Random-walk computation of similarities between nodes of a graph, with application to collaborative recommendation

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Abstract

This work presents a new perspective on characterizing the similarity between elements of a database or, more generally, nodes of a weighted and undirected graph. It is based on a Markov-chain model of random walk through the database. More precisely, we compute quantities (the **average commute time**, the **pseudoinverse of the Laplacian matrix** of the graph, etc) that provide similarities between any pair of nodes, having the nice property of increasing when the number of paths connecting those elements increases and when the "length" of paths decreases. It turns out that the square root of the average commute time is a Euclidean distance and that the pseudoinverse of the Laplacian matrix is a kernel (its elements are inner products closely related to commute times). A procedure for computing the subspace projection of the node vectors of the graph that preserves as much variance as possible in terms of the commute-time distance – a principal component analysis (PCA) of the graph – is also introduced. This graph PCA provides a nice interpretation to the "**Fiedler vector**", widely used for graph partitioning. The model is evaluated on a collaborative-recommendation task where suggestions are made about which movies people should watch based upon what they watched in the past. Experimental results on the MovieLens database show that the Laplacian-based similarities perform well in comparison with other methods. The model, which nicely fits into the so-called "statistical relational learning" framework, could also be used to compute document or word similarities, and, more generally, it could be applied to machine-learning and pattern-recognition tasks involving a database.

1 Introduction

Exploiting the graph structure of large repositories, such as digital documents repositories, the web environment, or large databases in general, is relevant to many areas of computer science. For instance, Kleinberg's suggestion to

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emphasize web pages that are hubs and authorities (see [41]; called the HITS algorithm) has been well received in the community (for a review, see [4]).

This work views a database as a collection of element sets connected by relationships. The model exploits the graph structure of the database to compute a similarity measure between elements (the work could have been presented as computing dissimilarities instead, and the word "proximities" used as a substitute for either). All the developments in this paper are valid in general for computing similarities between nodes of a **weighted** and **undirected graph**.

Computing similarities between pairs of elements allows, for instance, to determine the item that is most relevant (or similar) to a given item. Also, elements in a set can be assigned a category provided by elements from another set. Computing similarities between elements of the same set amounts to a clustering task.

For example, imagine a simple movie database with three sets of elements `people`, `movie`, and `movie_category`, and two relationships `has_watched`, between `people` and `movie`, and `belongs_to`, between `movie` and `movie_category`.

- Computing similarities between people allows to cluster them into groups with similar interest about watched movies.

- Computing similarities between people and movies allows to suggest movies to watch or not to watch.

- Computing similarities between people and movie categories allows to attach a most relevant category to each person.

The procedure used to compute similarities is based on a Markov-chain model. We define a **random walk** through the database by assigning a transition probability to each link. Thus, a random walker can jump from element to element and each element therefore represents a state of the Markov chain. The **average first-passage time** $m(k|i)$ (see, e.g., [39]) is the average number of steps needed by a random walker for reaching state k for the first time, when starting from state i. The symmetrized quantity $n(i,j) = m(j|i) + m(i|j)$, called the **average commute time** (see, e.g., [26]), provides a distance measure between any pair of states. The fact that this quantity is indeed a distance on a graph was proved independently by Klein & Randic [40] and Gobel & Jagers [26].

We will see later that $[n(i,j)]^{1/2}$, which is also a distance between nodes, takes a remarkable form; it will be called the **Euclidean Commute Time Distance** (ECTD). We also introduce the **average first-passage cost** $o(k|i)$ which generalizes the average first-passage time by assigning a cost to each transition.

Another quantity of interest, closely related to the ECTD is the **pseudoinverse of the Laplacian matrix** of the graph ($\mathbf{L}^+$). The elements of $\mathbf{L}^+$ are the inner products of the node vectors in a Euclidean space preserving the ECTD (i.e., a Euclidean space where the nodes are exactly separated by ECTD). $\mathbf{L}^+$

therefore provides a similarity measure between nodes and it is a valid kernel (a Gram matrix, see, e.g., [57]).

All these quantities have the nice property of decreasing (or increasing, depending on whether the quantity is a dissimilarity or a similarity measure) when the number of paths connecting two elements increases and when the "length" of any path decreases (communication is facilitated). In short, two elements are considered similar if there are many short paths connecting them. The "shortest path" or "geodesic" distance does not have the nice property of decreasing when connections between nodes are added: it does not capture the fact that strongly connected nodes are at a smaller distance than weakly connected ones. With a few notable exceptions (see the related work below), while being interesting alternatives to the well-known "shortest-path" distance on a graph [11], those quantities have not yet been fully exploited in the context of collaborative recommendation or, more generally, in pattern recognition and machine learning. This fact has, however, already been recognized in the field of mathematical chemistry where there were attempts to use the "commute-time" distance instead of the "shortest-path" distance [40].

This paper is an extended and improved follow-up of two previously published papers: [55, 25]. The former introduces our theoretical model based on a random-walk model while the latter presents preliminary experimental results obtained on the collaborative-recommendation task. The present paper contains proofs of the main results, a discussion of computational issues, and an account of substantially expanded experiments.

1.1 Some related work

Chebotarev & Shamis already proposed in [15] and [17] a similarity measure between nodes of a graph integrating indirect paths, based on the matrix-forest theorem. Interestingly, this quantity is also related to the Laplacian matrix of the graph. While the authors prove some nice properties about their similarity measure, no experiment investigating its effectiveness was performed. We will therefore investigate this matrix-forest based measure, together with other quantities, in Section 6.

Some authors recently considered similarity measures based on random-walk models. For instance, Harel & Koren [29] investigated the possibility of clustering data according to some random-walk related quantities, such as the probability of visiting a node before returning to the starting node. They showed that their algorithm is able to cluster arbitrary nonconvex shapes. White & Smyth [63], independently of our work, investigated the use of the average first-passage time as a similarity measure between nodes. Their purpose was to generalize the random-walk approach of Page et al. [48] by capturing a concept of "relative centrality" of a given node with respect to some other node of interest.

More recently, Newman [45] suggested a random-walk model to compute a "betweenness centrality" of a given node in a graph. This counts how often a node is traversed during a random walk between two other nodes. Then, this quantity is averaged over every pair of nodes, providing a general measure of betweenness [62] associated to each node.

3

Still another approach has been investigated by Faloutsos et al. [23] who extract the "most relevant" connected subgraph relating two nodes of interest, using a method based on electrical flows. In addition, Palmer & Faloutsos [49] define a similarity function between categorical attributes, called "refined escape probability", based on random walks and electrical networks. They show that this quantity provides a reasonably good measure for clustering and classifying categorical attributes. In a recent paper [44], Nadler et al. proposed a similarity measure between nodes of a graph based on a continuous-time diffusion process. They show that there are some interesting links between their model and our approach. We derived the discrete-time counterpart of their model and we are currently investigating its performance.

Very recently, Brand [10] proposed various quantities derived from the commute time for collaborative recommendation. He shows, as we do, that angular-based quantities perform much better than the commute time because the latter is quite sensible to the node degree. Their conclusions confirm our experimental results, as will be shown in Section 6.

Our approach based on a random-walk model on a graph is closely related to spectral-clustering and spectral-embedding techniques (for a recent account, see [20]), as detailed in [55]. Random-walk models on a graph also proved useful in the context of learning from labeled and unlabeled data (see, e.g., [64]).

1.2 Main contributions

In addition to suggesting quantities for computing similarities between nodes of a graph, this paper has four main contributions, three more theoretical and one more experimental:

1. We show that all the introduced quantities can be expressed in closed form in terms of the pseudoinverse of the Laplacian matrix of the graph. This generalizes results obtained by Klein & Randic [40], derived for the ECTD only, based on the electrical equivalence. Since the pseudoinverse of the Laplacian matrix plays a key role and has a nice interpretation in terms of random walk on a graph, we prove some of its properties.

2. We show that the pseudoinverse of the Laplacian matrix of the graph is a valid kernel (a Gram matrix; see for instance [57]). It therefore defines a kernel on a graph and can be interpreted as a similarity measure.

3. We show that the node space of the graph can be projected into a Euclidean subspace that approximately preserves the ECTD. This subspace is optimal in the following sense: it keeps as much variance of the projected data as possible (in terms of the ECTD). It is therefore an equivalent of principal components analysis (PCA) and classical multidimensional scaling (MDS), in terms of the ECTD. This provides a nice interpretation to the "Fiedler vector", widely used in graph partitioning.We also show that the ECTD PCA can be viewed as a special regularized Laplacian kernel, as introduced by Smola & Kondor [61].

4. From an experimental point of view, we show that these quantities can be used in the context of collaborative recommendation [18, 30, 33]. Indeed,

all the introduced concepts are illustrated on a collaborative-recommendation task where movies are suggested for people to watch from a database of previously watched movies. In particular the inner-product based quantities involving the Laplacian matrix provide good and stable results. We suggest that the same model could be used to compute document or word similarities, and, more generally, be applied to other pattern-recognition and machine-learning tasks involving a database.

We stress that our objective here is not to develop a state-of-the-art collaborative-recommendation system; rather, the application to collaborative recommendation aims to illustrate the interest of Markov-based similarity measures to nontrivial database-mining tasks. This approach fits quite naturally into the so-called "multi-relational data mining" and the "statistical relational learning" frameworks (see for instance [22] and other papers in the same issue of the SIGKDD newsletter).

