

# Forest matrices around the Laplacian matrix

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## Abstract

We study the matrices  $Q_k$  of in-forests of a weighted digraph  $\Gamma$  and their connections with the Laplacian matrix  $L$  of  $\Gamma$ . The  $(i, j)$  entry of  $Q_k$  is the total weight of spanning converging forests (*in-forests*) with  $k$  arcs such that  $i$  belongs to a tree rooted at  $j$ . The forest matrices,  $Q_k$ , can be calculated recursively and expressed by polynomials in the Laplacian matrix; they provide representations for the generalized inverses, the powers, and some eigenvectors of  $L$ . The normalized in-forest matrices are row stochastic; the normalized matrix of maximum in-forests is the eigenprojection of the Laplacian matrix, which provides an immediate proof of the Markov chain tree theorem. A source of these results is the fact that matrices  $Q_k$  are the matrix coefficients in the polynomial expansion of  $\text{adj}(\lambda I + L)$ . Thereby they are precisely Faddeev's matrices for  $-L$ .

*AMS classification:* 05C50; 15A48

*Keywords:* Weighted digraph; Laplacian matrix; Spanning forest; Matrix-forest theorem; Leverrier-Faddeev method; Markov chain tree theorem; Eigenprojection; Generalized inverse

## 1 Introduction

According to the matrix-tree theorem, the  $(i, j)$  cofactor of the Laplacian matrix of a weighted digraph equals the total weight of spanning converging trees rooted at vertex  $i$  of the digraph.

Fiedler and Sedláček [25] proved that the principal minor of the Laplacian matrix resulting by the removal of the rows and columns indexed by a set  $\mathcal{J}$  is equal to the total weight of in-forests with  $|\mathcal{J}|$  trees rooted at the vertices of  $\mathcal{J}$ .

These results are generalized by the *all minors matrix tree theorem* [17, 10] (see also [53]) which expresses arbitrary minors of the Laplacian matrix in terms of in-forests of the digraph.

We study the matrices,  $Q_k$ , of a digraph's in-forests: the  $(i, j)$  entry of  $Q_k$  is the total weight of in-forests with  $k$  arcs where  $i$  belongs to a tree converging to  $j$ . In this paper, we show that the forest matrices can be recursively calculated and represented by simple polynomials in the Laplacian matrix  $L$ ; in turn, the powers of  $L$  are linear combinations of  $Q_k$ 's. Further, we demonstrate that the forest matrices are useful to interpret a number

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of expressions that involve the Laplacian matrix, including those of the group and Moore-Penrose inverses, and some eigenvectors. Of special interest is the normalized matrix  $\tilde{J}$  of *maximum in-forests* of a digraph previously used [42, 43] to represent the long run transition probabilities of Markov chains. We prove that  $\tilde{J}$  is the eigenprojection of the Laplacian matrix corresponding to the eigenvalue 0 and study some properties of  $\tilde{J}$ .

A seminal result that enables one to give short algebraic proofs to these representations is the fact that matrices  $Q_k$  coincide with the matrix coefficients in the polynomial form of  $\text{adj}(\lambda I + L)$ :

$$\text{adj}(\lambda I + L) = \sum_{k=0}^{n-1} Q_{n-k-1} \lambda^k,$$

where  $\text{adj} A$  is the transposed matrix of cofactors of  $A$ . This expansion is a corollary to the *parametric matrix-forest theorem* [1] which expresses the entries of  $(I + \tau L)^{-1}$ ,  $\tau \in \mathbb{R}$  in terms of in-forests.

All results of this paper are applicable to unweighted digraphs (by taking all weights equal to one) and undirected graphs (by considering symmetric digraphs).

The paper is organized as follows. After the notation section, we briefly survey the major known results on the minors of the Laplacian (Kirchhoff) matrix of a weighted digraph (Section 3), give a new proof to the matrix-forest theorem for digraphs (Section 4), present a recursive method for calculating the forest matrices (Section 5), establish polynomial representations of the forest matrices (Sections 6), study the normalized matrix  $\tilde{J}$  of maximum in-forests (Section 7), consider  $L$  and  $\tilde{J}$  as linear transformations and show that  $\tilde{J}$  is the eigenprojection of  $L$ , which yields the *Markov chain tree theorem* (Section 8), and finally, express the generalized inverses of  $L$  in terms of the forest matrices (Section 9).

## 2 Notation

### 2.1 Graph definitions

For graph terminology, we mainly follow [30]. Suppose that  $\Gamma$  is a weighted digraph without loops,  $V(\Gamma) = \{1, \dots, n\}$ ,  $n > 1$ , is its set of vertices and  $E(\Gamma)$  its set of arcs. The weights of all arcs are strictly positive. Let  $W = (w_{ij})$  be the matrix of arc weights of  $\Gamma$ . Its  $(i, j)$  entry,  $w_{ij}$ , equals zero iff there is no arc from vertex  $i$  to vertex  $j$  in  $\Gamma$ . If  $\Gamma'$  is a subgraph of  $\Gamma$ , then the weight of  $\Gamma'$ ,  $w(\Gamma')$ , is the product of the weights of all its arcs; if  $\Gamma'$  does not contain arcs, then  $w(\Gamma') = 1$ . The weight of a nonempty set of digraphs  $\mathcal{G}$  is defined as follows:

$$w(\mathcal{G}) = \sum_{H \in \mathcal{G}} w(H); \quad w(\emptyset) = 0. \tag{1}$$

A *spanning* subgraph of  $\Gamma$  is a subgraph of  $\Gamma$  with vertex set  $V(\Gamma)$ . The *outdegree* of vertex  $v$  is the number of arcs that come from  $v$ . A *converging tree* is a weakly connected (i.e., its corresponding undirected graph is connected) digraph in which one vertex, called the *root*, has outdegree zero and the remaining vertices have outdegree one.

A converging tree is said to *converge* to its root. Spanning converging trees are sometimes called *in-arborescences*. A *converging forest* is a digraph all of whose weak components (i.e., maximal weakly connected subgraphs) are converging trees. The roots of these trees are the roots of the converging forest.

**Definition 1.** An *in-forest* is a spanning converging forest.

**Definition 2.** An in-forest  $F$  of a digraph  $\Gamma$  is called a *maximum in-forest* of  $\Gamma$  if  $\Gamma$  has no in-forest with a greater number of arcs than in  $F$ .

*Out-forests* which *diverge* from their roots and *maximum out-forests* are defined in the same manner. In this paper, we deal with in-forests, but a parallel theory can be developed for out-forests.

The notion of maximum in-forest of a digraph generalizes the concept of spanning converging tree (in-arborescence). If spanning converging trees of a digraph exist, they coincide with maximum in-forests; otherwise maximum in-forests inherit some of their properties. These properties were studied in [1].

It is easily seen that every maximum in-forest of  $\Gamma$  has the minimum possible number of converging trees; we call this number the *in-forest dimension* of  $\Gamma$  and denoted it by  $d$ . The number of arcs in any maximum in-forest is obviously  $n - d$ ; in general, the number of disjoint trees in a spanning forest with  $k$  arcs is  $n - k$ .

By  $\mathcal{F}^{\rightarrow*}(\Gamma) = \mathcal{F}^{\rightarrow*}$  and  $\mathcal{F}_k^{\rightarrow*}(\Gamma) = \mathcal{F}_k^{\rightarrow*}$  we denote the set of all in-forests of  $\Gamma$  and the set of all in-forests of  $\Gamma$  with  $k$  arcs, respectively;  $\mathcal{F}_k^{i \rightarrow *j}$  will designate the set of all in-forests with  $k$  arcs where  $i$  belongs to a tree converging to  $j$ ;  $\mathcal{F}^{i \rightarrow *j} = \cup_{k=0}^{n-d} \mathcal{F}_k^{i \rightarrow *j}$  is the set of such in-forests with any number of arcs. The notation  $\mathcal{F}_{(k)}^{\rightarrow*}$  will be used for the set of in-forests that consist of  $k$  trees. The  $\rightarrow*$  sign relates to in-forests; the corresponding notation for out-forests is  $\mathcal{F}^{*\rightarrow}$ , etc.

