end{bmatrix}$,

$Y = \begin{bmatrix} I & | & -\mathbf{1} \end{bmatrix}$. Then $I - T = XY$ so that $(I - T)^\# = X(YX)^{-2}Y$.

We have $Ye_n = -\mathbf{1}$, and it now follows that

$$(3.1) \qquad (YX)^{-1}Ye_n = \frac{-1}{1 + (1 - d_n)e_1^\top (I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}}(I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}.$$

Also, $(e_k - e_1)^\top X = ((1 - d_k)e_k - (1 - d_1)e_1)^\top (I - N)$, and it follows that

$$(3.2) \qquad\qquad\qquad (e_k - e_1)^\top X(YX)^{-1} = (e_k - e_1)^\top.$$

We find from (3.1) and (3.2) that

$$1 - x(e_k - e_1)^\top (I - T)^\# e_n = 1 - x(e_k - e_1)^\top X(YX)^{-1}(YX)^{-1}Ye_n =$$
$$1 + \frac{x}{1 + (1 - d_n)e_1^\top (I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}}(e_k - e_1)^\top (I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}.$$

Hence, $1 - x(e_k - e_1)^\top (I - T)^\# e_n = 1 + \frac{x}{1 - d_n}\frac{\sum_{j=1}^{k-1}\frac{1}{1-d_j}}{\sum_{j=1}^n \frac{1}{1-d_j}} > 0$. In particular, we find from

Lemma 3.9 that $\mathcal{K}(T_x) = \mathcal{K}(T) + \frac{x(1-d_n)\sum_{j=1}^n \frac{1}{1-d_j}}{(1-d_n)\sum_{j=1}^n \frac{1}{1-d_j} + x\sum_{j=1}^{k-1}\frac{1}{1-d_j}}(e_k - e_1)^\top ((I - T)^\#)^2 e_n$.

It remains to compute $(e_k - e_1)^\top ((I - T)^\#)^2 e_n$.

We have $((I - T)^\#)^2 = X(YX)^{-3}Y$. From (3.1) and (3.2), we deduce that $(e_k - e_1)^\top X(YX)^{-3}Ye_n$ has the same sign as $(e_1 - e_k)^\top (YX)^{-1}(I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}$.

Observe that for each $j = 1, \ldots, n-1$, the jth entry of $(I - N)^{-1}(I - \hat{D})^{-1}\mathbf{1}$ is $\sum_{\ell=j}^{n-1}\frac{1}{1-d_\ell}$. We also have $(e_1 - e_k)^\top (YX)^{-1} = \sum_{j=1}^{k-1}\frac{1}{1-d_j}e_j^\top - \frac{\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}}{\sum_{\ell=1}^n \frac{1}{1-d_\ell}}\sum_{j=1}^{n-1}\frac{1}{1-d_j}e_j^\top$. We thus find that $(e_k - e_1)^\top ((I - T)^\#)^2 e_n$ has the same sign as

$$(3.3) \qquad \sum_{\ell=1}^n \frac{1}{1-d_\ell}\left(\sum_{j=1}^{k-1}\frac{1}{1-d_j}\sum_{\ell=j}^{n-1}\frac{1}{1-d_\ell}\right) - \sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\sum_{j=1}^{n-1}\frac{1}{1-d_j}\sum_{\ell=j}^{n-1}\frac{1}{1-d_\ell}\right).$$

We claim that (3.3) is strictly positive.

In order to establish the claim, we rewrite (3.3) as follows:

$$\sum_{\ell=1}^n \frac{1}{1-d_\ell}\left(\sum_{j=1}^{k-1}\frac{1}{1-d_j}\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell} + \sum_{j=1}^{k-1}\frac{1}{1-d_j}\sum_{\ell=j}^{k-1}\frac{1}{1-d_\ell}\right)$$
$$- \sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\frac{1}{2}\left(\sum_{\ell=1}^{n-1}\frac{1}{1-d_\ell}\right)^2 + \frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{(1-d_\ell)^2}\right)$$
$$= \sum_{\ell=1}^n \frac{1}{1-d_\ell}\sum_{j=1}^{k-1}\frac{1}{1-d_j}\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell} + \sum_{\ell=1}^n \frac{1}{1-d_\ell}\left(\frac{1}{2}\left(\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\right)^2 + \frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{(1-d_\ell)^2}\right)$$

$$-\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\frac{1}{2}\left(\sum_{\ell=1}^{n-1}\frac{1}{1-d_\ell}\right)^2+\frac{1}{2}\sum_{\ell=1}^{n-1}\frac{1}{(1-d_\ell)^2}\right)$$