1.3 Outline of the paper

The paper is structured as follows. Section 2 introduces the random-walk model. Section 3 develops our similarity measures as well as the iterative formulae to compute them. Section 4 shows how the average first-passage time, the average first-passage cost, and the average commute time can be computed in closed form from the pseudoinverse of the Laplacian matrix of the graph. Section 5 introduces a subspace projection of the nodes of the graph that maximizes the variance of the projected data. Section 6 specifies our experimental methodology and illustrates the concepts with experimental results obtained on the MovieLens database. Section 7 is the conclusion.

2   A Markov-chain model of database navigation

A weighted graph G is associated with a database in the following obvious way: database elements correspond to nodes of the graph and database links correspond to edges. In our movie example, each element of the `people`, `movie`, and `movie_category` sets corresponds to a node of the graph, and each `has_watched` and `belongs_to` link is expressed as an edge.

The weight w_{ij} of the edge connecting node i and node j should be set to some meaningful value, with the following convention: the more important the relation between node i and node j, the larger the value of w_{ij}, and consequently the easier the communication through the edge. We require the weights to be both positive ($w_{ij} > 0$) and symmetric ($w_{ij} = w_{ji}$). For instance, for an `has_watched` edge, the weight could be set to the number of times that the person watched the corresponding movie. The elements a_{ij} of the symmetric adjacency matrix $\mathbf{A}$ of the graph are defined as usual as: $a_{ij} = w_{ij}$ if node i is connected to node j and $a_{ij} = 0$ otherwise.

Thus, people who watch the same kind of movies, and therefore have similar taste, will be connected by a comparatively larger number of short paths. On the contrary, for people with different interests, there will be fewer paths connecting them and these paths will be longer.

The Markov chain describing the sequence of nodes visited by a random walker is called a random walk. A random variable $s(t)$ contains the current state of the Markov chain at time t: if the random walker is in state i at time t, then $s(t) = i$. The random walk is defined with the following single-step transition probabilities of jumping from any state or node $i = s(t)$ to an adjacent node $j = s(t+1)$: $\mathrm{P}(s(t+1) = j | s(t) = i) = a_{ij}/a_{i.} = p_{ij}$, where $a_{i.} = \sum_{j=1}^{n} a_{ij}$.

The transition probabilities depend only on the current state and not on the past ones (first-order Markov chain). Since the graph is connected, the Markov chain is irreducible, that is, every state can be reached from any other state. If this is not the case, the Markov chain can be decomposed into closed subsets of states which are independent (there is no communication between them), each closed subset being irreducible, and the procedure can be applied independently on these closed subsets.

If we denote the probability of being in state i at time t by $\pi_i(t) = \mathrm{P}(s(t) = i)$ and we define $\mathbf{P}$ as the transition matrix with entries $p_{ij} = \mathrm{P}(s(t+1) = j | s(t) = i)$, the evolution of the Markov chain is characterized by $\boldsymbol{\pi}(t+1) = \mathbf{P}^{\mathrm{T}}\boldsymbol{\pi}(t)$, with $\boldsymbol{\pi}(0) = \boldsymbol{\pi}^0$ and where T is the matrix transpose. This provides the state probability distribution $\boldsymbol{\pi}(t) = [\pi_1(t), \pi_2(t), ..., \pi_n(t)]^{\mathrm{T}}$ at time t once the initial distribution $\boldsymbol{\pi}^0$ is known. For more details on Markov chains, the reader is invited to consult standard textbooks (e.g., [39, 47]).

3 Average first-passage time/cost and average commute time

This section reviews two basic quantities that can be computed from the definition of the Markov chain, that is, from its transition probability matrix: the average first-passage time and the average commute time. We also introduce the average first-passage cost which generalizes the average first-passage time. Relationships allowing to compute these quantities are just introduced without proof (see, e.g., [39] or [47] for a more formal treatment).

The **average first-passage time** $m(k|i)$ is defined as the average number of steps that a random walker, starting in state $i \neq k$, will take to enter state k for the first time [47]. More precisely, we define the minimum time until hitting state k, when starting from state i, as $T_{ik} = \min{(t \geq 0 \mid s(t) = k \text{ and } s(0) = i)}$ for one realization of the stochastic process. The random walker will pass through k repeatedly; the minimum time corresponds to its first passage. The average first-passage time is the expectation of this quantity: $m(k|i) = E[T_{ik}|s(0) = i]$.

In a similar way, the **average first-passage cost** $o(k|i)$ is the average cost incurred by the random walker starting from state i to reach state k for the first time. The cost of each transition is given by $c(j|i)$ for any states i, j. Notice that $m(k|i)$ is a special case of $o(k|i)$ obtained when $c(j|i) = 1$ for all i, j.

The recurrence relations for computing $m(k|i)$ and $o(k|i)$ can easily be ob-

tained by first-step analysis [39, 47, 54]:

$$\begin{cases} m(k|k) = 0 \\ m(k|i) = 1 + \sum_{j=1}^{n} p_{ij}\, m(k|j), \text{ for } i \neq k \end{cases} \quad (1)$$

$$\begin{cases} o(k|k) = 0 \\ o(k|i) = \sum_{j=1}^{n} p_{ij}\, c(j|i) + \sum_{j=1}^{n} p_{ij}\, o(k|j), \text{ for } i \neq k \end{cases} \quad (2)$$

These formulae are quite obvious: to go from state i to state k, first go to any adjacent state j and proceed from there. These quantities can be computed by iterating these recurrence relations, by using some dedicated algorithms developed in the Markov-chain community (see for instance [39]), or by using the pseudoinverse of the Laplacian matrix of the graph, as shown in this paper (see Section 4).

A closely related quantity, the **average commute time** $n(i,j)$ is defined as the average number of steps that a random walker, starting in state $i \neq j$, will take to enter state j for the first time and go back to i. That is, $n(i,j) = m(j|i) + m(i|j)$. Notice that, while $n(i,j)$ is symmetric by definition, $m(i|j)$ is not.

As shown by [26, 40], the average commute time is a distance measure since, for any states i, j, k: (1) $n(i,j) \geq 0$, (2) $n(i,j) = 0$ if and only if $i = j$, (3) $n(i,j) = n(j,i)$, and (4) $n(i,j) \leq n(i,k) + n(k,j)$. It will be referred to as the "**commute-time distance**". Because of a close relationship between the random-walk model and electrical networks theory, this distance is also called "**resistance distance**". Indeed, $n(i,j)$ is proportional to the effective resistance between node i and node j of the corresponding network, where a resistance w_{ij}^{-1} is assigned to each edge. We will show in Section 4 that $[n(i,j)]^{1/2}$, which is also a distance on the graph, takes a remarkable form.

As already mentioned, the commute-time distance between two points has the desirable property of decreasing when the number of paths connecting the two points increases and when the length of paths decreases (see [21] for a proof based on electrical networks theory). This is indeed an intuitively satisfying property of the effective resistance of the equivalent electrical network [14, 21]. The usual **shortest-path distance** (also called geodesic distance) does not have this property: the shortest-path distance does not capture the fact that strongly connected nodes are closer than weakly connected nodes.

Methods for computing the quantities defined above are based on algorithms introduced in the Markov-chain community or on iterative procedures (Equation (1)). For instance, Kemeny & Snell proposed a general method in the appendix of their book [39] (see also [34] or [50]).

4 Computation of the basic quantities with $\mathbf{L}^+$

In this section, we show how formulae for computing the average first-passage time, the average first-passage cost, and the average commute time can be derived from Equations (1) and (2), by using the Moore-Penrose pseudoinverse of the Laplacian matrix of the graph ($\mathbf{L}^+$), which plays a fundamental role and has a number of interesting properties. The developments in this section are inspired by the work of Klein & Randic [40] who proved, based on the electrical equivalence, that the effective resistance (equivalent to the average commute time) can be computed from the Laplacian matrix. We extend their results by showing how the formula computing the average commute time in terms of $\mathbf{L}^+$ can be directly derived from Equation (1), and by providing formulae for the average first-passage time and the average first-passage cost.

4.1 The pseudoinverse of the Laplacian matrix

The symmetric Laplacian matrix $\mathbf{L}$ of the graph is defined in the usual manner, $\mathbf{L} = \mathbf{D} - \mathbf{A}$, where $\mathbf{D} = \mathrm{diag}(a_{i\cdot})$ with $d_{ii} = [\mathbf{D}]_{ii} = a_{i\cdot} = \sum_{j=1}^{n} a_{ij}$, if there are n nodes in total. We suppose that the graph is connected, that is, any node can be reached from any other node. In this case, $\mathbf{L}$ has rank $n - 1$ [19]. If $\mathbf{e}$ is a column vector made of 1's (i.e., $\mathbf{e} = [1, 1, ..., 1]^{\mathrm{T}}$, where T denotes the matrix transpose) and $\mathbf{0}$ is a column vector made of 0's, $\mathbf{Le} = \mathbf{0}$ and $\mathbf{e}^{\mathrm{T}}\mathbf{L} = \mathbf{0}^{\mathrm{T}}$ hold: $\mathbf{L}$ is doubly centered. The null space of $\mathbf{L}$ is therefore the one-dimensional space spanned by $\mathbf{e}$. Moreover, one can easily show that $\mathbf{L}$ is symmetric and positive semidefinite (see for instance [19]).