Let

$$\sigma_k = w(\mathcal{F}_k^{\rightarrow*}), \quad k = 0, 1, \dots, \quad (2)$$

$$\sigma = w(\mathcal{F}^{\rightarrow*}) = \sum_{k=0}^{n-d} \sigma_k. \quad (3)$$

By (2) and (1),  $\sigma_k = 0$  whenever  $k > n - d$ , and  $\sigma_0 = 1$ .

We will also consider the parametric value

$$\sigma(\tau) = \sum_{k=0}^{n-d} \sigma_k \tau^k, \quad (4)$$

which is the total weight of in-forests in  $\Gamma$  provided that all arc weights are multiplied by  $\tau$ .

Let

$$s_k = \sum_{j=0}^k \sigma_j, \quad k = 0, \dots, n - d \quad (5)$$

be the total weight of in-forests of  $\Gamma$  with at most  $k$  arcs. Then, by definition,  $s_{n-d} = \sigma$ .

Finally,

$$s_k(\tau) = \sum_{j=0}^k \sigma_j \tau^j, \quad k = 0, \dots, n-d, \quad (6)$$

whence  $s_{n-d}(\tau) = \sigma(\tau)$ .

## 2.2 Matrix definitions

For any  $n \times n$  matrix  $A$ , let  $A(\overline{\mathcal{I}} | \overline{\mathcal{J}})$ , where  $\mathcal{I}, \mathcal{J} \subseteq \{1, \dots, n\}$ , be the submatrix of  $A$  obtained by the removal of the rows indexed by  $\mathcal{I}$  and the columns indexed by  $\mathcal{J}$ . For a complex matrix  $A$ ,  $A^*$  is the conjugate transpose (Hermitian adjoint) and  $A^T$  the transpose of  $A$ .

The *Laplacian* (or *row Laplacian*) matrix of a weighted digraph  $\Gamma$  is the  $n \times n$  matrix  $L = L(\Gamma) = (\ell_{ij})$  with entries  $\ell_{ij} = -w_{ij}$  when  $j \neq i$  and  $\ell_{ii} = -\sum_{k \neq i} \ell_{ik}$ ,  $i, j = 1, \dots, n$ . The *column Laplacian* matrix  $L' = L'(\Gamma) = (\ell'_{ij})$  differs from  $L$  by the diagonal only:  $\ell'_{ij} = -w_{ij}$  when  $j \neq i$  and  $\ell'_{ii} = -\sum_{k \neq i} \ell'_{ki}$ ,  $i, j = 1, \dots, n$ . The *Kirchhoff* (or *row Kirchhoff*) matrix [65] is  $K = L'^T$ ; the *column Kirchhoff* matrix is  $K' = L^T$ . These four singular matrices are generalizations of the Laplacian (Kirchhoff) matrix of an undirected graph. In what follows, we deal with the Laplacian matrix  $L(\Gamma)$  and reformulate for it some results originally obtained for the other matrices.

Throughout let  $\Gamma$  be a fixed digraph. Consider the *matrices*

$$Q_k = (q_{ij}^k), \quad k = 0, 1, \dots,$$

of *in-forests* of  $\Gamma$  with  $k$  arcs: the entries of  $Q_k$  are

$$q_{ij}^k = w(\mathcal{F}_k^{i \rightarrow *j}). \quad (7)$$

By (7) and (1),  $Q_k = 0$  whenever  $k > n-d$ , and  $Q_0 = I$ .

The *matrix of all in-forests* is

$$Q = (q_{ij}) = \sum_{k=0}^{n-d} Q_k \quad (8)$$

with entries  $q_{ij} = w(\mathcal{F}^{i \rightarrow *j})$ .

We will also consider the *normalized matrices of forests*:

$$J_k = \sigma_k^{-1} Q_k, \quad k = 0, \dots, n-d, \quad (9)$$

$$J = \sigma^{-1} Q, \quad (10)$$

and the parametric matrices

$$Q(\tau) = \sum_{k=0}^{n-d} Q_k \tau^k, \quad (11)$$

$$J(\tau) = \sigma^{-1}(\tau) Q(\tau), \quad \tau \geq 0, \quad (12)$$

where  $\sigma_k$ ,  $\sigma$ , and  $\sigma(\tau)$  are defined by (2)–(4).

The *normalized matrix of maximum in-forests*  $J_{n-d}$  will be also denoted by  $\tilde{J}$ :

$$\tilde{J} = J_{n-d}.$$

In the case of undirected graphs, the entries of  $\tilde{J}$  are the same within every connected component. In the directed case, this matrix possesses nontrivial properties determined by the properties of maximum in-forests, cf. [1].

**Proposition 1.** *The matrices  $J_k$ ,  $k = 0, \dots, n-d$ ,  $J$ , and  $J(\tau)$  are row stochastic.*

**Proof of Proposition 1.** Every row sum of  $Q_k$ ,  $k = 0, \dots, n-d$ , is  $\sigma_k$ . Indeed, for every  $i = 1, \dots, n$ , we have

$$\sum_{j=1}^n q_{ij}^k = \sum_{j=1}^n w(\mathcal{F}_k^{i \rightarrow *j}) \stackrel{(*)}{=} w\left(\bigcup_{j=1}^n \mathcal{F}_k^{i \rightarrow *j}\right) = w(\mathcal{F}_k^{\rightarrow *}) = \sigma_k.$$

In the  $(*)$  passage, we used the fact that  $\mathcal{F}_k^{i \rightarrow *j_1} \cap \mathcal{F}_k^{i \rightarrow *j_2} = \emptyset$  whenever  $j_1 \neq j_2$ . Thus, the nonnegative matrices  $J_k = \sigma_k^{-1} Q_k$  are row stochastic. Now the stochasticity of  $J$  and  $J(\tau)$  follows from their definitions.  $\square$

The aim of this paper is to interpret, in terms of the forest matrices, a number of expressions that involve the Laplacian matrix as well as to provide polynomial expressions for the forest matrices themselves.

### 3 Preliminaries

This section briefly surveys some known results on the minors of a digraph’s Laplacian matrix.

The oldest result of this kind is the *matrix-tree theorem* by Tutte [64, 65], although some authors (e.g., [10]; cf. [52]) trace it back to Sylvester [63] and its proof to Borchardt [9].

**Theorem 1.** *For every  $i, j \in V(\Gamma)$ ,  $\ell^{ij} = w(\mathcal{T}^{\rightarrow *i})$  holds, where  $\ell^{ij}$  is the cofactor of the  $(i, j)$  entry of  $L$  and  $\mathcal{T}^{\rightarrow *i}$  is the set of all spanning trees converging to  $i$  in  $\Gamma$ .*

As stated in [34], “This small formula opens a world of opportunities.”

Tutte [65] formulated this theorem for the diagonal cofactors of the Kirchhoff matrix. A version that involves all cofactors of the Laplacian and the column Laplacian matrices can be found in [30]. We do not describe multiple analogues of the matrix-tree theorem here.