$$=\sum_{\ell=1}^{n}\frac{1}{1-d_\ell}\sum_{j=1}^{k-1}\frac{1}{1-d_j}\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell}+\frac{1}{2}\sum_{\ell=1}^{n}\frac{1}{1-d_\ell}\left(\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\right)^2$$

$$+\frac{1}{2}\sum_{\ell=1}^{n}\frac{1}{1-d_\ell}\sum_{\ell=1}^{k-1}\frac{1}{(1-d_\ell)^2}-\frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\right)^2-\frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell}\right)^2$$

$$-\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell}-\frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\sum_{\ell=1}^{n-1}\frac{1}{(1-d_\ell)^2}$$

$$=\frac{1}{2}\sum_{j=k}^{n}\frac{1}{1-d_j}\left(\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\right)^2+\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell}\sum_{\ell=k}^{n}\frac{1}{1-d_\ell}$$

$$-\frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\left(\sum_{\ell=k}^{n-1}\frac{1}{1-d_\ell}\right)^2+\frac{1}{2}\sum_{\ell=k}^{n}\frac{1}{1-d_\ell}\sum_{\ell=1}^{k-1}\frac{1}{(1-d_\ell)^2}$$

$$-\frac{1}{2}\sum_{\ell=1}^{k-1}\frac{1}{1-d_\ell}\sum_{\ell=k}^{n-1}\frac{1}{(1-d_\ell)^2}.$$

Inspecting this final expression, we see that (3.3) is strictly positive. The conclusion now follows readily. ∎

Theorem 3.11 *Suppose that $d_j \in [0,1)$, $j = 1,\dots,n$ and that P is an $n \times n$ partial stochastic matrix with $p_{j,j} = d_j$, $j = 1,\dots,n$ and all other entries unspecified. Let $D = \mathrm{diag}(d_1,\dots,d_n)$. Then $T \in SC(P)$ with $\mathcal{K}(T) = m(P)$ if and only if $T = D + (I - D)C$, where C is a cyclic permutation matrix for a cycle of length n.*

Proof Suppose that $T \in SC(P)$ and that T cannot be written as $D + (I - D)C$, for any n-cyclic permutation matrix C. Let the number of positive off-diagonal entries in T be ℓ. We claim that $\mathcal{K}(T) > m(P)$, and proceed by induction on ℓ.

If $\ell = n$, then from the proof of Theorem 3.6, we find that for some $k < n$, $\mathcal{K}(T) = \frac{(\sum_{j=1}^{k}\frac{1}{1-d_j})^2-\sum_{j=1}^{k}\frac{1}{(1-d_j)^2}}{2\sum_{j=1}^{k}\frac{1}{1-d_j}} + \sum_{j=k+1}^{n}\frac{1}{1-d_j}$. The conclusion then follows from Lemma 3.5.

Suppose now that $\ell > n$ (here we mimic the approach of Proposition 2.3). Then there are indices j, k_1, k_2 such that $t_{j,k_1}, t_{j,k_2} > 0$. If $(e_{k_1} - e_{k_2})^\top((I-T)^\#)^2 e_j \neq 0$, then we may perturb T slightly in the jth row to produce a matrix $\hat{T} \in SC(P)$ such that $\mathcal{K}(\hat{T}) < \mathcal{K}(T)$. On the other hand, if $(e_{k_1} - e_{k_2})^\top((I-T)^\#)^2 e_j = 0$, then there is a matrix $\tilde{T} \in SC(P)$ such that $\mathcal{K}(\tilde{T}) = \mathcal{K}(T)$ and $\tilde{T}$ has $\ell - 1$ positive off-diagonal entries. If $\tilde{T}$ is not of the form $D + (I - D)C$ for any n-cyclic permutation matrix C, then $\mathcal{K}(\tilde{T}) > m(P)$ by the induction hypothesis. Suppose now that $\tilde{T} = D + (I - D)C$ for some n-cyclic permutation matrix C, and without loss of generality, C corresponds to the permutation $1 \to 2 \to \cdots \to n \to 1$. In that case, T is permutationally similar to a matrix $T_x = D + (I - D)C + xe_n(e_k - e_1)^\top$ for some $x > 0$. Then $\mathcal{K}(T) = \mathcal{K}(T_x) > m(P)$, the strict inequality following from Lemma 3.10. ∎

4 *P* with all specified entries in one row

In this section, we consider the case that the $n \times n$ partial stochastic matrix P has n specified entries, all lying in a common row. By applying a permutation similarity if necessary, we may assume, without loss of generality, that the specified entries are in row n, and take the values $r_0, r_1, \ldots, r_{n-1}$, with r_0 on the diagonal of P, with the remaining values occupying positions $(n, 1), \ldots, (n, n-1)$. Throughout this section, we assume that $r_j \geq 0$, $j = 0, \ldots, n-1$, and $\sum_{j=0}^{n-1} r_j = 1$.