The **Moore-Penrose pseudoinverse** of $\mathbf{L}$ (see for instance [5]) will be denoted by $\mathbf{L}^+$, with elements $l_{ij}^+ = [\mathbf{L}^+]_{ij}$. The concept of pseudoinverse generalizes the matrix inverse to matrices that are not of full rank or not square. It provides closed-form solutions to systems of linear equations for which there is no exact solution (in which case it provides a solution in the least-square sense) or when there is an infinity of solutions (in which case it provides the solution closest to the origin). A thorough treatment of matrix pseudoinverses and their applications can be found in [8].

Appendix A reviews some useful properties of $\mathbf{L}^+$, in particular, that: (1) $\mathbf{L}^+$ is symmetric, (2) if ($\lambda_i \neq 0, \mathbf{u}_i$) are (eigenvalues, eigenvectors) of $\mathbf{L}$, then ($\lambda_i^{-1} \neq 0, \mathbf{u}_i$) are corresponding (eigenvalues, eigenvectors) of $\mathbf{L}^+$; if ($\lambda_j = 0, \mathbf{u}_j$) are (eigenvalues, eigenvectors) of $\mathbf{L}$, then they are also (eigenvalues, eigenvectors) of $\mathbf{L}^+$, (3) $\mathbf{L}^+$ is doubly centered, and (4) $\mathbf{L}^+$ is positive semidefinite. Moreover it can be shown that $\mathbf{L}^+$ can be computed with the following formula (see [52], chapter 10):

$$\mathbf{L}^+ = \left(\mathbf{L} - \frac{\mathbf{ee}^{\mathrm{T}}}{n}\right)^{-1} + \frac{\mathbf{ee}^{\mathrm{T}}}{n} \tag{3}$$

where n is the number of nodes.

4.2 The average first-passage time/cost and average commute time

Appendix B shows that the average first-passage time and the average first-passage cost can be computed in terms of $\mathbf{L}^+$ from Equations (1) and (2). A similar formula (see Appendix C) is derived for the average commute time, which is repeated here:

$$n(i,j) = V_G \left(l_{ii}^+ + l_{jj}^+ - 2l_{ij}^+ \right) \qquad (4)$$

where V_G is the volume of the graph ($V_G = \sum_{k=1}^n d_{kk}$). This formula was also obtained by using the electrical equivalent of the average commute time (the effective resistance) in [40]; see also [54].

If we define $\mathbf{e}_i$ as the ith column of $\mathbf{I}$, $\mathbf{e}_i = [\underset{1}{0}, ..., \underset{i-1}{0}, \underset{i}{1}, \underset{i+1}{0}, ..., \underset{n}{0}]^{\mathrm{T}}$, Equation (4) takes the remarkable form:

$$n(i,j) = V_G \left(\mathbf{e}_i - \mathbf{e}_j \right)^{\mathrm{T}} \mathbf{L}^+ (\mathbf{e}_i - \mathbf{e}_j) \qquad (5)$$

where each node i is *represented by a unit vector* $\mathbf{e}_i$ (a **node vector**) in the node space (the space spanned by $\{\mathbf{e}_i\}$).

We observe that $[n(i,j)]^{1/2}$ is a **distance** in the Euclidean space spanned by the node vectors of the graph since $\mathbf{L}^+$ is positive semidefinite. It will therefore be called the **Euclidean Commute-Time Distance** (ECTD). This is nothing else than a **Mahalanobis distance** with a weighting matrix $\mathbf{L}^+$.

4.3 Computational issues

If the number of nodes is too large, the direct computation based on the pseudoinverse becomes intractable; in this case, one may use iterative techniques (such as those based on Equations (1) or (2)) and on the sparseness of the transition probabilities matrix [28, 53].

Another alternative that proved useful for computing $\mathbf{L}^+$ for sparse graphs is based on a sparse Cholesky factorization of the Laplacian matrix. First, observe that the ith column of $\mathbf{L}^+$, $\mathbf{l}_i^+ = \mathrm{col}_i(\mathbf{L}^+)$, can be obtained by (see [31], pp. 440-441) the following procedure:

1. Compute the projection of the basis vector $\mathbf{e}_i$ on the column space of $\mathbf{L}$; this projection is provided by $\mathbf{y}_i = \mathrm{proj}_{\mathbf{L}}(\mathbf{e}_i) = (\mathbf{I} - \mathbf{e}\mathbf{e}^{\mathrm{T}}/n)\mathbf{e}_i$.

2. Find a solution, $\mathbf{l} = \mathbf{l}_i^{*+}$, of the equation $\mathbf{L}\mathbf{l} = \mathbf{y}_i$, where $\mathbf{y}_i$ is the projection of $\mathbf{e}_i$ on the column space of $\mathbf{L}$.

3. Project the result, $\mathbf{l}_i^{*+}$, on the row space, $\mathbf{l}_i^+ = \mathrm{proj}_{\mathbf{L}}(\mathbf{l}_i^{*+}) = (\mathbf{I} - \mathbf{e}\mathbf{e}^{\mathrm{T}}/n)\mathbf{l}_i^{*+}$ (since $\mathbf{L}^+$ is symmetric its row space is equal to its column space).

It can be easily shown, based on the electrical equivalence, that $\mathbf{l}_i^+$ represents the centered (summing to zero) voltage at each node when (1) a unit current is injected in node i and (2) a current $1/n$ is removed from any node.

The main idea is to find one solution of $\mathbf{L}\mathbf{l} = \mathbf{y}_i$ in step 2 by using the Cholesky factorization. We first observe that, since the columns of $\mathbf{L}$ are linearly dependent, we can arbitrarily set one element of $\mathbf{l}$, say the last one, to zero:

$l_n = 0$. Then, we note that the n resulting equations are redundant (the rows of $\mathbf{L}$ and $\mathbf{y}_i$ sum to zero), and we can delete one of these equations, say the last one, without change. The resulting system of equations is equivalent to $\widehat{\mathbf{L}}\widehat{\mathbf{l}} = \widehat{\mathbf{y}}_i$ where $\widehat{\mathbf{L}}$ is the Laplacian matrix from which we have deleted the last column and row. In a same way, $\widehat{\mathbf{l}}$ and $\widehat{\mathbf{y}}_i$ are the $\mathbf{l}$ and $\mathbf{y}_i$ vectors from which we removed the last row. The $(n-1) \times (n-1)$ matrix $\widehat{\mathbf{L}}$, called the reduced Laplacian matrix, is of full rank and positive definite. A Cholesky factorization, $\widehat{\mathbf{L}} = \mathbf{R}\mathbf{R}^{\mathrm{T}}$, is performed. If $\widehat{\mathbf{L}}$ is sparse, the lower-triangular factor $\mathbf{R}$ is sparse as well, although less sparse than the original matrix $\mathbf{L}$. It is therefore useful to first compute a permutation of the original adjacency matrix $\mathbf{A}$ in order to obtain a "band" matrix. Once the factorization has been computed, one solution of $\widehat{\mathbf{L}}\widehat{\mathbf{l}} = \mathbf{R}\mathbf{R}^{\mathrm{T}}\widehat{\mathbf{l}} = \widehat{\mathbf{y}}_i$, call it $\widehat{\mathbf{l}}_i^{*+}$, can easily be obtained by back-substitution ($\mathbf{R}$ is lower-triangular and sparse). A solution to $\mathbf{L}\mathbf{l} = \mathbf{y}_i$ in step 2 is therefore $(\mathbf{l}_i^{*+})^{\mathrm{T}} = \left[\widehat{\mathbf{l}}_i^{*+}, 0\right]$.

This procedure allows to compute the columns of $\mathbf{L}^+$ "on demand". By using this procedure, we were able to compute the elements of $\mathbf{L}^+$ for sparse graphs of about 150000 nodes.

Still another viable approach, based on a truncated series expansion, is proposed by Brand in [10]. Finally, the special case of a bipartite graph (as the movie database) is developed in [32], where the authors propose an optimized method for computing the pseudoinverse of the Laplacian matrix in this situation.

5 Maximum variance subspace projection of the node vectors

5.1 Mapping to a Euclidean space preserving the ECTD

Based on the eigenvector decomposition of $\mathbf{L}^+$, the node vectors $\mathbf{e}_i$ can be mapped into a new Euclidean space that preserves the ECTD (see Appendix D): $n(i,j) = V_G (\mathbf{x}_i' - \mathbf{x}_j')^{\mathrm{T}}(\mathbf{x}_i' - \mathbf{x}_j') = V_G \|\mathbf{x}_i' - \mathbf{x}_j'\|^2$ where we made the transformations $\mathbf{e}_i = \mathbf{U}\mathbf{x}_i$ (or $\mathbf{x}_i = \mathbf{U}^{\mathrm{T}}\mathbf{e}_i$), $\mathbf{x}_i' = \boldsymbol{\Lambda}^{1/2}\mathbf{x}_i$, and where $\mathbf{U}$ is an orthonormal matrix made of the eigenvectors of $\mathbf{L}^+$ (ordered in decreasing order of corresponding eigenvalue λ_k) and $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_k)$. So, in this new n-dimensional Euclidean space, the transformed node vectors $\mathbf{x}_i'$ are **exactly separated** (according to the standard Euclidean distance) by ECTD.