By definition,  $L$  has the form  $L = D - W$ , where  $W$  is the nonnegative matrix of arc weights and  $D$  is the diagonal matrix ensuring the zero row sums of  $L$ . Therefore, by Geršgorin’s theorem, the real part of each nonzero eigenvalue of  $L$  is positive. Thus,  $L$  is a singular M-matrix (see, e.g., [7, Theorem 4.6 in Chapter 6]). One of the consequences is that all the principal minors of  $L$  are nonnegative. Fiedler and Sedláček [25] obtained an interpretation of all principal minors of the Laplacian matrix in terms of spanning forests:

**Theorem 2.** For any  $\mathcal{J} \subseteq \{1, \dots, n\}$ ,  $\det L(\overline{\mathcal{J}} | \overline{\mathcal{J}}) = w(\mathcal{F}^{\rightarrow* \mathcal{J}})$  holds, where  $\mathcal{F}^{\rightarrow* \mathcal{J}}$  is the set of in-forests for which  $\mathcal{J}$  is the set of roots.

Later this theorem was formulated and proved in [11]. Its special case with undirected graphs and  $|\mathcal{J}| = 2$  was discovered and employed earlier in the theory of electrical networks (see, e.g., [55]). Fiedler and Sedláček stated their result for the column Laplacian matrix and out-forests. Generally, to get interpretations for the minors of the column Laplacian matrix  $L'(\Gamma)$ , it suffices to observe that for the digraph obtained from  $\Gamma$  by the reversal of all arcs, the Laplacian matrix coincides with  $K(\Gamma) = L'^T(\Gamma)$  and the in-forests are in a weight preserving correspondence with the out-forests of  $\Gamma$ .

Let

$$\varphi(\lambda) = \det(\lambda I + L) = \sum_{k=0}^n c_{n-k} \lambda^k \quad (13)$$

be the characteristic polynomial of  $-L$  and let  $\sigma_k$  be as defined in (2).

**Proposition 2.** In (13),  $c_k = \sigma_k$ ,  $k = 0, \dots, n$ .

In view of Theorem 2, this proposition follows from the fact that  $c_k$  is equal to the sum of the  $k \times k$  principal minors of  $L$ . In the case of undirected unweighted multigraphs, Proposition 2 is due to Kelmans [36, 37], who was probably the first [35] to study the Laplacian characteristic polynomial (see also discussion in [52, p. 42] and [21, Sections 1.2, 1.5], and [8, Theorem 7.5]); some extensions are given in [4, the last statement on p. 236] and [20, Theorem 2]. An alternative representation for the coefficients of the Laplacian characteristic polynomial can be found in [26].

Since  $\sigma_k = 0$  if and only if  $k > n - d$  ( $k = 0, 1, \dots$ ), Proposition 2 implies

**Corollary 1.** The multiplicity of 0 as the eigenvalue of  $L$  is  $d$ .

Another immediate consequence of Proposition 2 is

**Corollary 2.**  $\sigma_k = \sum_{\mathcal{J}: |\mathcal{J}|=k} \prod_{j \in \mathcal{J}} \lambda_j$ ,  $k = 0, \dots, n$ ,

where  $\lambda_1, \dots, \lambda_n$  are the eigenvalues of  $L$  and  $\mathcal{J}$  are the subsets of  $\{1, \dots, n\}$ .

Chen [17, p. 313, Problems 4.14 and 4.16] proposed an extension of the matrix-tree theorem to additional minors of the Laplacian matrix and Chaiken [10] gave a similar graph interpretation to all minors of  $L'$ . Moon [53] obtained a more general expansion which applies to all minors of arbitrary matrices; Chaiken's theorem and a number of W.K. Chen's expansions follow from his result as special cases. Minoux [51] generalized Chaiken's theorem to semirings and Bapat et al. [5] to mixed graphs (where each arc is either directed or undirected). Other useful graph interpretations of minors and determinants are given in [45].

We do not quote these results here, but we employ Chaiken's formulation [10] of the *all minors matrix tree theorem* in the proof of a *matrix-forest theorem* in the following section.

## 4 Another matrix-forest theorem

The following theorem [13, 15] provides expressions for the forest matrices  $Q$  and  $J$  (see (8) and (10)) in terms of the cofactors and the determinant of  $I + L$ , where  $I$  is the identity matrix.

**Theorem 3.**  $Q = \text{adj}(I + L)$  and  $\sigma = \det(I + L)$ . Thus,  $J = (I + L)^{-1}$ .

For the properties of  $(I + L)^{-1}$ , see [15, 16, 46, 47].

It was mentioned in [15] that a quick way to prove the matrix-forest theorem is to employ the all minors matrix tree theorem, more specifically, to apply the first formula (without number) on page 328 in [10]. Below we give a complete inference of Theorem 3 from the all minors matrix tree theorem. Note that a self-contained proof of the matrix-forest theorem for unweighted multigraphs can be found in [62]. Another inference based on some results of [36, 37, 25, 45] was given in [13] for the case of weighted multidigraphs and multigraphs. Undirected and unweighted analogies of Theorem 3 have been presented in [46, 47] (with the proof based on Chaiken's theorem) and [14].

In the following proof of Theorem 3, we employ a standard trick which enables one to reduce many novel statements about forests to known statements about trees or forests. Versions of this trick have been used in many papers, e.g., [4, 10, 12, 17, 28, 33, 34, 38, 46, 47, 56].<sup>1</sup> We formalize it by

**Definition 3.** Let  $\Gamma$  be a weighted digraph. The digraph  $\widehat{\Gamma}$  with vertex set  $V(\widehat{\Gamma}) = V(\Gamma) \cup \{0\}$ , arc set  $E(\widehat{\Gamma}) = E(\Gamma) \cup \{(j, 0) : j \in V(\Gamma)\}$ , the weights of arcs in  $E(\widehat{\Gamma}) \cap E(\Gamma)$  the same as for  $\Gamma$ , and  $w((j, 0)) = 1$ ,  $j \in V(\Gamma)$ , will be called the *ground extension* of  $\Gamma$ .<sup>2</sup>

**Observation 1.** Let  $\widehat{\Gamma}$  be the ground extension of  $\Gamma$ . Let  $U = I + L(\Gamma)$ ,  $\widehat{L} = L(\widehat{\Gamma})$ . Then for any  $\mathcal{I}, \mathcal{J} \subseteq V(\Gamma)$ ,  $U(\overline{\mathcal{I}} | \overline{\mathcal{J}}) = \widehat{L}(\overline{\mathcal{I} \cup \{0\}} | \overline{\mathcal{J} \cup \{0\}})$  holds.

By virtue of Observation 1, if one has expressions for all minors of the Laplacian matrices  $L$  (say, those provided by the all minors matrix tree theorem), then expressions for all minors of matrices  $I + L$  are got gratis. The following lemma establishes a correspondence between the forests in  $\Gamma$  and some forests in  $\widehat{\Gamma}$ . The lemma is formulated here in a form useful for expressing all minors of  $I + L$ .

**Lemma 1.** Consider  $\mathcal{I} = \{i_1, \dots, i_k\} \subseteq V(\Gamma)$ ,  $\mathcal{J} = \{j_1, \dots, j_k\} \subseteq V(\Gamma)$ ,  $0 \leq k \leq n$ , and the set of in-forests  $\mathcal{F}^{\rightarrow*} \cap \left( \prod_{u=1}^k \mathcal{F}^{i_u \rightarrow *j_u} \right)$  in  $\Gamma$ . Then there exists a weight preserving one-to-one correspondence between this set and the set  $\widehat{\mathcal{F}}_{\mathcal{I}\mathcal{J}}^{\rightarrow*}$  of in-forests  $F \in \widehat{\mathcal{F}}^{0 \rightarrow *0} \cap \left( \prod_{u=1}^k \widehat{\mathcal{F}}^{i_u \rightarrow *j_u} \right)$  in  $\widehat{\Gamma}$  such that the  $F$ 's consist of exactly  $k + 1$  trees.