As in Section 2, we consider a $T \in SC(P)$ that minimizes Kemeny's constant, and in view of Proposition 2.3, we focus on the case that the first $n-1$ rows of T are $(0,1)$. That leads to two possibilities for the directed graph of T: either there is a cycle in the subgraph induced by vertices $1, \ldots, n-1$ or every cycle passes through vertex n. The next two results address those cases.

Proposition 4.1   *Suppose that the first $n-1$ rows of the stochastic matrix T are $(0,1)$, the directed graph of T has a cycle on vertices $1, \ldots, k$, that T has a single essential class, and that the last row of T is specified, with diagonal entry r_0. Then $\mathcal{K}(T) = \frac{2n-k-3}{2} + \frac{1}{1-r_0}$. In particular, $\mathcal{K}(T) \geq \frac{n-2}{2} + \frac{1}{1-r_0}$, with equality if $k = n-1$.*

Proof   Write T as $T = \left[\begin{array}{c|c|c} C & 0 & 0 \\ \hline X & N & 0 \\ \hline u^{\top} & v^{\top} & r_0 \end{array}\right]$, where C is the adjacency matrix of the k-cycle, N is a $(0,1)$ matrix of order $n-k-1$, and $u^{\top}, v^{\top}$ are vectors whose entries comprise $r_1, \ldots, r_{n-1}$. The directed graph of N cannot contain a cycle, otherwise the fact that N is $(0,1)$ implies that T has more than one essential class. Consequently, N is nilpotent.

We now find that $\mathcal{K}(T) = \mathcal{K}(C) + \mathrm{trace}((I-N)^{-1}) + \frac{1}{1-r_0} = \frac{k-1}{2} + n - k - 1 + \frac{1}{1-r_0}$. The conclusion follows.   ∎

Proposition 4.2   *Suppose that the first $n-1$ rows of the stochastic matrix T are $(0,1)$ and that every cycle in the directed graph of T goes through vertex n. Suppose that in the last row of T, the entries $r_1, \ldots, r_{n-1}$ appear in positions $1, \ldots, n-1$ (in some order) and that the (n,n) entry is r_0. Partition the vertices of the directed graph associated with T into sets $A_0 = \{n\}, A_1, \ldots, A_{d-1}$ where A_j is the set of vertices at distance j from n, and $d-1$ is the maximum distance from n. For each $j = 0, \ldots, d-1$, let $\tilde{r}_j = \sum_{k \in A_j} r_k$. Then*
$$\mathcal{K}(T) = n - 1 - \frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{2\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}.$$

Proof   We proceed by induction on n and note that the case $n = 2$ is straightforward. Henceforth, we suppose that $n \geq 3$. We subdivide the rest of the proof into two cases.

Case 1, the first $n-1$ rows of T are distinct.

In this case, we have $d = n$, and each A_j consists of a single vertex. Without loss of generality, we may write T as $\left[\begin{array}{c|c} N & e_{n-1} \\ \hline u^{\top} & \tilde{r}_0 \end{array}\right]$, where N is the nilpotent matrix of order $n-1$ with ones on the superdiagonal and zeros elsewhere, and where the entries

in $u^\top$ correspond to $r_1, \ldots, r_{n-1}$. Indeed, in the notation of the statement, $u_j = \tilde{r}_{n-j}$, $j = 1, \ldots, n-1$.

Applying Lemma 3.2, we find that

$$\mathcal{K}(T) = \operatorname{trace}((I - N)^{-1}) - \frac{1}{1 + u^\top (I - N)^{-1}\mathbf{1}}\operatorname{trace}((I - N)^{-1}\mathbf{1}u^\top(I - N)^{-1})$$

$$= n - 1 - \frac{1}{1 + u^\top(I - N)^{-1}\mathbf{1}}u^\top(I - N)^{-1}(I - N)^{-1}\mathbf{1}.$$

The desired expression now follows from a computation.

Case 2, among the first $n - 1$ rows of T, two rows are the same.

For concreteness, but without loss of generality, we may assume that the first two rows of T are equal to $e_3^\top$. We may then write T as $T = \left[\begin{array}{c|c} 0^\top & e_1^\top \\ 0^\top & e_1^\top \\ \hline T_1 & T_2 \end{array}\right]$, where T_1 is $(n-2) \times 2$, T_2 is $(n-2) \times (n-2)$, the first $n-3$ rows of $\left[\begin{array}{c|c} T_1 & T_2 \end{array}\right]$ are $(0,1)$, and the last row of $\left[\begin{array}{c|c} T_1 & T_2 \end{array}\right]$ consists of the entries $r_1, \ldots, r_{n-1}$ in the first $n-1$ positions and r_0 in the last position.