Appendix E shows that the $\mathbf{x}_i'$ are centered and that the elements of the pseudoinverse of the Laplacian matrix are the **inner products** of the transformed node vectors, $l_{ij}^+ = \mathbf{x}_i'^{\mathrm{T}}\mathbf{x}_j'$. Therefore, $\mathbf{L}^+$ is a **kernel** (a Gram matrix) and can be considered as a **similarity matrix** for the nodes (as in the vector-space model in information retrieval). It therefore defines a new kernel on a graph, like the von Neumann kernel [58], the diffusion kernel [42], and the recently introduced regularized Laplacian kernel [35, 61]. In fact, it can easily be shown that the $\mathbf{L}^+$ kernel can be obtained from the regularized Laplacian kernel by using a special regularization operator (see the end of Section 5.2). This result is worth mentioning since, once a meaningful kernel has been defined on a

graph, a number of interesting measures come almost for free (kernel PCA, etc.; see for instance [57]). We are currently comparing various other well-defined kernels on a graph on the same collaborative recommendation task.

One key issue here is to assess which of the **distance-based measures** (for instance the ECTD) or the **inner-product based measures** (for instance $\mathbf{L}^+$) perform better for collaborative recommendation. It is well-known that, for the vector-space model of information retrieval, inner-product based measures outperform Euclidean distances when computing proximities between documents [3]. In the present case, ECTD are Euclidean distances, while $\mathbf{L}^+$ contains the inner products of node vectors. In this framework, another measure of interest is the **cosine** of node vectors, which is defined as

$$\cos^+(i,j) = l_{ij}^+ / \sqrt{l_{ii}^+ l_{jj}^+} \tag{6}$$

5.2 Subspace projection of the node vectors (the principal component analysis of a graph)

$\mathbf{L}^+$ can be approximated by retaining only the $m < (n-1)$ first eigenvectors (the smallest eigenvalue is 0) of its eigenvector decomposition:

$$\widetilde{\mathbf{L}}^+ = \sum_{k=1}^{m} \lambda_k \, \mathbf{u}_k \mathbf{u}_k^{\mathrm{T}} \tag{7}$$

where the $\mathbf{u}_k$ are the eigenvectors of $\mathbf{L}^+$ and λ_k the corresponding eigenvalues (see Appendix D for details). A new transformation of the node vectors is therefore defined by $\widetilde{\mathbf{x}}_i = \widetilde{\mathbf{U}}^{\mathrm{T}} \mathbf{e}_i$ and $\widetilde{\mathbf{x}}'_i = \widetilde{\mathbf{\Lambda}}^{1/2} \widetilde{\mathbf{x}}_i$, where $\widetilde{\mathbf{U}} = [\mathbf{u}_1, \mathbf{u}_2, ..., \mathbf{u}_m, \mathbf{0}, ..., \mathbf{0}]$ and $\widetilde{\mathbf{\Lambda}} = \mathrm{diag}[\lambda_1, \lambda_2, ..., \lambda_m, 0, ..., 0]$. The $\widetilde{\mathbf{x}}'_i$ are column vectors containing zeroes from position $m+1$ on: $\widetilde{\mathbf{x}}' = [\widetilde{x}'_1, \widetilde{x}'_2, ..., \widetilde{x}'_m, 0, ..., 0]^{\mathrm{T}}$. This subspace is thus an m-dimensional space where the ECTD are approximately preserved. A bound on this approximation can easily be derived: $||n(i,j) - \widetilde{n}(i,j)|| \leq V_G \sum_{k=m+1}^{n-1} \lambda_k$.

This decomposition is similar to Principal Component Analysis (PCA) in the sense that the projection of the node vectors in this subspace has maximal variance (in terms of ECTD) among all the possible candidate projections (see [55]; see also Appendix F). This is related, in a number of interesting ways, with both spectral clustering (see, e.g., [59, 20], and our work [55]) and spectral embedding [6, 7].

Moreover, it is easy to show that performing a multidimensional scaling on the ECTD gives exactly the same results as the PCA. Indeed, classical multidimensional scaling [9] amounts to performing the spectral decomposition of the matrix given by $-(1/2)\,\mathbf{J}\mathbf{N}\mathbf{J}$, and to retaining the first m eigenvalues and eigenvectors, where $\mathbf{J}$ is the centering matrix ($\mathbf{J} = \mathbf{I} - \mathbf{e}\mathbf{e}^{\mathrm{T}}/n$) and $\mathbf{N}$ is the ECTD distance matrix ($[\mathbf{N}]_{ij} = n(i,j)$). It is not difficult to show that $-(1/2)\,\mathbf{J}\mathbf{N}\mathbf{J}$ is nothing else than $\mathbf{L}^+$ (times V_G), so that both formulations are equivalent [9].

As for PCA, we expect that the first few principal components contain most of the information about the basic structure of the graph and that the remaining

components related to smaller eigenvalues represent noise. If this is true, appropriate results are obtained by keeping only a few components of the PCA. For example, keeping only two or three components allows to visualize the graph.

Both $\mathbf{L}$ and $\mathbf{L}^+$ have rank $(n-1)$. They have the same set of eigenvectors and inverse eigenvalues. Thus, we need not explicitly compute the pseudoinverse of $\mathbf{L}$ in order to find the projection. We need to compute only the m smallest (except $\lambda_n = 0 = \lambda_n^+$) eigenvectors (that is, with lowest eigenvalue) of $\mathbf{L}$, which are the largest of $\mathbf{L}^+$.

This result shows that the $\widetilde{\mathbf{L}}^+$ similarity matrix is a regularized Laplacian kernel (as defined in [42]) with a regularization factor given by $r(\lambda_i) = \lambda_i^{-1}$ for the smallest m (non-null) eigenvalues λ_i of $\mathbf{L}$ and $r(\lambda_i) = 0$ for the remaining eigenvalues. It trivially penalizes the largest eigenvalues of $\mathbf{L}$, by "cutting" them off in the regularized Laplacian kernel.

Finally, notice that this graph PCA provides a nice interpretation to the "**Fiedler vector**" [24, 43], widely used for graph partitioning [13, 51]: the Fiedler vector simply contains the projections of the node vectors on the first principal component $\mathbf{u}_1$ of the graph. Indeed, the Fiedler vector corresponds to the smallest nonzero eigenvalue of the Laplacian matrix, which is also the first eigenvector $\mathbf{u}_1$ of $\mathbf{L}^+$.

6   Experiments

6.1   Experimental methodology

Remember that each element of the `people` and the `movie` sets corresponds to a node of the graph. Each node of the `people` set is connected by an edge to each movie watched by the corresponding person. The results shown here do not take into account the numerical value of the ratings provided by the persons but only the fact that a person has or has not watched a movie (i.e., entries in the person-movie matrix are 0's and 1's). Our experiments do not take the `movie_category` set into account so that comparisons between the various scoring algorithms remain fair. Indeed, three standard scoring algorithms (i.e., maximum frequency, cosine, and nearest-neighbour algorithms) cannot naturally use the `movie_category` set to rank the movies.

6.1.1   Data set

Our experiments were performed on a real movie database from the web-based recommender system MovieLens (http://www.movielens.umn.edu). We used a sample of their database as suggested in [56]: enough persons (i.e., 943 persons) were randomly selected to obtain 100,000 ratings (considering only persons that had rated 20 or more movies on a total of 1682 movies).

A **preliminary experiment** was performed to tune the parameters of several scoring algorithms (we do not show the corresponding results in this paper), namely parameter α of the Katz method, the number of dimensions for PCA CT, the similarity measure for the k nearest-neighbour algorithm, and the number k of neighbours for each scoring algorithm when using the indirect method (see Section 6.1.3). The database was divided into a `training set` and a `test set`. The `test set` contains exactly 10 ratings for each of the 943 persons (about

10, 000 ratings), while the `training set` contains the remaining ratings (about 90, 000 ratings).

In the **main experiment**, the data set was divided into n subsets ($n = 10$) and the scoring algorithm was executed n times (10-fold cross-validation). Each time, one of the n subsets was used as the `test set` while the other $n-1$ subsets were merged into a `training set`. Then the average result was computed. Notice that no link between a specific person and a specific movie belongs both to the `training set` and to the `test set` and that, for each person, the `test set` may contain any number of movies.

For each person, each scoring algorithm described in Section 6.1.4 computes from the `training set` a ranked list of preferences about movies, expressed as similarities (scores) between people nodes and movie nodes. From that information, we retain a ranked list of all the movies *that the person has not watched*, according to the `training set`.

6.1.2 Performance evaluation

To evaluate the scoring algorithms described in Section 6.1.4, we compared their performance using three measures: (1) the degree of agreement (which is a variant of Somers'D [60]), (2) a percentile score, and (3) a recall score. The `test set` contains, for each person, a set of movies that the person has actually watched and that are not linked to that person in the `training set`. Those movies are part of the ranked list supplied by each scoring algorithm from the `training set`.

Degree of agreement. To compute the degree of agreement, we consider each pair of movies where one movie (say, $M1$) is in the `test set` for that person (the movie has actually been watched by that person) and the other movie (say, $M2$) is not in the `test set` nor in the training set for that person (the movie has not been watched by that person). A scoring algorithm ranks the pair in the correct order if, in the ranked list computed from the `training set`, movie $M1$ precedes movie $M2$. The individual degree of agreement is thus the percentage of pairs ranked in the correct order with respect to the total number of pairs [60]. The idea here is that the scoring algorithm should favour the movies that have indeed been watched by ranking them before those that have not been watched.