**Proof of Lemma 1.** Let  $F \in \mathcal{F}^{\rightarrow*} \cap \left( \prod_{u=1}^k \mathcal{F}^{i_u \rightarrow *j_u} \right)$ . To define the corresponding forest in  $\widehat{\mathcal{F}}_{\mathcal{I}\mathcal{J}}^{\rightarrow*}$ , consider the replica  $F'$  of  $F$  in  $\widehat{\Gamma}$  and attach the arcs  $(r, 0)$  to it, where the  $r$ 's are the

<sup>1</sup>Note that one more expedient is to identify the roots of all trees in a forest, which converts the forest into a tree [21, 25, 36, 37, 54, 13].

<sup>2</sup>In [34]  $\widehat{\Gamma}$  is called the *cone* of  $\Gamma$ .

roots of  $F'$  that are not in  $\mathcal{J}$ . The resulting in-forest consists of exactly  $k+1$  trees and belongs to  $\widehat{\mathcal{F}}_{\mathcal{I}\mathcal{J}}^{\rightarrow*}$ . Conversely, for any  $\widehat{F} \in \widehat{\mathcal{F}}_{\mathcal{I}\mathcal{J}}^{\rightarrow*}$ , consider its restriction to  $V(\Gamma)$  as the corresponding forest of  $\Gamma$ . Obviously, this correspondence is one-to-one and the corresponding forests share the weight.  $\square$

**Proof of Theorem 3.** Consider the ground extension  $\widehat{\Gamma}$  of  $\Gamma$ . By Observation 1, if  $U = I + L(\Gamma)$ ,  $U^{ij}$  is the  $(i, j)$  entry of  $\text{adj } U$ , and  $\widehat{L} = L(\widehat{\Gamma})$ , then

$$U^{ij} = (-1)^{i+j} \det U(\overline{\{j\}} | \overline{\{i\}}) = (-1)^{i+j} \det \widehat{L}(\overline{\{0, j\}} | \overline{\{0, i\}}). \quad (14)$$

Let  $\widehat{\mathcal{F}}_{(2)}^{0 \rightarrow *0, i \rightarrow *j}$  be the set of in-forests  $F \in \widehat{\mathcal{F}}^{0 \rightarrow *0} \cap \widehat{\mathcal{F}}^{i \rightarrow *j}$  that consist of two trees. Denoting by  $\text{inv}\{0 \rightarrow 0, i \rightarrow j\}$  the number of violations of monotonicity in the two-element correspondence  $\{0 \rightarrow 0, i \rightarrow j\}$ , which is obviously zero, and using the all minors matrix tree theorem [10, 53], we get

$$\begin{aligned} \det \widehat{L}(\overline{\{0, j\}} | \overline{\{0, i\}}) &= (-1)^{|\{k \in V(\Gamma) : k < j\}| + |\{k \in V(\Gamma) : k < i\}|} \sum_{F \in \widehat{\mathcal{F}}_{(2)}^{0 \rightarrow *0, i \rightarrow *j}} (-1)^{\text{inv}\{0 \rightarrow 0, i \rightarrow j\}} w(F) \\ &= (-1)^{j+i-2} w(\widehat{\mathcal{F}}_{(2)}^{0 \rightarrow *0, i \rightarrow *j}). \end{aligned} \quad (15)$$

In the first passage, we used the fact that  $\widehat{\mathcal{F}}^{i \rightarrow *0} = \emptyset$ .

Lemma 1 implies  $w(\widehat{\mathcal{F}}_{(2)}^{0 \rightarrow *0, i \rightarrow *j}) = w(\mathcal{F}^{i \rightarrow *j})$ , so, from (14) and (15), we get

$$U^{ij} = (-1)^{2i+2j-2} w(\mathcal{F}^{i \rightarrow *j}) = w(\mathcal{F}^{i \rightarrow *j}) = q_{ij}.$$

By Observation 1, Theorem 1, and Lemma 1,  $\det U = \det \widehat{L}(\overline{\{0\}} | \overline{\{0\}}) = w(\widehat{\mathcal{F}}_{(1)}^{0 \rightarrow *0}) = w(\mathcal{F}^{\rightarrow*}) = \sigma$  (cf. [33, Eq. (37)] and [34, 7.2 and 7.3]). This completes the proof.  $\square$

**Remark 1.** Obviously, the positivity of arc weights is needed for the last statement of Theorem 3 only; the first two statements are preserved for digraphs with arbitrary arc weights.

**Remark 2.** Note that the cofactors and the determinant of  $I + L$ , in the case of an unweighted undirected graph  $G$ , have been expressed in [28] in terms of spanning trees and 2-forests in the ground extension of  $G$  (for the case of weighted graphs, cf. [39, Theorem 2.3]). Ref. [28] also discusses the idea of using graph invariants related to  $(I + L)^{-1}$  in the study of the graph isomorphism problem. We surmise that the forest matrices  $Q_k$  also have some potential in this respect.

It is easily seen that  $I + \tau L$  with  $\tau \geq 0$  are nonsingular M-matrices, so their inverses are nonnegative. In the next section, the following parametric matrix-forest theorem [1] will be helpful:

**Theorem 3'.** For any  $\tau \in \mathbb{R}$ ,  $Q(\tau) = \text{adj}(I + \tau L)$  and  $\sigma(\tau) = \det(I + \tau L)$ . Thus, for any  $\tau \geq 0$ ,  $J(\tau) = (I + \tau L)^{-1}$ .

To prove this theorem, it suffices to apply Theorem 3 to the weighted digraph  $\Gamma'(\tau)$  that differs from  $\Gamma$  in the weights of arcs only: for all  $i, j = 1, \dots, n$ ,  $w'_{ij}(\tau) = \tau w_{ij}$ . By Remark 1, the nonnegativity of  $\tau$  is needed for the last statement of Theorem 3' only.



## 5 A method for calculating $Q_1, \dots, Q_{n-d}$

We first show that  $Q_1, \dots, Q_{n-d}$  are the matrix coefficients in the polynomial expansion of  $\text{adj}(\lambda I + L)$ .

**Proposition 3.**  $\text{adj}(\lambda I + L) = \sum_{k=0}^{n-d} Q_k \lambda^{n-k-1}$ .

**Proof of Proposition 3.** If  $\lambda = 0$ , then the right-hand side is zero whenever  $d > 1$  and it reduces to  $Q_{n-1}$  when  $d = 1$  (we put  $\lambda^0 \equiv 1$ ). This is equal to  $\text{adj}(\lambda I + L)$  by Theorem 1. For any  $\lambda \neq 0$ , let  $\tau = \lambda^{-1}$ . Using Theorem 3' we get

$$\text{adj}(\lambda I + L) = \text{adj} \lambda(I + \tau L) = \lambda^{n-1} Q(\tau) = \lambda^{n-1} \sum_{k=0}^{n-d} Q_k \tau^k = \sum_{k=0}^{n-d} Q_k \lambda^{n-k-1}. \quad \square \quad (16)$$

Proposition 3 underlies an easy algorithm for calculating  $Q_1, \dots, Q_{n-d}$  and  $\sigma_1, \dots, \sigma_{n-d}$ .

**Proposition 4.** For any  $k = 0, 1, \dots$ ,

$$Q_{k+1} = (-L)Q_k + \sigma_{k+1}I, \quad (17)$$

$$\sigma_{k+1} = \frac{\text{tr}(LQ_k)}{k+1}. \quad (18)$$

**Proof of Proposition 4.** Since, by Proposition 3,  $Q_0, \dots, Q_n$  are the matrix coefficients in the polynomial form of  $\text{adj}(\lambda I + L)$ , where  $\lambda I + L$  is the characteristic matrix of  $-L$  and, by Proposition 2,  $\sigma_0, \dots, \sigma_n$  are the coefficients of the characteristic polynomial of  $-L$ , the equations [27, §3 of Chapt. 4]  $Q_{k+1} = \sigma_{k+1}I - LQ_k$ ,  $k = 0, 1, \dots$ , take place.