We may factor T as UV where $U = \left[\begin{array}{c|c} \mathbf{1} & 0^\top \\ \hline 0 & I \end{array}\right]$, $V = \left[\begin{array}{c|c} 0^\top & e_1^\top \\ \hline T_1 & T_2 \end{array}\right]$. Here the rows of U are partitioned as 2 rows/$(n-2)$ rows, and the columns are partitioned as 1 column/$(n-2)$ columns, while the rows of V are partitioned as 1 row/$(n-2)$ rows, and the columns are partitioned as 2 columns/$(n-2)$ columns. The eigenvalues of T consist of 0, along with the eigenvalues of the $(n-1) \times (n-1)$ matrix $VU = \left[\begin{array}{c|c} 0 & e_1^\top \\ \hline T_1\mathbf{1} & T_2 \end{array}\right]$. Observe that since the first $n-3$ rows of T_1 are $(0,1)$ with at most one 1 in each row, $T_1\mathbf{1}$ is necessarily $(0,1)$ in its first $n-3$ positions. Observe also that $\mathcal{K}(T) = \mathcal{K}(UV) = 1 + \mathcal{K}(VU)$.

Note that the induction hypothesis applies to VU, and in particular that in the directed graph of T, vertices 1 and 2 of T (which correspond to vertex 1 of VU) are at the same distance from n. Applying the induction hypothesis to VU, we find that $\mathcal{K}(VU) = n - 2 - \frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{2\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}$. The expression for $\mathcal{K}(T)$ now follows. ∎

From Proposition 4.2, in order to minimize Kemeny's constant when one row of P is specified, we would like to maximize $\frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}$ over the various choices of d and the subsets $A_1, \ldots, A_{d-1}$. The next result is useful in that regard.

Lemma 4.3 *Suppose that $d < n$ and that we have the partition $A_0, A_1, \ldots, A_{d-1}$, where $|A_{j_0}| \geq 2$, say with $\ell \in A_{j_0}$. Consider the partition $A'_j, j = 0, \ldots, d$ with $A'_j = A_j, j \in \{0, \ldots, d-1\} \smallsetminus \{j_0\}, A'_{j_0} = A_{j_0} \smallsetminus \{\ell\}, A'_d = \{\ell\}$. Let $g = \frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}$ be associated with the original partition $A_0, A_1, \ldots, A_{d-1}$, and let $h = \frac{\sum_{j=0}^{d} j(j+1)\tilde{r}'_j}{\sum_{j=0}^{d}(j+1)\tilde{r}'_j}$ be associated with the modified partition $A'_0, \ldots, A'_d$. Then $h \geq g$.*

Proof   Observe that $\tilde{r}'_j = \tilde{r}_j$ for $j = 0, \ldots, d-1$, $j \ne j_0$, while $\tilde{r}'_{j_0} = \tilde{r}_{j_0} - r_\ell$, $\tilde{r}_d = r_\ell$. It now follows that h can be written as $h = \frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j + (d-j_0)(d+j_0+1)r_\ell}{\sum_{j=0}^{d-1}(j+1)\tilde{r}_j + (d-j_0)r_\ell}$. A computation now reveals that $h - g$ has the same sign as $r_\ell(d-j_0)\big((d+j_0+1)\sum_{j=0}^{d-1}(j+1)\tilde{r}_j - \sum_{j=0}^{d-1} j(j+1)\tilde{r}_j\big) = r_\ell(d-j_0)\sum_{j=0}^{d-1}(j+1)\tilde{r}_j(d+j_0+1-j)$, which is clearly nonnegative. ∎

Remark 4.4   From Lemma 4.3, we see that in order to maximize $\frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}$, it suffices to consider the case that $d = n$, and that each A_j consists of a single index. It follows that the corresponding stochastic matrices are of the form

$$
\begin{bmatrix}
0 & 1 & 0 & \ldots & 0 & 0 \\
0 & 0 & 1 & 0 & \ldots & 0 \\
\vdots & & & \ddots & & \vdots \\
0 & 0 & \ldots & 0 & 1 & 0 \\
0 & 0 & \ldots & 0 & 0 & 1 \\
r_{\sigma(n-1)} & r_{\sigma(n-2)} & \cdots & r_{\sigma(2)} & r_{\sigma(1)} & r_0
\end{bmatrix}
$$

for permutations $\sigma \in S_{n-1}$.

Here is one of the main results in this section.