The results discussed in the next section compute a single global degree of agreement for all the persons by averaging out the individual degrees of agreement. A degree of agreement of 50% (50% of all the pairs are in correct order and 50% are in bad order) is equivalent to a random ranking. A degree of agreement of 100% means that the proposed ranking is identical to the ideal ranking.

Percentile. The individual percentile score is simply the position (in %) that the median movie in the list from the `test set` occupies in the whole list of ranked movies from the `training set`. For instance, if the `test set` contains three movies, ranked in 10th, 15th and 40th position, and there are 100 ranked movies in total, the percentile score will be 15%. A random ranking would provide a percentile score of about 50%. This measure should be as low as possible for good performance (near 0% for a perfect model). The global percentile score is obtained by averaging the individual percentile scores of all persons.

13

Recall. The recall score is the average (on all persons) of the proportion (in %) of movies from the `test set` that appear among the *top n* of the ranked list from the `training set`, for some given n. This measure should be as high as possible for good performance. A recall score of 100% indicates that the scoring algorithm always positioned the movies in the `test set` among the *top n* of the ranked list. We computed the recall for the *top* 10 and the *top* 20 movies (for a total of 1682 movies).

6.1.3 Direct method versus indirect method for recommendation

We have used three methods to determine which movies to suggest to a particular person based on computing similarities between pairs of nodes:

Direct method: use each scoring algorithm to compute the similarities between a given *person* and all the *movies*. Movies are presented in decreasing order of the similarity values.

User-based indirect method: first, use each scoring algorithm as in the direct method to compute the similarities (denoted $\text{sim}(p_0, p)$) between a given *person* p_0 and all the other *persons* p; then, for p_0, compute from its k nearest neighbours (in the present case, nearest neighbours are persons) the *predicted value* (or preference) of each movie. The predicted value of movie m_0 for person p_0 is computed as a sum, weighted by $\text{sim}(p_0, p)$, of the values of a the link weight (0 or 1) of movie m_0 for the k persons p closest to person p_0:

$$\text{pred}(p_0, m_0) = \frac{\sum_{p=1}^{k} \text{sim}(p_0, p) \ a_{pm_0}}{\sum_{p=1}^{k} \text{sim}(p_0, p)} \qquad (8)$$

where a_{pm_0} is 1 if person p watched movie m_0 and 0 otherwise. The higher the predicted value $\text{pred}(p_0, m_0)$, the stronger the recommendation that person p_0 should watch movie m_0. For each scoring algorithm, we systematically varied the number k of neighbours $(1, 2, ..., 10, 20, ..., 100)$ and we kept the value of k providing the best result. Notice that the value of k depends on the measure used to evaluate the performance (see Section 6.1.2).

Movie-based indirect method: this corresponds to the methodology proposed by Karypis in its SUGGEST approach [37]. First, use each scoring algorithm as in the direct method to compute the similarities (denoted $\text{sim}(m_0, m)$) between a given *movie* and all the other *movies* (in the present case, nearest neighbours are movies); then, for a given person p_0, compute from the k nearest neighbours of the movies watched by p_0 the predicted value of each movie. The predicted value of movie m_0 for person p_0 is computed as a sum, weighted by $\text{sim}(m_0, m)$, of the values of the link weight (0 or 1) of movie m_0 for the k nearest movies m of movie m_0:

$$\text{pred}(p_0, m_0) = \frac{\sum_{m=1}^{k} \text{sim}(m_0, m) \ a_{p_0 m}}{\sum_{m=1}^{k} \text{sim}(m_0, m)} \qquad (9)$$

where $a_{p_0 m}$ is defined as before. The movies are proposed to person p_0 in decreasing order of predicted values. As for the user-based indirect method, we

optimized the number of neighbours. This way to suggest movies is equivalent to the SUGGEST method proposed in [37].

Notice that, if the algorithm provides a dissimilarity measure $\mathrm{dis}(i,j)$, we use $(\max - \mathrm{dis}(i,j))/(\max - \min)$ to convert it into a similarity measure.

6.1.4 Scoring algorithms

Twelve scoring, or ranking, algorithms are compared. The person-independent maximum-frequency algorithm (MaxF) will serve as a reference to appreciate the quality of the other scoring algorithms. Six scoring algorithms are based on our random-walk model: the average commute time (normal and PCA-based), the average first-passage time (one-way and return, see later), and the pseudoinverse of the Laplacian matrix (normal and $\cos^+$). The other algorithms are standard techniques: k-nearest neighbours techniques, cosine coefficient, Katz' method, and the shortest-path algorithm. We also include the random-forest based similarity measure proposed in [15]. We now describe these algorithms in more detail.

Maximum-frequency (MaxF). This scoring algorithm simply ranks the movies by the number of persons who watched them. In other words, movies are suggested to each person in order of decreasing popularity. The ranking is thus the same for all the persons. MaxF is equivalent to basing the decision only on the a priori probabilities in supervised classification. Notice that MaxF can only be used in the direct method.

Average commute time (CT). We use the average commute time $n(i,j)$ to rank the elements of the considered set, where i and j are elements of the database. For instance, if we want to suggest movies to people using the direct method, we compute the average commute time between `people` elements and `movie` elements. The lower the value is, the more similar the two elements are. In the sequel, this quantity will simply be referred to as *"commute time"*.

Principal component analysis based on ECTD (PCA CT). In Section 5, we showed that, based on the eigenvector decomposition of $\mathbf{L}^+$, the nodes can be mapped into a new Euclidean space (with more than 2600 dimensions in this case) that preserves the ECTD, or a m-dimensional subspace keeping as much variance as possible, in terms of ECTD.

Thus, after performing a PCA and keeping a given number of principal components, we recompute the distances in this reduced subspace. These approximate ECTD between people and movies are then used to rank the movies for each person. We varied the dimension m of the subspace from 10 to 2620 by step of 10. The best results were obtained for 60 principal components ($m = 60$).

Average first-passage time (One-way). In a similar way, we use the average first-passage time $m(i|j)$, to compute a similarity score between element i and element j of the database. This quantity will simply be referred to as *"one-way time"*.

Average first-passage time (Return). As a similarity between element i and element j of the database, this scoring algorithm uses $m(j|i)$ (the transpose of $m(i|j)$), that is, the average time used to reach j when starting from i. This quantity will simply be referred to as *"return time"*.

15

Pseudoinverse of the Laplacian matrix ($\mathbf{L}^+$). $\mathbf{L}^+$ provides a similarity measure ($\mathrm{sim}(i,j) = l_{ij}^+$) since it is the matrix containing the inner products of the node vectors in the Euclidean space where the nodes are exactly separated by the ECTD. Once we have computed the similarity matrix, movies are ranked according to their similarity with the person. In addition, we used the same procedure as for the "PCA CT": rely on the principal components analysis subspace. Since we did not observe any improvement in comparison with $\mathbf{L}^+$, we do not show the results here.

Cosine based on $\mathbf{L}^+$ ($\mathbf{cos}^+$). This scoring algorithm computes similarities from Equation (6) to rank the movies.

k-nearest neighbours (kNN). This scoring algorithm can be represented by the following rule: to classify a new item, choose the most frequent class of the k-nearest example in the training set as measured by a similarity coefficient. Using a nearest-neighbour technique requires a measure of "closeness" or "similarity". The choice of a similarity measure (see [36]) includes to consider the nature of the variables (discrete, continuous, binary), the scales of measurement (nominal, ordinal, interval, ratio), and specific knowledge about the subject matter.

We now detail the procedure used for performing a k-nearest neighbours in the *user-based indirect method* (see Section 6.1.3). The procedure used for performing a k-nearest neighbours in the *movie-based indirect method* is similar and does not require further explanations. In the case of our movie database, pairs of items are compared on the basis of the presence or absence of certain features, i.e., watching a particular movie. The presence or absence of a feature is described mathematically by using a binary variable, which takes the value 1 if the feature is present (i.e., if person i has watched movie j) and the value 0 if the feature is absent (i.e., if person i has not watched movie j). More precisely, each person i is characterized by a binary vector $\mathbf{v}_i$ encoding the movies that that person watched. The dimension of this vector is equal to the number of movies. The k-nearest neighbours of person i are computed by taking the k nearest $\mathbf{v}_j$ according to a given similarity measure between binary vectors, $\mathrm{sim}(i,j) = s(\mathbf{v}_i, \mathbf{v}_j)$. We performed systematic comparisons between eight different such measures s (listed in [36], p.674) and for different values of k ($= 1, 2, ..., 10, 20, ..., 100$). The best scores (for all the performance measures) were obtained with the "a ratio of 1-1 matches to mismatches with 0-0 matches excluded". Notice that the k-nearest neighbours is an indirect method that cannot be used in the direct method.

Cosine coefficient (Cosine). The cosine coefficient between persons i and j, which measures the strength and the direction of a linear relationship between two variables, is defined by $\mathrm{sim}(i,j) = \mathrm{cosine}(i,j) = (\mathbf{v}_i{}^{\mathrm{T}}\mathbf{v}_j)/(\|\mathbf{v}_i\| \, \|\mathbf{v}_j\|)$. We again systematically varied the number k of neighbours ($= 1, 2, ..., 10, 20, ..., 100$). The cosine coefficient algorithm is also an indirect method that cannot be used in the direct method.