To prove (18), it suffices to take the traces on the left and on the right of (17) and use the fact that

$$\text{tr} Q_k = (n - k)\sigma_k, \quad k = 0, 1, \dots,$$

which holds since every in-forest with  $k$  arcs has  $n - k$  roots.  $\square$

Note that, by virtue of Propositions 2 and 3, the recurrent application of (18) and (17) starting with  $Q_0 = I$  coincides with the Leverrier-Faddeev algorithm [23, 27] applied to calculate the characteristic polynomial of  $-L$ .

Consider now a few corollaries to Proposition 4. First, in what follows we will need a recurrence formula for the row stochastic matrices  $J_k$ . It is:

$$J_{k+1} = \frac{\sigma_k}{\sigma_{k+1}}(-L)J_k + I, \quad k = 0, \dots, n - d - 1. \quad (19)$$

Second, the matrices  $LQ_k$  prevailing in Proposition 4 have a noteworthy graph interpretation. Let  $\Gamma_k$  be the *digraph of in-forests with  $k$  arcs* of  $\Gamma$ , i.e., the digraph on vertex set  $V(\Gamma_k) = V(\Gamma)$  whose matrix of arc weights results from  $Q_k$  by putting zeros on the main diagonal. In other words,  $(i, j) \in E(\Gamma_k)$  whenever  $j \neq i$  and  $q_{ij}^k > 0$ ;  $q_{ij}^k$  is the weight of such arc. Evidently,  $\Gamma_1 = \Gamma$ .

**Proposition 5.**  $LQ_k$  is the Laplacian matrix of  $\Gamma_{k+1}$ ,  $k = 0, 1, \dots$

**Proof of Proposition 5.** By Proposition 4,  $LQ_k = \sigma_{k+1}I - Q_{k+1}$ , so the off-diagonal entries of  $LQ_k$  coincide with those of  $L(\Gamma_{k+1})$ . To complete the proof, note that every row sum of  $LQ_k$  is zero, since every row sum of both  $\sigma_{k+1}I$  and  $Q_{k+1}$  is  $\sigma_{k+1}$ .  $\square$

Finally, Proposition 4 provides a recurrent formula for the Laplacian matrices  $L_k := L(\Gamma_k)$ :

$$L_{k+1} = L \left( -L_k + \frac{\text{tr } L_k}{k} I \right), \quad k = 1, 2, \dots$$

We are going to discuss the application of digraphs  $\Gamma_k$  to the analysis of  $\Gamma$  elsewhere.

## 6 Forest matrices as polynomials in the Laplacian matrix

It follows from Proposition 4 that the forest matrices  $Q_k$ ,  $Q$ , and  $Q(\tau)$  are polynomials in  $L$ . As a corollary, the powers of  $L$  are linear combinations of  $Q_0, \dots, Q_{n-d}$ .

First, it is straightforward to prove

$$\textbf{Proposition 6.} \quad Q_k = \sum_{i=0}^k \sigma_{k-i} (-L)^i, \quad k = 0, 1, \dots$$

These expressions are closely related to the characteristic polynomial of  $-L$  (13) which, by Proposition 2, can be represented as  $\varphi(\lambda) = (\dots((\sigma_0 \lambda + \sigma_1)\lambda + \sigma_2)\lambda + \dots + \sigma_{n-1})\lambda + \sigma_n$ . To find  $\varphi(\lambda)$ , one can successively calculate  $\varphi_0(\lambda) = \sigma_0$ ,  $\varphi_1(\lambda) = \sigma_0 \lambda + \sigma_1$ ,  $\varphi_2(\lambda) = (\sigma_0 \lambda + \sigma_1)\lambda + \sigma_2, \dots, \varphi_n(\lambda) = \varphi(\lambda)$ . It is easily seen now that  $Q_k = \varphi_k(-L)$ ,  $k = 0, \dots, n$ .

**Corollary 3.** *The matrices  $Q_k$ ,  $k = 0, 1, \dots$ , commute with all matrices with which  $L$  commutes, in particular, with  $L$ ,  $Q(\tau)$ , and each other.*

By Theorems 3 and 3',  $Q = \text{adj}(I + L)$  and  $Q(\tau) = \text{adj}(I + \tau L)$ . Proposition 6, (8), and (11) provide a polynomial form of  $Q$  and  $Q(\tau)$ .

**Proposition 7.**

$$\begin{aligned} Q &= \sum_{k=0}^{n-d} s_{n-d-k} (-L)^k = \text{adj}(I + L), \\ Q(\tau) &= \sum_{k=0}^{n-d} s_{n-d-k}(\tau) (-\tau L)^k = \text{adj}(I + \tau L), \end{aligned} \quad (20)$$

where  $s_i$  and  $s_i(\tau)$  are defined in (5) and (6).

By (16),  $\text{adj}(\lambda I + L) = \lambda^{n-1} Q(\tau)$ , where  $\lambda \neq 0$  and  $\tau = 1/\lambda$ . Combining this with (20) and (6), we obtain

$$\textbf{Corollary 4.} \quad \text{adj}(\lambda I + L) = \sum_{k=0}^{n-d} s'_{n-d-k}(\lambda) (-L/\lambda)^k,$$

where  $s'_i(\lambda) = \sum_{j=0}^i \sigma_j \lambda^{n-j-1}$ ,  $i = 0, \dots, n-d$ , and  $\lambda \neq 0$ .

Corollary 4 and Proposition 3 can be considered as dual representations of  $\text{adj}(\lambda I + L)$ .

It follows from Proposition 6 that the powers of  $L$  are linear combinations of  $Q_0, \dots, Q_{n-d}$ , but the coefficients are more complicated than before.

**Proposition 8.** For  $m = 0, 1, \dots$ ,  $(-L)^m = \sum_{k=0}^m \alpha_k Q_{m-k}$  holds, where  $\alpha_0 = 1$ ,

$$\alpha_k = \sum_{(p_1, \dots, p_k): \sum ip_i = k} (-1)^{\sum p_i} \frac{(\sum p_i)!}{\prod (p_i!)} \prod \sigma_i^{p_i}, \quad k = 1, \dots, m, \quad (21)$$

$p_i$  are nonnegative integers, and all sums and products in (21), except for the first sum, range from  $i = 1$  to  $k$ .

A nice property of these linear combinations is that the coefficients  $\alpha_k$  do not depend on  $m$  (similarly to Proposition 6). For instance,

$$\begin{aligned} L &= -(Q_1 - \sigma_1 I), \\ L^2 &= Q_2 - \sigma_1 Q_1 - (\sigma_2 - \sigma_1^2)I, \\ L^3 &= -(Q_3 - \sigma_1 Q_2 - (\sigma_2 - \sigma_1^2)Q_1 - (\sigma_3 - 2\sigma_2 \sigma_1 + \sigma_1^3)I), \\ L^4 &= Q_4 - \sigma_1 Q_3 - (\sigma_2 - \sigma_1^2)Q_2 - (\sigma_3 - 2\sigma_2 \sigma_1 + \sigma_1^3)Q_1 \\ &\quad - (\sigma_4 - 2\sigma_3 \sigma_1 - \sigma_2^2 + 3\sigma_2 \sigma_1^2 - \sigma_1^4)I. \end{aligned}$$

**Proof of Proposition 8.** We first prove, by induction on  $m$ , the identity

$$(-L)^m = \sum_{k=0}^m \alpha'_k Q_{m-k} \quad (22)$$

with  $\alpha'_0 = 1$  and

$$\alpha'_k = \sum_{(\beta(1), \dots, \beta(n_\beta)): \sum \beta(i) = k} \prod (-\sigma_{\beta(i)}), \quad k = 1, \dots, m, \quad (23)$$

where  $\beta(i)$  are positive integers,  $n_\beta$  is the variable number of entries in  $(\beta(1), \dots, \beta(n_\beta))$ , and the unmarked sum and product range from  $i = 1$  to  $n_\beta$ .