Theorem 4.5   *Suppose that P is an $n \times n$ partial stochastic matrix where row n has been specified as $p_{n,j} = r_{n-j}$, $j = 1, \ldots, n$, and all remaining entries are unspecified. Then*

$$
m(P) = \min\left\{ \frac{n-2}{2} + \frac{1}{1-r_0},\, n-1 - \frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{2(1 + \sum_{j=1}^{n-1} j r_{\sigma(j)})} \right\},
$$

where the minimum is taken over all permutations σ of $\{1, \ldots, n-1\}$.

Proof   Adopting the notation of Proposition 4.2, it follows from Lemma 4.3 that in order to maximize $\frac{\sum_{j=0}^{d-1} j(j+1)\tilde{r}_j}{\sum_{j=0}^{d-1}(j+1)\tilde{r}_j}$, it suffices to consider $d = n$, $A_0 = \{n\}$, and $A_j = \{\sigma(j)\}$ for some permutation σ of $\{1, \ldots, n-1\}$. From the fact that $(\tilde{r}_0 =)r_0 = 1 - \sum_{k=1}^{n-1} r_{\sigma(k)}$, it follows that $\frac{\sum_{j=0}^{n-1} j(j+1)\tilde{r}_j}{\sum_{j=0}^{n-1}(j+1)\tilde{r}_j} = \frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{(1 + \sum_{j=1}^{n-1} j r_{\sigma(j)})}$. The conclusion now follows from Propositions 4.1 and 4.2. ∎

Remark 4.6   In the case that $r_0 \geq \frac{n-2}{n}$, we have $\frac{n-2}{2} + \frac{1}{1-r_0} \geq n-1$. In that case, the expression for $m(P)$ simplifies to $\min_{\sigma \in S_{n-1}}\left\{ n-1 - \frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{2(1 + \sum_{j=1}^{n-1} j r_{\sigma(j)})} \right\}$.

On its face, Theorem 4.5 leaves us in the position of evaluating $(n-1)! + 1$ expressions, then choosing the minimum. Our next task is to reduce the number of permutations to be considered in Theorem 4.5. The following result is useful in that regard.

Proposition 4.7 *Suppose that $1 \le j_1 < j_2 \le n-1$. Form the sequence $\hat{r}_1, \hat{r}_2, \ldots, \hat{r}_{n-1}$ from $r_1, r_2, \ldots, r_{n-1}$ by exchanging r_{j_1} and r_{j_2}. Then $\frac{\sum_{j=0}^{n-1} j(j+1)\hat{r}_j}{\sum_{j=0}^{n-1}(j+1)\hat{r}_j} - \frac{\sum_{j=0}^{n-1} j(j+1)r_j}{\sum_{j=0}^{n-1}(j+1)r_j}$ is positive, zero, or negative according as $(r_{j_1} - r_{j_2})\left(j_1 + j_2 + 1 - \frac{\sum_{j=0}^{n-1} j(j+1)r_j}{\sum_{j=0}^{n-1}(j+1)r_j}\right)$ is positive, zero, or negative.*

Proof Observe that

$$\frac{\sum_{j=0}^{n-1} j(j+1)\hat{r}_j}{\sum_{j=0}^{n-1}(j+1)\hat{r}_j} = \frac{\sum_{j=0}^{n-1} j(j+1)r_j + (r_{j_1} - r_{j_2})(j_2 - j_1)(j_1 + j_2 + 1)}{\sum_{j=0}^{n-1}(j+1)r_j + (r_{j_1} - r_{j_2})(j_2 - j_1)}.$$

A computation reveals that

$$\frac{\sum_{j=0}^{n-1} j(j+1)\hat{r}_j}{\sum_{j=0}^{n-1}(j+1)\hat{r}_j} - \frac{\sum_{j=0}^{n-1} j(j+1)r_j}{\sum_{j=0}^{n-1}(j+1)r_j} =$$
$$\frac{(r_{j_1} - r_{j_2})(j_2 - j_1) \sum_{j=0}^{n-1}(j+1)r_j(j_1 + j_2 + 1 - j)}{\sum_{j=0}^{n-1}(j+1)\hat{r}_j \sum_{j=0}^{n-1}(j+1)r_j}.$$

The conclusion follows. ∎

We always have $\frac{\sum_{j=1}^{n-1} j(j+1)r_j}{1 + \sum_{j=1}^{n-1} jr_j} \le n-1$, with equality if and only if $r_{n-1} = 1, r_j = 0$, $j = 0, \ldots, n-1$. That case is excluded from consideration in the following result.