Katz (Katz). This similarity index has been proposed in the social sciences field and has been recently rediscovered in the context of collaborative recommendation [33] and kernel methods where it is known as the von Neumann kernel [57]. Katz proposed in [38] a method of computing similarities, taking into account not only the number of direct links between items but, also, the

16

number of indirect links (going through intermediaries) between items. The similarity matrix is

$$\mathbf{K} = \alpha \mathbf{A} + \alpha^2 \mathbf{A}^2 + ... + \alpha^n \mathbf{A}^n + ... = (\mathbf{I} - \alpha \mathbf{A})^{-1} - \mathbf{I} \qquad (10)$$

where $\mathbf{A}$ is the adjacency matrix and α is a constant which has the force of a probability of effectiveness of a single link ($\text{sim}(i,j) = k_{ij} = [\mathbf{K}]_{ij}$). A n-step chain or path, then, has a probability α^n of being effective. In this sense, α actually measures the attenuation in a link, $\alpha = 0$ corresponding to complete attenuation and $\alpha = 1$ to absence of any attenuation. For the series to be convergent, α must be less than the inverse of the spectral radius of $\mathbf{A}$.

For the experiment, we systematically varied the value of α ($\alpha = (0.05, 0.10, ..., 0.95)$ * (spectral radius)$^{-1}$) and we present only the results obtained by the best model (namely, $\alpha = 0.05$ * (spectral radius)$^{-1}$).

Random-forest based algorithm (RFA). The similarity matrix introduced by Chebotarev & Shamis in [15, 17] is

$$\mathbf{T} = (\mathbf{I} + \mathbf{L})^{-1} \qquad (11)$$

where $\mathbf{L}$ is the Laplacian matrix. This similarity measure has an interesting interpretation in terms of the matrix-forest theorem [15, 17]. Suppose that $F^i(G) = F^i$ is the set of all spanning forests rooted on node i of graph G, and $F^{ij}(G) = F^{ij}$ is the set of those spanning rooted forests for which nodes i and j belong to the same tree rooted at i. A spanning rooted forest is an acyclic subgraph of G that has the same nodes set as G and one marked node (a root) in each component. It is shown in [15, 17] that the matrix $(\mathbf{I} + \mathbf{L})^{-1}$ exists and that $[(\mathbf{I} + \mathbf{L})^{-1}]_{ij} = \epsilon(F^{ij})/\epsilon(F^i)$ where $\epsilon(F^{ij})$ and $\epsilon(F^i)$ are the total weights of forests that belong to F^{ij} and F^i respectively. The elements of this matrix are therefore called "relative forest accessibilities" between nodes. It can be shown that this matrix is a similarity measure ($\text{sim}(i,j) = t_{ij} = [\mathbf{T}]_{ij}$), having the natural properties of a similarity (triangular property for similarities, among others [16]). It has recently been rediscovered and used in the context of documents ranking [35]. It is clear that this similarity measure is closely related to $\mathbf{L}^+$. Indeed, $(\mathbf{I} + \mathbf{L})^{-1}$ and $\mathbf{L}^+$ have the same set of eigenvectors, and their eigenvalues are related by $\lambda_i^{\text{RFA}} = \lambda_i^{\mathbf{L}^+}/(1 + \lambda_i^{\mathbf{L}^+})$. This operation is similar to a kind of regularization of the Laplacian matrix.

Shortest-path algorithm (Dijkstra). This algorithm solves a shortest path problem for a directed and connected graph with nonnegative edge weights. As a distance between two elements of the database, we compute the shortest path between these two elements. We do not show in the sequel the results of the shortest path algorithm. Indeed, it seems that, for example using the direct method, nearly each movie can be reached from any person with a shortest path distance of 3. The degree of agreement is therefore close to 50% because of the large number of ties, and the detailed results are of little interest.

6.2 Cross-validation results

Thus, for each step of the cross-validation and for each person, we first select the movies that have not been watched. Then, we rank them according to all the

described scoring algorithms and the methods to use them (direct, user-based indirect or movie-based indirect method). We compare the proposed ranking with the `test set` (if the ranking procedure performs well, we expect watched movies belonging to the `test set` to be on top of the list) by using the three measures of performance.

6.2.1 Results and discussion

All the results are summarized in Table 2, which shows the three performance measures: the degree of agreement (Agreement), the percentile score (Percentile), and the recall, considering either the top 10 of the ranked list (Recall 10) or the top 20 of the ranked list (Recall 20). The standard deviation of the results (STD) across the 10 cross-validation sets is also reported, as well as the optimal number of neighbours (Neighbours), when applicable.

Table 2 shows that, when using the **direct method** to rank the movies for each user, the best results are obtained by $\mathbf{L}^+$, $\cos^+$, and RFA. Notice that we use a paired t-test to determine if there is a significant difference (with a p-value smaller than 10^{-2}) between the results of the various scoring algorithms. The best results, for each measure of performance and for each method (i.e., direct, user-based indirect, or movie-based indirect), are displayed in bold in each row of the table, based on the t-test.

In the **user-based indirect method**, the bests results are obtained by $\mathbf{L}^+$ and RFA. In particular, the best degree of agreement and percentile are provided by $\mathbf{L}^+$ whereas the best recall scores (either the recall 10, or the recall 20) are obtained by both scoring algorithms with no significant difference. In the **movie-based indirect method**, kNN and RFA provide the best results.

When looking at the global performance (regardless of the direct or indirect way the similarities are computed) of the various scoring algorithms, Table 2 shows that $\mathbf{L}^+$, kNN, Cosine, $\cos^+$, and RFA are the best scoring algorithms in terms of both performance and stability of the results. The **best results overall** are obtained by the kNN, used in the movie-based indirect method (as proposed in the SUGGEST method, [37]), when considering the degree of agreement or the percentile, by $\mathbf{L}^+$ and RFA, used in the user-based indirect method, when considering the recall scores (considering either the top 10 or the top 20). We also observe that the user-based indirect method provides better recommendations than the movie-based indirect method for $\mathbf{L}^+$ and RFA, and for both kNN and Cosine but only for recall scores.

All the dissimilarity measures (i.e., CT, One-way and Return) are clearly less efficient (except the Return in the user-based indirect method) and seem to present a lack of stability (the results highly depends on the method used). We observe that CT and One-way give better results in the direct method than in the indirect method and that their direct recommendations are very similar to simply suggest the most popular movies (MaxF), most likely because they are both dominated by the stationary distribution, as stated in [10]. Indeed, Brand [10] showed that the commute time is highly sensitive to the degree of the node (which is equal to the stationary distribution up to a scaling factor when considering a simple random walk on a graph). His work therefore provides an

explanation of the bad performances obtained by the dissimilarity measures, and confirms our results.

The fact that the inner products ($\mathbf{L}^+$, $\cos^+$, and RFA) provide better results than the corresponding distance measures (CT, PCA CT, One-way, and Return) shows that, in these experiments, the *angle between the node vectors* is a much more predictive measure than the distance between the nodes. The situation is therefore quite similar to what we observe in information retrieval. This result was also pointed out by Brand [10].

In conclusion, three similarity measures provide very good and stable performance: $\mathbf{L}^+$, RFA and the simple nearest neighbours technique (kNN). We also clearly observe that using the most efficient scoring algorithms ($\mathbf{L}^+$, RFA) in the indirect method improves the results, in comparison with the direct method. It is not clear, however, which of the two different indirect methods (user-based or movie-based) perform best. Indeed, kNN provides slightly better results in the movie-based indirect method, while we observe the opposite for $\mathbf{L}^+$ and RFA.

Correlations between the ranking algorithms. The Kendall rank-order correlation coefficient provides a measure of the degree of association or correlation between two sets of rankings (see [60] for details; its range is $[0, 1]$ with 1 corresponding to a perfect association and 0.5 corresponding to no association at all). Table 3 shows the average correlations between the rankings provided by all the ranking algorithms.

Firstly, we observe that the values of the correlations are quite low (rarely more than 0.75). This can be partially explained by the features of the database. There are actually many movies that have been watched by few people (2 or less). These movies have a small influence on the measure of performance (i.e., it is rare to find one of them in the movies belonging to the `test set` for a specific user) whereas they have some influence on the Kendall scores, because of their quantity (remember that a Kendall score is computed using the whole rankings provided by the considered scoring algorithms).

We observe that, as discussed in the previous section, MaxF is positively correlated with CT, PCA CT, and One-way used in the direct method. On the other hand, $\mathbf{L}^+$, $\cos^+$, Katz, and RFA are negatively correlated with MaxF. Thus, these methods do not always favor best-sellers.

6.2.2 Computing times

In this section, we perform a comparison of the computing time (on a Pentium 4, 2.80 GHz) for all the implemented scoring algorithms and the ways defined to use them (direct, user-based indirect or movie-based indirect method). Notice that we do not use (for none scoring algorithm) the sparseness of the adjacency matrix $\mathbf{A}$ in order to reduce the computing times.