For the basis of induction, observe that  $(-L)^0 = I = \alpha'_0 Q_0$ . Let (22)–(23) be valid for  $(-L)^0, \dots, (-L)^{m-1}$ . By Proposition 6,

$$(-L)^m = \alpha'_0 Q_m - \sum_{i=0}^{m-1} \sigma_{m-i} (-L)^i. \quad (24)$$

Substituting (22) in the right-hand side of (24) and interchanging the two sums we obtain:

$$(-L)^m = \alpha'_0 Q_m + \sum_{k=1}^m \alpha_k^{(m)} Q_{m-k},$$

where

$$\alpha_k^{(m)} = \sum_{i=1}^k (-\sigma_i) \alpha'_{k-i}, \quad k = 1, \dots, m.$$

It is easily seen that  $\alpha_k^{(m)} = \alpha'_k$ ,  $k = 1, \dots, m$ , thereby the induction step has succeeded.

Next, for an arbitrary positive integer  $k$ , consider any vector  $(\beta(1), \dots, \beta(n_\beta))$  with positive integer entries such that  $\sum_{i=1}^{n_\beta} \beta(i) = k$  (see (23)). Let  $p_j = |\{i : \beta(i) = j\}|$ ,  $j = 1, \dots, k$ . Classifying the set of vectors  $(\beta(1), \dots, \beta(n_\beta))$  such that  $\sum \beta(i) = k$  by the equality of the corresponding vectors  $(p_1, \dots, p_k)$ , we see that every such a class contains  $(\sum p_i)! / \prod (p_i!)$  members. This implies that  $\alpha_k = \alpha'_k$ ,  $k = 0, 1, \dots$ , (cf. (21) and (23)) and thus, completes the proof.

## 7 The matrix of maximum in-forests

In this section, we study some properties of the normalized matrix  $\tilde{J} = J_{n-d}$  of maximum in-forests. Let  $\mu_\lambda(A)$  stand for the multiplicity of  $\lambda$  as the eigenvalue of a square matrix  $A$ .

- Proposition 9.** (i)  $L\tilde{J} = \tilde{J}L = LQ_{n-d} = Q_{n-d}L = 0$ ;  
(ii)  $\tilde{J}J_k = J_k\tilde{J} = \tilde{J}$ ,  $k = 0, \dots, n-d$ ;  
(iii)  $\tilde{J}$  is a projection:  $\tilde{J}^2 = \tilde{J}$ ;  
(iv)  $\text{rank } \tilde{J} = \mu_1(\tilde{J}) = \text{tr } \tilde{J} = d$ ;  $\mu_0(\tilde{J}) = n-d$ .

**Proof of Proposition 9.** (i) Putting  $k = n-d$  in (17) and using the facts that  $Q_{n-d+1} = 0$  and  $\sigma_{n-d+1} = 0$ , we get  $LQ_{n-d} = 0$ . The other identities follow from Corollary 3 and (9).

(ii) Multiplying (19) by  $\tilde{J}$  and using item (i) and Corollary 3, we get the required statement, whose special case is (iii).

(iv) Each maximum in-forest of  $\Gamma$  has  $d$  roots, hence  $\text{tr } Q_{n-d} = d\sigma_{n-d}$  and  $\text{tr } \tilde{J} = \text{tr}(\sigma_{n-d}^{-1}Q_{n-d}) = d$ . Since  $\tilde{J}$  is idempotent,  $\text{rank } \tilde{J} = \mu_1(\tilde{J}) = \text{tr } \tilde{J}$ , so  $\mu_0(\tilde{J}) = n-d$ .  $\square$

The following connection between the spectra of  $L$  and  $L + \alpha\tilde{J}$ ,  $\alpha \in \mathbb{C}$ , will be used in the sequel.

**Proposition 10.** (i) *The spectrum of  $L + \alpha\tilde{J}$  consists of all nonzero eigenvalues of  $L$  with their multiplicities and  $\alpha$  with  $\mu_\alpha(L + \alpha\tilde{J}) = d$ .* (ii)  $L + \alpha\tilde{J}$  is nonsingular whenever  $\alpha \neq 0$ .

**Proof of Proposition 10.** (i) Let  $p(\lambda) = \sigma_{n-d}^{-1} \sum_{i=0}^{n-d} \sigma_{n-d-i}(-\lambda)^i$ . By Proposition 6,  $\tilde{J} = \sigma_{n-d}^{-1}Q_{n-d} = p(L)$ , so  $L + \alpha\tilde{J} = L + \alpha p(L)$ . Therefore, by [27, Theorem 3 in Chapt. 4], all eigenvalues of  $L + \alpha\tilde{J}$  are  $\lambda'_i = \lambda_i + \alpha p(\lambda_i)$ , where  $\lambda_i$ ,  $i = 1, \dots, n$ , are all eigenvalues of  $L$  with their multiplicities. By (i) of Proposition 9,  $L\tilde{J} = 0 = Lp(L)$ , whence  $\lambda p(\lambda)$  is an annihilating polynomial for  $L$ . Therefore, for each  $\lambda_i$ , a nonzero eigenvalue of  $L$ , we have  $p(\lambda_i) = 0$ , hence  $\lambda'_i = \lambda_i$ . Otherwise, if  $\lambda_i = 0$ , then  $\lambda'_i = \alpha$ , since  $p(0) = 1$  by definition of  $p(\lambda)$ . Finally, by Corollary 1,  $\mu_0(L) = d$ , thus  $\mu_\alpha(L + \alpha\tilde{J}) = d$ . This implies (ii).  $\square$

**Proposition 11.**  $\tilde{J} = \lim_{\tau \rightarrow \infty} J(\tau) = \lim_{\tau \rightarrow \infty} (I + \tau L)^{-1}$ .

**Proof of Proposition 11.** Using Theorem 3' and the definition (12) of  $J(\tau)$ , we have

$$\begin{aligned} \lim_{\tau \rightarrow \infty} (I + \tau L)^{-1} &= \lim_{\tau \rightarrow \infty} J(\tau) = \lim_{\tau \rightarrow \infty} \left( \sum_{k=1}^{n-d} \sigma_k \tau^k \right)^{-1} \sum_{k=1}^{n-d} Q_k \tau^k \\ &= \lim_{\tau \rightarrow \infty} \left( \sum_{k=1}^{n-d} \sigma_k \tau^{k-n-d} \right)^{-1} \sum_{k=1}^{n-d} Q_k \tau^{k-n-d} = \sigma_{n-d}^{-1} Q_{n-d} = \tilde{J}. \end{aligned}$$

## 8 $L$ and $\tilde{J}$ as “complementary” linear transformations

For a complex matrix  $A$ , let  $\mathcal{R}(A)$  and  $\mathcal{N}(A)$  denote its range and null space, respectively. Recall that the *index* of a square matrix  $A$ ,  $\text{ind } A$ , is the smallest nonnegative integer  $k$  for which  $\text{rank}(A^{k+1}) = \text{rank}(A^k)$ . The *eigenprojection*<sup>3</sup> at 0 of  $A$  [57] or, for short, the *eigenprojection of  $A$*  [58] is the idempotent matrix  $B$  such that  $\mathcal{R}(B) = \mathcal{N}(A^\nu)$  and  $\mathcal{N}(B) = \mathcal{R}(A^\nu)$ , where  $\nu = \text{ind } A$ . In other words,  $B$  is the projection on  $\mathcal{N}(A^\nu)$  along  $\mathcal{R}(A^\nu)$ . The eigenprojection is unique, because an idempotent matrix is uniquely determined by its range and null space (see, e.g., [6, p. 50]).<sup>4</sup>