Proposition 4.8 *Suppose that $r_0, r_1, \ldots, r_{n-1} \ge 0$, $\sum_{j=0}^{n-1} r_j = 1$ and that $\gamma \equiv \frac{\sum_{j=1}^{n-1} j(j+1)r_j}{1 + \sum_{j=1}^{n-1} jr_j}$ maximizes $\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{1 + \sum_{j=1}^{n-1} jr_{\sigma(j)}}$ over all permutations σ of $\{1, \ldots, n-1\}$. Let $\rho_j, j = 1, \ldots, n - 1$ denote the sequence $r_1, \ldots, r_{n-1}$ written in nondecreasing order. Assume that $\gamma < n-1$.*
  (a) If $\gamma < 4$, then $r_j = \rho_j, j = 1, \ldots, n-1$.
  (b) If $\gamma \notin \mathbb{N}, \gamma > 4$, let $k = \lfloor \gamma \rfloor$. Then

$$r_j = \rho_{k-2j}, j = 1, \ldots, \left\lfloor \frac{k-1}{2} \right\rfloor; r_j = \rho_{2j-k+1}, j = \left\lceil \frac{k}{2} \right\rceil, \ldots, k-2;$$

(4.1) $r_j = \rho_j, j = k-1, \ldots, n-1.$

  (c) If $\gamma = k \in \mathbb{N}$ for some $k = 4, \ldots, n-2$, set $\ell = \lfloor \frac{k}{2} \rfloor$. The ordering given by (4.1) maximizes $\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{1 + \sum_{j=1}^{n-1} jr_{\sigma(j)}}$. The other maximizing orderings can be obtained from (4.1) by choosing a subset $\{j_1, \ldots, j_m\} \subseteq \{1, \ldots, \ell-1\}$ and exchanging r_{j_i} and r_{k-1-j_i}, $i = 1, \ldots, m$.

Proof The key observation is that from Proposition 4.7, it must be the case that for indices $1 \le j_1 < j_2 \le n-1$, $(r_{j_1} - r_{j_2})(j_1 + j_2 + 1 - \gamma) \le 0$.
  (a) If $\gamma < 4$, then $j_1 + j_2 + 1 - \gamma > 0$, and the conclusion follows.
  (b) Since $\gamma \notin \mathbb{N}, k < \gamma < k+1$. From Proposition 4.7, we find that $r_j \ge r_{k-j-1}$ for $j = 1, \ldots, \lfloor \frac{k-2}{2} \rfloor, r_j \le r_{k-j}$ for $j = 1, \ldots, \lfloor \frac{k-1}{2} \rfloor$, and $r_j \le r_{j+1}$ for $j \ge \lfloor \frac{k-1}{2} \rfloor$.

Suppose that k is odd, with $k = 2\ell + 1$. Then $r_{2\ell-j+1} \geq r_j \geq r_{2\ell-j}, j = 1, \ldots, \ell - 1$ and $r_j \leq r_{j+1}, j \geq \ell$. It now follows that $r_j = \rho_{2\ell-2j+1}, j = 1, \ldots, \ell, r_j = \rho_{2j-2\ell}, j = \ell + 1, \ldots, 2\ell - 1$, and $r_j = \rho_j, j \geq 2\ell$. A similar argument applies if k is even, and we may then express the odd and even cases in unified form as (4.1).

(c) From Proposition 4.7, we find that $r_j \geq r_{k-j-2}, j = 1, \ldots, \lfloor \frac{k-3}{2} \rfloor, r_j \leq r_{k-j}, j = 1, \ldots, \lfloor \frac{k-1}{2} \rfloor$, and $r_j \leq r_{j+1}, j \geq \lfloor \frac{k-1}{2} \rfloor$. Note also from Proposition 4.7 that for $j = 1, \ldots, \lfloor \frac{k-3}{2} \rfloor$, we have $r_{k-j} \geq r_{k-j-1} \geq r_{k-j-2}$.

If $k = 2\ell + 1$ is odd, we then have $r_j \geq r_{2\ell-j-1}, j = 1, \ldots, \ell - 1, r_j \leq r_{2\ell-j+1}, j = 1, \ldots, \ell, r_j \leq r_{j+1}, j \geq \ell$. We also have $r_{2\ell-j+1} \geq r_{2\ell-j} \geq r_{2\ell-j-1}, j = 1, \ldots, \ell - 1$. In particular, $r_{2\ell-j+1} \geq r_j, r_{2\ell-j} \geq r_{2\ell-j-1}, j = 1, \ldots, \ell - 1$ and $r_j \leq r_{j+1}, j \geq \ell$. If it happens to be the case that $r_j \geq r_{2\ell-j}$ for each $j = 1, \ldots, \ell - 1$, then we recover the ordering (4.1). On the other hand, if there are indices $j_1, \ldots, j_m \in \{1, \ldots, \ell - 1\}$ for which $r_{j_i} < r_{2\ell-j_i}, i = 1, \ldots, m$, we may perform a sequence of m switches that exchange the entries r_{j_i} and $r_{2\ell-j_i}, i = 1, \ldots, m$. According to Proposition 4.7, those exchanges leave the value of the objective function unchanged. We deduce that any maximizing ordering can be constructed by starting with the ordering in (4.1), then possibly exchanging r_{j_i} and $r_{2\ell-j_i}, i = 1, \ldots, m$ for indices $j_1, \ldots, j_m \in \{1, \ldots, \ell - 1\}$.