Table 1 shows the time, in seconds (using the Matlab `cputime` function), needed by each scoring algorithm to compute, from the adjacency matrix $\mathbf{A}$, a $n \times n$ matrix whose element i,j is a similarity measure between node i and node j. Notice that this matrix could be computed offline so that it could take very little time to provide an online recommendation.

All these scoring algorithms were implemented in Matlab. We used, in order to compute the similarity matrices, Equation (4) for the average commute

time, the method suggested by Kemeny & Snell ([39], p. 218) for the average first-passage times (one-way and return), Equation (3) for $\mathbf{L}^+$ and the derived $\cos^+$, and Equations (10) and (11) (both by inverting the matrix in Matlab) for respectively Katz and RFA similarity matrices. Notice also that, for the principal components analysis, we first had to compute the $\mathbf{L}^+$ matrix, then take out its eigenvectors and eigenvalues (using the Matlab `svd` function) and finally compute the derived distances.

MaxF	CT	PCA CT	One-way	Return	$\mathbf{L}^+$	$\cos^+$	kNN	Cosine	Katz	RFA
0	327	1308	630	630	25	228	114	202	25	25

Table 1: Time (in sec) needed to compute predictions for all the non-watched movies and all the users.

We observe that the slowest methods are the distance-based scoring algorithms (i.e., CT, PCA CT, One-way, and Return) and the $\cos^+$ method. The fastest scoring algorithms (if we do not consider the MaxF algorithm which provides nearly immediate results) are $\mathbf{L}^+$, Katz, and RFA.

7   Conclusions and further work

We have proposed a general procedure for computing similarities between elements of a database. It is based on a Markov-chain model of random walk through a graph representation of the database. More precisely, we compute quantities (the average first-passage time, the average commute time, and the pseudoinverse of the Laplacian matrix) that provide similarity measures between any pair of elements of a connected graph. These similarity measures can be used in order to compare items belonging to database tables that are not necessarily directly connected. They rely on the degree of connectivity between these elements. While the theoretical framework has been developed in the case of a weighted, undirected, graph, the notions of average first-passage time and average commute time also apply to **directed** graphs. However, the nice interpretation in terms of the pseudoinverse of the Laplacian matrix does not apply in this case (still, see [1, 2] for potential generalizations to directed graphs).

We showed through experiments performed on the MovieLens database that inner-product based quantities perform well in comparison with standard scoring algorithms. In fact, as already stressed in [40], the proposed quantities provide a very general mechanism for computing similarities between nodes of a graph by exploiting its structure.

More precisely, the experiments showed that three similarity measures provide good and stable performance: the pseudoinverse of the Laplacian matrix, the random-forest based similarity measure, and the simple nearest-neighbour technique (the latter when used in an item-based indirect method, such as that proposed in the SUGGEST methodology [37]). However, for the nearest neighbour, two parameters need to be adjusted: the number of neighbours and the similarity between binary vectors, while the Laplacian pseudo-inverse and the random-forest based measures do not need any parameter tuning in the direct

method and only the number of neighbours in the indirect methods. Moreover, the pseudoinverse of the Laplacian matrix and the random-forest based similarity measure are much more generic than the nearest neighbour since they provide similarity measures between any two elements of a database.

The main drawback of this method is that it does not scale well for large databases. Indeed, the Markov model has as many states as elements in the database. For large databases, we have to rely on iterative formulas or approximate algorithms, and on the sparseness of the matrix.

We are now working on other generalizations of standard multivariate statistical methods to the mining of databases, such as discriminant analysis. We are also comparing the various kernels on a graph that have been proposed in the literature on the same collaborative recommendation task. Finally, we are working on generalizations to directed weighted graphs for which the weights are not necessarily positive.

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Acknowledgments

	MaxF	CT	PCA CT	One-way	Return	L^+	$\cos^+$	kNN	Cosine	Katz	RFA
Direct method (in %)											
Agreement	85.98	85.98	86.90	85.96	80.11	91.11	90.52	/	/	88.38	**91.12**
STD	*0.32*	*0.33*	*0.32*	*0.33*	*0.32*	*0.17*	*0.24*	/	/	*0.30*	*0.17*
Percentile	10.73	10.73	10.04	10.74	17.88	**6.52**	7.37	/	/	8.93	**6.53**
STD	*0.45*	*0.45*	*0.54*	*0.45*	*0.44*	*0.30*	*0.39*	/	/	*0.41*	*0.30*
Recall 10	11.02	11.11	12.97	11.09	0.34	16.31	**17.24**	/	/	14.97	16.65
STD	*0.23*	*0.23*	*0.36*	*0.24*	*0.05*	*0.33*	*0.45*	/	/	*0.29*	*0.35*
Recall 20	17.43	17.57	21.77	17.54	1.07	26.39	26.16	/	/	23.11	**26.72**
STD	*0.43*	*0.43*	*0.67*	*0.44*	*0.16*	*0.48*	*0.50*	/	/	*0.41*	*0.53*
User-based indirect method (in %)											
Agreement	/	81.87	91.66	81.83	92.35	**92.90**	90.77	92.64	92.66	90.07	92.85
STD	/	*0.31*	*0.25*	*0.31*	*0.27*	*0.22*	*0.18*	*0.16*	*0.18*	*0.30*	*0.22*
Neighbours	/	100	100	100	100	100	40	100	70	30	100
Percentile	/	13.07	6.47	13.09	5.65	**5.19**	7.20	5.53	5.68	7.61	5.41
STD	/	*0.53*	*0.39*	*0.52*	*0.34*	*0.34*	*0.30*	*0.48*	*0.41*	*0.32*	*0.36*
Neighbours	/	100	60	100	100	60	30	50	30	30	60
Recall 10	/	10.93	18.57	10.91	20.56	**21.43**	17.18	20.76	20.68	17.07	**21.32**
STD	/	*0.35*	*0.39*	*0.35*	*0.23*	*0.41*	*0.31*	*0.33*	*0.22*	*0.48*	*0.38*
Neighbours	/	100	60	100	80	40	50	50	60	50	50
Recall 20	/	17.35	28.67	17.35	31.14	**32.20**	26.37	31.13	31.29	25.41	**32.28**
STD	/	*0.36*	*0.37*	*0.38*	*0.30*	*0.40*	*0.46*	*0.39*	*0.42*	*0.32*	*0.49*
Neighbours	/	100	60	100	60	50	50	50	40	30	40
Movie-based indirect method (in %)											
Agreement	/	61.28	90.74	85.76	83.25	92.13	89.52	**93.27**	92.78	86.80	92.21
STD	/	*1.06*	*0.26*	*0.51*	*0.24*	*0.22*	*0.16*	*0.22*	*0.17*	*0.26*	*0.17*
Neighbours	/	50	80	50	100	70	90	100	100	100	100
Percentile	/	35.02	7.13	10.91	14.64	5.76	8.72	**4.93**	5.26	10.41	5.42
STD	/	*2.78*	*0.40*	*0.42*	*0.74*	*0.24*	*0.26*	*0.32*	*0.26*	*0.40*	*0.24*
Neighbours	/	30	40	50	90	40	90	40	40	100	60
Recall 10	/	4.00	12.01	11.13	1.39	16.41	6.65	18.92	17.29	5.82	**19.84**
STD	/	*0.63*	*0.34*	*0.56*	*0.11*	*0.65*	*0.23*	*0.27*	*0.26*	*0.32*	*0.39*
Neighbours	/	40	20	100	20	40	30	20	20	100	60
Recall 20	/	6.93	20.80	17.45	3.88	27.98	12.59	**30.81**	28.72	10.77	**30.91**
STD	/	*0.80*	*0.34*	*0.62*	*0.22*	*0.50*	*0.30*	*0.38*	*0.44*	*0.48*	*0.39*
Neighbours	/	30	20	50	20	40	30	20	30	90	40

Table 2: Average results obtained by performing a 10-fold cross-validation by the various scoring algorithms, and the three methods defined to use them (direct, user-based indirect, and movie-based indirect).

	CT	PCA CT	One-way	Return	$\mathbf{L}^+$	$\cos^+$	kNN	Cosine	Katz	RFA
Direct method										
MaxF	0.7468	0.6303	0.7470	0.5248	0.2880	0.2861	/	/	0.2762	0.2870
CT		0.6298	0.9526	0.5251	0.2881	0.2861	/	/	0.2760	0.2871
PCA CT			0.6297	0.5369	0.3915	0.3873	/	/	0.3796	0.3906
One-way				0.5251	0.2882	0.2861	/	/	0.2761	0.2871
Return					0.4896	0.4827	/	/	0.4796	0.4890
$\mathbf{L}^+$						0.7222	/	/	0.7117	0.7309
$\cos^+$							/	/	0.7137	0.7172
kNN								/	/	/
Cosine									/	/
Katz										0.7127
User-based indirect method										
MaxF	0.2791	0.3263	0.2796	0.3865	0.3579	0.3263	0.3524	0.3502	0.2978	0.3557
CT		0.6695	0.7338	0.6075	0.6360	0.6681	0.6415	0.6442	0.6964	0.6378
PCA CT			0.6696	0.5903	0.6132	0.6494	0.6175	0.6193	0.6565	0.6272
One-way				0.6071	0.6359	0.6681	0.6412	0.6437	0.6961	0.6377
Return					0.5930	0.5988	0.5935	0.5941	0.6022	0.5930
$\mathbf{L}^+$						0.6223	0.6141	0.6148	0.6279	0.6327
$\cos^+$							0.6268	0.6302	0.6561	0.6239
kNN								0.6198	0.6326	0.6151
Cosine									0.6349	0.6159
Katz										0.6301
Movie-based indirect method										
MaxF	0.3520	0.4108	0.2749	0.4979	0.4109	0.3435	0.3837	0.3772	0.4570	0.4207
CT		0.5585	0.6547	0.4990	0.5565	0.4238	0.5715	0.5792	0.5363	0.4600
PCA CT			0.5902	0.5065	0.5392	0.5255	0.5492	0.5546	0.5210	0.5143
One-way				0.5023	0.5872	0.6544	0.6124	0.6207	0.5461	0.5748
Return					0.5049	0.5165	0.5029	0.5052	0.5016	0.5048
$\mathbf{L}^+$						0.5699	0.5653	0.5652	0.5269	0.5514
$\cos^+$							0.5848	0.5972	0.5405	0.5621
kNN								0.5897	0.5284	0.5689
Cosine									0.5310	0.5666
Katz										0.5273

Table 3: Correlation matrix containing the Kendall score for each pair of scoring algorithms, for the three methods defined to use them (direct, user-based indirect, and movie-based indirect).