Since  $L\tilde{J} = 0$  (Proposition 9), we have  $\mathcal{R}(L^*) \cap \mathcal{R}(\tilde{J}) = \{\mathbf{0}\}$ , where  $L^* = L^T$ . Similarly,  $\tilde{J}L = 0$  implies  $\mathcal{R}(\tilde{J}^*) \cap \mathcal{R}(L) = \{\mathbf{0}\}$ . Consequently, by [44, Theorem 11],  $L$  and  $\tilde{J}^*$  are *rank additive*, i.e.,  $\text{rank}(L + \tilde{J}^*) = \text{rank } L + \text{rank } \tilde{J}^*$ . Corollary 1 implies that  $\text{rank } L \geq n - d$ , whereas, by Proposition 9,  $\text{rank } \tilde{J}^* = d$ . Since  $\text{rank}(L + \tilde{J}^*) \leq n$ , we have  $\text{rank } L = n - d$  and  $\text{rank}(L + \tilde{J}^*) = n$ . Now  $L\tilde{J} = \tilde{J}L = 0$  implies  $\mathcal{N}(L) = \mathcal{R}(\tilde{J})$  and  $\mathcal{N}(\tilde{J}) = \mathcal{R}(L)$ . Furthermore, by Proposition 10,  $\text{rank}(L + \tilde{J}) = n$ , hence  $L$  and  $\tilde{J}$  are rank additive. It follows now from [44, Theorem 11] that  $\mathcal{R}(L) \cap \mathcal{R}(\tilde{J}) = \{\mathbf{0}\}$ . Since  $\mathcal{R}(\tilde{J}) = \mathcal{N}(L)$ , we get  $\mathcal{R}(L) \cap \mathcal{N}(L) = \{\mathbf{0}\}$ , which, by [6, p. 165], implies  $\text{ind } L = 1$ . The latter fact together with  $\mathcal{R}(\tilde{J}) = \mathcal{N}(L)$ ,  $\mathcal{N}(\tilde{J}) = \mathcal{R}(L)$ , and  $\tilde{J}^2 = \tilde{J}$  imply that  $\tilde{J}$  is the eigenprojection of  $L$  (alternatively, this follows from Proposition 11 and [48, Theorem 3.1]). We proved

**Proposition 12.** (i)  $L + \tilde{J}^*$  is nonsingular.

(ii)  $\text{rank } L = n - \text{rank } \tilde{J} = n - d$ .

(iii)  $\mathcal{N}(L) = \mathcal{R}(\tilde{J})$  and  $\mathcal{R}(L) = \mathcal{N}(\tilde{J})$ .

(iv)  $\mathcal{R}(L) \cap \mathcal{R}(\tilde{J}) = \{\mathbf{0}\}$ .

(v)  $\text{ind } L = 1$ .

(vi)  $\tilde{J}$  is the eigenprojection of  $L$ .

It is known [57, p. 194], [59, Theorem 7.a.3] that for every finite homogeneous Markov chain with a transition matrix  $P$ , the *long run transition matrix*  $P^\infty = \lim_{k \rightarrow \infty} \frac{1}{k} \sum_{t=0}^{k-1} P^t$  is the eigenprojection of  $P$  at 1, which is the eigenprojection of  $I - P$ .<sup>5</sup> On the other hand,  $I - P$  is exactly the Laplacian matrix  $L$  of the weighted digraph without loops whose arc weights are equal to the corresponding transition probabilities. Therefore  $\tilde{J}$ , the eigenprojection of  $L$ , coincides with  $P^\infty$ . The fact that  $P^\infty$  coincides with the normalized matrix of maximum

<sup>3</sup>The eigenprojections are also called *principal idempotents* [66, 32].

<sup>4</sup>Note that for every  $A \in \mathbb{C}^{n \times n}$  s.t.  $\text{ind } A = \nu$  and every idempotent matrix  $B$ , each of the following conditions is equivalent to  $B$  being the eigenprojection of  $A$ :

(i)  $\mathcal{R}(B) = \mathcal{N}(A^\nu)$  and  $\mathcal{R}(B^*) = \mathcal{N}((A^*)^\nu)$  [57];

(ii)  $A^\nu B = BA^\nu = 0$  and  $\text{rank } A^\nu + \text{rank } B = n$  [67, 69].

(iii)  $AB = BA$  and  $A + \alpha B$  is nonsingular for all  $\alpha \neq 0$  [41] (cf. (ii) of Proposition 10);

(iv)  $AB = BA$ ,  $A + \alpha B$  is nonsingular for some  $\alpha \neq 0$ , and  $AB$  is nilpotent [41];

(v)  $AB = BA$ ,  $AB$  is nilpotent, and  $AU = I - B = VA$  for some  $U, V \in \mathbb{C}^{n \times n}$  [31];

(vi)  $B$  commutes with all matrices commuting with  $A$ ,  $AB$  is nilpotent, and  $B \neq 0$  if  $A$  is singular [40];

Moreover, the eigenprojection of  $A$  is  $I - AA^D$ , where  $A^D$  is the Drazin inverse of  $A$  (see Section 9).

<sup>5</sup>This also follows from Meyer’s Theorem 2.2 in [49]. Indeed, by this theorem,  $P^\infty = I - (I - P)(I - P)^\#$ , where  $(I - P)^\#$  is the group inverse of  $I - P$ , and the right-hand side is the eigenprojection of  $I - P$ , as mentioned in the next section.

in-forests of the digraph corresponding to a Markov chain is the so called *Markov chain tree theorem* [42, 43]. Thus, item (vi) of Proposition 12 provides an immediate proof of this theorem.

By virtue of Proposition 9, every nonzero column of  $\tilde{J}$  (or  $Q_{n-d}$ ) is an eigenvector of  $L$  that corresponds to the zero eigenvalue. Moreover, it follows from  $\mathcal{N}(L) = \mathcal{R}(\tilde{J})$  (Proposition 12) that the nonzero columns of  $\tilde{J}$  span the null space of  $L$ . Since, by (16),  $Q(\tau)$  is proportional to  $\text{adj}(\lambda I - (-L))$  at  $\lambda = \tau^{-1}$ ,  $Q(\tau)$  can be used to generate some eigenvectors of  $L$  that correspond to its nonzero eigenvalues. For completeness, we give a proof of this fact.

**Proposition 13.** *Let  $\lambda_i \neq 0$  be an eigenvalue of  $L$ . Then every nonzero column of  $Q(-\lambda_i^{-1})$  is an eigenvector of  $L$  that corresponds to  $\lambda_i$ .*

**Proof of Proposition 13.** Let  $X = \lambda_i I - L$ . Then  $\det X = 0$ . Using Theorem 3' and the fact that for every square matrix  $Y$ ,  $Y \text{adj} Y = (\det Y)I$  holds, we get

$$(\lambda_i I - L) Q(-\lambda_i^{-1}) = X \text{adj}(I - \lambda_i^{-1} L) = \lambda_i^{1-n} X \text{adj} X = \lambda_i^{1-n} (\det X) I = 0.$$

This implies the desired statement.

## 9 Forest matrices and generalized inverses of $L$

The *Moore-Penrose generalized inverse*  $A^+$  of a rectangular complex matrix  $A$  is the unique matrix  $X$  such that

$$AXA = A, \quad XAX = X, \quad (AX)^* = AX, \quad (XA)^* = XA.$$

For an arbitrary square matrix  $A$ , its *Drazin inverse*,  $A^D$ , is the unique matrix  $X$  satisfying the equations

$$A^{\nu+1} X = A^\nu, \quad XAX = X, \quad AX = XA,$$

where  $\nu = \text{ind } A$ . If  $\nu = 0$ , then  $A^D = A^{-1}$ ; if  $\nu \leq 1$ , then  $A^D$  is referred to as the *group inverse*,  $A^\#$ , i.e., the unique matrix  $X$  such that

$$AXA = A, \quad XAX = X, \quad AX = XA.$$

As applied to the Laplacian matrices of graphs, the generalized inverses were considered in connection with the analysis of electrical networks (providing “resistance distance”), Markov chains, and some preference aggregation problems (more specifically, estimation from paired comparisons), in constructing geometrical representations of graphs (with applications to chemistry, social networks, etc.), in control, cluster analysis, and parallel computing. There is a huge literature on generalized inverses within the last years. For multiple representations of the Drazin inverse, see, e.g., [68, 19, 18].