If $k = 2\ell$ is even, then as above we find that $r_j \geq r_{2\ell-j-2}, j = 1, \ldots, \ell - 2, r_j \leq r_{2\ell-j}, j = 1, \ldots, \ell - 1, r_j \leq r_{j+1}, j \geq \ell - 1$, and $r_{2\ell-j} \geq r_{2\ell-j-1} \geq r_{2\ell-j-2}, j = 1, \ldots, \ell - 2$. If it happens to be the case that $r_j \geq r_{2\ell-j-1}, j = 1, \ldots, \ell - 1$, then we generate the ordering (4.1). On the other hand, if there are indices $j_1, \ldots, j_m \in \{1, \ldots, \ell - 1\}$ for which $r_{j_i} < r_{2\ell-j_i-1}, i = 1, \ldots, m$, we may perform a sequence of m switches that exchange r_{j_i} and $r_{2\ell-j_i-1}, i = 1, \ldots, m$. From Proposition 4.7, those exchanges leave the value of the objective function unchanged. We deduce that any maximizing ordering can be constructed by starting with (4.1), then possibly exchanging r_{j_i} and $r_{2\ell-j_i-1}, i = 1, \ldots, m$ for indices $j_1, \ldots, j_m \in \{1, \ldots, \ell - 1\}$. ∎

Remark 4.9   We emphasize that the ordering in (4.1) depends on the specific value of k.

Corollary 4.10   *Suppose that P is an $n \times n$ partial stochastic matrix where row n has been specified as $p_{n,j} = r_{n-j}, j = 1, \ldots, n$, and all remaining entries are unspecified. Suppose further that $r_j < 1, j = 0, \ldots, n - 1$. Let $\rho_j, j = 1, \ldots, n - 1$ denote the sequence $r_1, \ldots, r_{n-1}$ written in nondecreasing order. For each $k = 4, \ldots, n - 2$, let $r_j^{(k)}$ denote the ordering of (4.1) associated with k. Then*

$$m(P) = \min \left\{ \frac{n-2}{2} + \frac{1}{1-r_0}, n - 1 - \frac{\sum_{j=1}^{n-1} j(j+1)\rho_j}{2(1 + \sum_{j=1}^{n-1} j\rho_j)}, \right.$$
$$\left. n - 1 - \frac{\sum_{j=1}^{n-1} j(j+1) r_j^{(4)}}{2(1 + \sum_{j=1}^{n-1} j r_j^{(4)})}, \ldots, n - 1 - \frac{\sum_{j=1}^{n-1} j(j+1) r_j^{(n-2)}}{2(1 + \sum_{j=1}^{n-1} j r_j^{(n-2)})} \right\}.$$

Corollary 4.11   *Suppose that $3 \leq n \leq 5$. Then*

$$m(P) = \min \left\{ \frac{n-2}{2} + \frac{1}{1-r_0}, n - 1 - \frac{\sum_{j=0}^{n-1} j(j+1)\rho_j}{2 \sum_{j=0}^{n-1} (j+1)\rho_j} \right\}.$$

Remark 4.12 In this remark, we show how, for each $k = 4, \ldots, n - 2$, there is a sequence $r_0, r_1, \ldots, r_{n-1}$ such that the optimal ordering corresponds to that given by (4.1) for the parameter k. Fix such a k and suppose that $\gamma \in [k, k + 1)$.

Suppose that $\varepsilon \in (0, \frac{1}{2})$ and select a vector $c \in \mathbb{R}^{n-2}$ with $c_j \geq 0$, $j = 1, \ldots, n - 2$ and $\sum_{j=1}^{n-2} c_j = 1$. Now set $\hat{r}_j = \varepsilon c_j$, $j = 1, \ldots, n - 2$, and $\hat{r}_{n-1} = 1 - \varepsilon$. Fix a k with $4 \leq k \leq n - 2$ and assume that $\hat{r}_1, \ldots, \hat{r}_{n-1}$ has the ordering given by (4.1) corresponding to k. Fix $\gamma \in [k, k + 1)$, define r_0 via

$$1 - r_0 = \frac{\gamma}{(1 - \varepsilon)(n - 1)(n - \gamma) + \varepsilon \sum_{j=1}^{n-2} jc_j(j + 1 - \gamma)}$$

and set $r_j = (1 - r_0)\hat{r}_j$, $j = 1, \ldots, n - 1$. (We note that $r_0 \in (0, 1)$ for all sufficiently small $\varepsilon > 0$.) For notational convenience, we suppress the dependence on ε and γ. It is straightforward to determine that $\frac{\sum_{j=0}^{n-1} j(j+1)r_j}{\sum_{j=0}^{n-1}(j+1)r_j} = \gamma$. Observe also that for all sufficiently small $\varepsilon > 0$ and any permutation σ of $\{1, \ldots, n - 1\}$, $\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{r_0 + \sum_{j=1}^{n-1}(j+1)r_{\sigma(j)}} = \gamma + O(\varepsilon)$. In particular, for any such ε and σ, $\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{r_0 + \sum_{j=1}^{n-1}(j+1)r_{\sigma(j)}} < k + 1$. We deduce that

$$\max\left\{\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{r_0 + \sum_{j=1}^{n-1}(j+1)r_{\sigma(j)}} \,\middle|\, \sigma \in S_{n-1}\right\} \in [\gamma, k + 1).$$ If $k < \gamma$, then Proposition 4.8(b) applies, and hence the unique ordering of $r_1, \ldots, r_{n-1}$ that yields the maximum is in fact given by (4.1).

Suppose now that $\gamma = k$. If it were the case that

$$\max\left\{\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{r_0 + \sum_{j=1}^{n-1}(j+1)r_{\sigma(j)}} \,\middle|\, \sigma \in S_{n-1}\right\} > \gamma,$$

then Proposition 4.8(b) would necessitate that the ordering (4.1) yields the maximum value, a contradiction (since that ordering yields the value γ). Consequently, we find that $\max\left\{\frac{\sum_{j=1}^{n-1} j(j+1)r_{\sigma(j)}}{r_0 + \sum_{j=1}^{n-1}(j+1)r_{\sigma(j)}} \,\middle|\, \sigma \in S_{n-1}\right\} = k$.

Finally, we note that for this sequence, and sufficiently small $\varepsilon > 0$, we have $\frac{n}{2} + \frac{1}{1-r_0} = \frac{n}{2} + \frac{(n-1)(n-\gamma)}{\gamma} + O(\varepsilon)$, while the ordering given by (4.1) corresponds to $n - 1 - \frac{\gamma}{2}$. It now follows that $\frac{n}{2} + \frac{1}{1-r_0}$ is strictly greater than the minimum value of Kemeny's constant.

We close the paper with a brief example.

Example 4.13 Suppose that $n = 6, r_0 = 0$, and $0 \leq a \leq \frac{1}{2}$. Consider the values $\frac{1-a}{2}, \frac{1-a}{2}, \frac{a}{2}, \frac{a}{2}, 0$ as the remaining specified entries in last row of the partial stochastic matrix P. From Corollary 4.10, it suffices to consider r_1, r_2, r_3, r_4, r_5 in one of the following two orders: $0, \frac{a}{2}, \frac{a}{2}, \frac{1-a}{2}, \frac{a}{2}; \frac{a}{2}, 0, \frac{a}{2}, \frac{1-a}{2}, \frac{a}{2}$. The first ordering yields $\mathcal{K}_1(a) \equiv \frac{30-4a}{11-4a}$ for Kemeny's constant, while the second ordering yields $\mathcal{K}_2(a) = \frac{30-7a}{11-5a}$ for Kemeny's constant, so that by Corollary 4.10, $m(P) = \min\{3, \mathcal{K}_1(a), \mathcal{K}_2(a)\}$. A few computations show that $\mathcal{K}_2(a) < \mathcal{K}_1(a) < 3$ for $0 < a < \frac{3}{8}$ and $3 < \mathcal{K}_1(a) < \mathcal{K}_2(a)$

for $\frac{3}{8} < a \leq \frac{1}{2}$. We deduce that $m(P) = \mathcal{K}_2(a)$ for $a \in \left[0, \frac{3}{8}\right]$, while $m(P) = 3$ for $a \in \left[\frac{3}{8}, \frac{1}{2}\right]$.

By contrast, we note that some orderings of r_1, r_2, r_3, r_4, r_5 yield values of Kemeny's constant that are well separated from $m(P)$. For example, if r_1, r_2, r_3, r_4, r_5 are ordered as $\frac{1-a}{2}, \frac{1-a}{2}, \frac{a}{2}, \frac{a}{2}, 0$, the corresponding value of Kemeny's constant is $\frac{8a+21}{4a+5}$, which lies in the interval $\left[\frac{25}{7}, \frac{21}{5}\right]$ when $0 \leq a \leq \frac{1}{2}$.

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