In this section, we present a few relations between the  $L^\#$  and the forest matrices and one representation for  $L^+$ . In the case of symmetric  $L$ , where  $L^\# = L^+$ , some of these expressions are given in [16].<sup>6</sup>

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<sup>6</sup>For symmetric  $L$ , interesting representations for  $L^\# = L^+$  were proposed in [24], [39, Theorem 2.2], and, in case of weighted trees, in [39] and [3, Theorem 3]. In [22, Theorem 3] a combinatorial interpretation of the Campbell-Youla inverse (the symmetric generalized inverse with the zero diagonal) of  $L$  is given.

For an arbitrary square matrix  $A$ ,  $AA^D$  is the unique projection on  $\mathcal{R}(A^\nu)$  along  $\mathcal{N}(A^\nu)$  [6, p. 173]. Then  $I - AA^D$  is the projection on  $\mathcal{N}(A^\nu)$  along  $\mathcal{R}(A^\nu)$ . Therefore,  $I - AA^D$  is the eigenprojection of  $A$  [57, 58]. Combining this with items (v) and (iv) of Proposition 12, we obtain

**Proposition 14.**  $\tilde{J} = I - LL^\#$ .

The fact that  $\tilde{J}$  is the eigenprojection of  $L$  helps interpret, in terms of in-forests, the expressions of generalized inverses of  $L$  that involve the eigenprojection of  $L$ .

**Proposition 15.**

- (i) For any  $\alpha \neq 0$ ,  $L^\# = (L + \alpha\tilde{J})^{-1} - \alpha^{-1}\tilde{J}$ , whence  $L^\# = \lim_{|\alpha| \rightarrow \infty} (L + \alpha\tilde{J})^{-1}$ .
- (ii) For any  $\alpha \neq 0$ ,  $L^\# = (L + \alpha\tilde{J})^{-1}(I - \tilde{J})$ .
- (iii)  $L^\# = \frac{\sigma_{n-d-1}}{\sigma_{n-d}} (J_{n-d-1} - \tilde{J})$ .
- (iv)  $L^\# = \lim_{\tau \rightarrow \infty} \tau (J(\tau) - \tilde{J})$ .

**Remarks on Proposition 15.** (i), (iii), and (iv) were presented in [2]. (i) results by substituting  $\tilde{J}$  for the eigenprojection in the expression of group inverse employed in [50, p. 150] (for its proof see [60, Theorem 4.2]; related expressions appeared in [49, Theorem 5.5] and [58, last line on p. 646], where ‘+’ must be replaced by ‘-’). (ii) is obtained by the same substitution in the representation of Drazin inverse given in [40] (the case with  $\alpha = 1$  appeared in [58]) or by multiplying (i) by  $LL^\# = I - \tilde{J}$ . In view of Propositions 2 and 3, (iii) follows from the expression of Drazin inverse discovered independently by Hartwig [32, Eq. (13)] and Gower [29, Theorem 1].

The matrices  $L + \alpha\tilde{J}$  are the “complementary perturbations” [50] of  $L$ . Matrices of this kind are important for the analysis of M-matrices and singular systems of equations. In particular, a matrix  $A$  with eigenprojection  $B$  and nonpositive off-diagonal entries is an M-matrix if and only if for some  $c > 0$ ,  $(A + \alpha B)^{-1}$  is nonnegative when  $\alpha \in (0, c)$  [50]. If  $A$  is an M-matrix, then  $(A + \alpha B)^{-1}$ ,  $\alpha \in (0, c)$ , make up a class of *nonnegative nonsingular commuting weak inverses* for  $A$  [50].  $(L + \alpha\tilde{J})^{-1}$  can be represented as a linear combination of forest matrices using (i) and (iii) of Proposition 15:

$$(L + \alpha\tilde{J})^{-1} = \frac{\sigma_{n-d-1}}{\sigma_{n-d}} (J_{n-d-1} + \beta\tilde{J}),$$

where  $\beta = \frac{\sigma_{n-d}}{\alpha\sigma_{n-d-1}} - 1$ . This throws some light on the nonnegativity of  $(L + \alpha\tilde{J})^{-1}$ : if  $\alpha \in (0, \frac{\sigma_{n-d}}{\sigma_{n-d-1}})$  then  $(L + \alpha\tilde{J})^{-1}$  is a positive combination of  $J_{n-d-1}$  and  $\tilde{J}$ . Based on this, we termed  $(L + \alpha\tilde{J})^{-1}$  the *matrices of dense in-forests* of  $\Gamma$ . These and the inverse “uniform diagonal perturbations”  $(L + \alpha I)^{-1}$  can serve to measure proximity between digraph vertices [2]. Note in this connection that by [60, Corollary 4.4],  $(L + \alpha\tilde{J})_{ij}^{-1} > 0$  for all  $\alpha > 0$  sufficiently small if and only if vertex  $j$  is accessible from  $i$  in  $\Gamma$ , and the same is true for  $(L + \alpha I)_{ij}^{-1}$ . By Theorem 3',  $(L + \alpha I)^{-1}$  is proportional to  $J(\tau)$  with  $\tau = 1/\alpha$ .

We conclude with one expression for the Moore-Penrose inverse of  $L$ .

Consider the matrix  $Z := L + \tilde{J}^*$  which is nonsingular by Proposition 12. Using the identity  $L\tilde{J} = 0$  (Proposition 9), we get  $(Z^*)^{-1}Z^{-1} = (ZZ^*)^{-1} = (\tilde{J}^*\tilde{J} + LL^*)^{-1}$ .

**Proposition 16** [2].  $L^+ = L^*(ZZ^*)^{-1} = L^*(\tilde{J}^*\tilde{J} + LL^*)^{-1}$ .

One method to prove this is to check the conditions in the definition of Moore-Penrose inverse by direct computation using Proposition 9 and the facts that  $(ZZ^*)^{-1}$  commutes with  $LL^*$  and  $\tilde{J}^*\tilde{J}$  and that  $LL^*(ZZ^*)^{-1}$  and  $\tilde{J}^*\tilde{J}(ZZ^*)^{-1}$  are symmetric [2]. Alternatively, Proposition 16 can be proved by employing the Penrose formula  $A^+ = A^*(AA^*)^+$ , the fact that  $(AA^*)^+ = (AA^*)^\#$  (since  $AA^*$  is Hermitian) and an expression of  $(AA^*)^\#$  such as those given in (i) and (ii) of Proposition 15.

## 10 A concluding remark

It is instructive to compare the ‘‘Laplacian graph mathematics’’ we touched upon in this paper with the corresponding results on the adjacency characteristic matrix, see, e.g., [21, Sections 1.4, 1.9.1, 1.9.5 and others] and the articles by Kasteleyn and Ponstein cited therein, [61], and so on. This comparison suggests that the Laplacian mathematics is based on trees in the same sense as the ‘‘adjacency graph mathematics’’ is based on routes and circuits. We mean that a number of expressions related with the adjacency characteristic matrix can be interpreted in terms of routes and circuits, whereas the counterparts of these expressions related with the Laplacian characteristic matrix involve spanning forests for their interpretation.

## Acknowledgements

This work was supported in part by the Russian Foundation for Basic Research under grants 01–01–10732-z and 02–01–00614-a. The authors thank a referee for a careful reading of the paper and many thoughtful suggestions.

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