A Some useful properties of the pseudoinverse of the Laplacian matrix

A.1 $\mathbf{L}^+$ is symmetric

Since $\mathbf{L}$ is symmetric and, for any matrix $\mathbf{M}$, $(\mathbf{M}^{\mathrm{T}})^+ = (\mathbf{M}^+)^{\mathrm{T}}$ (see [5]), we easily obtain $\mathbf{L}^+ = (\mathbf{L}^{\mathrm{T}})^+ = (\mathbf{L}^+)^{\mathrm{T}}$. Therefore, $\mathbf{L}^+$ is symmetric.

A.2 $\mathbf{L}^+$ has rank $n-1$ and is doubly centered

An EP matrix $\mathbf{M}$ is a matrix that commutes with its pseudoinverse, i.e., $\mathbf{M}^+\mathbf{M} = \mathbf{M}\mathbf{M}^+$. Since $\mathbf{L}$ is real symmetric, it is automatically an EP-matrix (see [5], p. 253). In particular, the following property of EP matrices is worth mentioning:

If $(\lambda_i \neq 0, \mathbf{u}_i)$ are (eigenvalues, eigenvectors) of $\mathbf{L}$, then $(\lambda_i^{-1} \neq 0, \mathbf{u}_i)$ are corresponding (eigenvalues, eigenvectors) of $\mathbf{L}^+$. On the other hand, if $(\lambda_j = 0, \mathbf{u}_j)$ are (eigenvalues, eigenvectors) of $\mathbf{L}$, then they are also (eigenvalues, eigenvectors) of $\mathbf{L}^+$.

In particular, this implies that
1. $\mathbf{L}^+$ has rank $n-1$ and has the same null space as $\mathbf{L}$: $\mathbf{L}^+\mathbf{e} = 0$ ($\mathbf{e} = [\mathbf{1}, \mathbf{1}, \ldots, \mathbf{1}]^{\mathrm{T}}$ is the eigenvector associated to $\lambda_n = 0$).
2. The previous property shows that $\mathbf{L}^+$ is doubly centered (the sum of its columns and the sum of its rows are both zero), just like $\mathbf{L}$ (see also [52], chapter 10, for a discussion of this topic).

Other properties of EP-matrices are described in [5] or [12].

A.3 $\mathbf{L}^+$ is positive semidefinite

Indeed, from the previous property, the eigenvalues of $\mathbf{L}$ and $\mathbf{L}^+$ have the same sign and $\mathbf{L}$ is positive semidefinite; therefore $\mathbf{L}^+$ is also positive semidefinite.

B Computation of the average first-passage time/cost in terms of $\mathbf{L}^+$

Let us start from Equations (2), rewritten as 13

$$o(k|i) \;=\; \sum_{j=1}^{n} p_{ij}c(j|i) + \sum_{j=1}^{n} p_{ij}o(k|j), \text{ for } i \neq k \tag{12}$$

$$o(k|i) \;=\; r_i + \sum_{j=1}^{n} p_{ij}o(k|j), \text{ for } i \neq k \tag{13}$$

where $r_i = \sum_{j=1}^{n} p_{ij}c(j|i)$ for $i = 1\ldots n$, and $o(k|k) = 0$ for all k. The corresponding $n \times 1$ column vector made of r_i is $\mathbf{r}$.

Let us renumber the states so that state k becomes state n, the last state of the Markov model, and rewrite Equation (13) in matrix form. The equation will refer to vectors and matrices where the nth row and the nth column have been deleted; we denote by $\widehat{\mathbf{o}}$, $\widehat{\mathbf{r}}$ and $\widehat{\mathbf{P}}$ the vectors/matrices obtained from

$\mathbf{o}$, $\mathbf{r}$ and $\mathbf{P}$ by suppressing their nth row and column. We thus obtain $\widehat{\mathbf{o}} = \widehat{\mathbf{r}} + \widehat{\mathbf{P}}\widehat{\mathbf{o}} = \widehat{\mathbf{r}} + \widehat{\mathbf{D}}^{-1}\widehat{\mathbf{A}}\widehat{\mathbf{o}}$, where the column vector $\widehat{\mathbf{o}}$ has elements $[\widehat{\mathbf{o}}]_i = o(n|i)$ and $\widehat{\mathbf{P}} = \widehat{\mathbf{D}}^{-1}\widehat{\mathbf{A}}$. As long as there is no isolated node (with no edge associated to it), $\widehat{\mathbf{D}}$ can be inverted. If we pre-multiply this last equation by $\widehat{\mathbf{D}}$, we obtain $\widehat{\mathbf{D}}\widehat{\mathbf{o}} = \widehat{\mathbf{D}}\widehat{\mathbf{r}} + \widehat{\mathbf{A}}\widehat{\mathbf{o}}$; therefore $(\widehat{\mathbf{D}} - \widehat{\mathbf{A}})\widehat{\mathbf{o}} = \widehat{\mathbf{D}}\widehat{\mathbf{r}}$. By defining $\mathbf{b} = \mathbf{Dr}$, we finally obtain $\widehat{\mathbf{L}}\widehat{\mathbf{o}} = \widehat{\mathbf{b}}$ and, since $\mathbf{L}$ has rank $n-1$, $\widehat{\mathbf{L}}$ is of full rank. We therefore have $\widehat{\mathbf{L}}^+ = \widehat{\mathbf{L}}^{-1}$, so that

$$\widehat{\mathbf{o}} = \widehat{\mathbf{L}}^{-1}\widehat{\mathbf{b}} = \widehat{\mathbf{L}}^+\widehat{\mathbf{b}} \tag{14}$$

or $o(n|i) = \sum_{j=1}^{n-1} \widehat{l}_{ij}^{-1} b_j$, for $i \neq n$.

We could solve these equations for all the nodes being node n in turn, but this would be quite inefficient. Instead, we will express the elements of $\widehat{\mathbf{L}}^+$ in terms of the elements of $\mathbf{L}^+$ in order to obtain a more general equation (valid for all the nodes). This can easily be done thanks to the formula computing the pseudoinverse of a general $m \times n$ matrix $\mathbf{M}_n = [\mathbf{M}_{n-1}\ \mathbf{a}]$ obtained by appending a $m \times 1$ column vector $\mathbf{a}$ to the $m \times (n-1)$ matrix $\mathbf{M}_{n-1}$ (see, e.g., [5, 8]).

Before going into the details, here is a sketch of the main idea. From the $(n-1) \times (n-1)$ matrix $\widehat{\mathbf{L}}^{-1}$, we construct $\mathbf{L}^+$ by first adding a column vector to $\widehat{\mathbf{L}}$ and then a row vector, in order to obtain $\mathbf{L}$ and its corresponding pseudoinverse $\mathbf{L}^+$. Consequently we first obtain from $\widehat{\mathbf{L}}^{-1}$ a new $(n-1) \times n$ matrix, $\mathbf{M}_n = [\widehat{\mathbf{L}}\ \mathbf{a}]$, and compute its pseudoinverse $\mathbf{M}_n^+$ Then we add a row vector $\mathbf{a}'^{\mathrm{T}}$ to $\mathbf{M}_n$ in order to finally obtain $\mathbf{L} = \begin{bmatrix} \mathbf{M}_n \\ \mathbf{a}'^{\mathrm{T}} \end{bmatrix}$ and its pseudoinverse.

Here is the general formula (see, e.g., [5, 8]) allowing to compute the pseudoinverse of a matrix $\mathbf{M}_n = [\ \mathbf{M}_{n-1}\ \mathbf{a}]$ in terms of the pseudoinverse of $\mathbf{M}_{n-1}$:

$$\mathbf{M}_n^+ = \begin{bmatrix} \mathbf{M}_{n-1} & \mathbf{a} \end{bmatrix}^+ = \begin{bmatrix} \mathbf{M}_{n-1}^+ - \mathbf{db}^{\mathrm{T}} \\ \mathbf{b}^{\mathrm{T}} \end{bmatrix} \tag{15}$$

where we define $\mathbf{d} = \mathbf{M}_{n-1}^+\mathbf{a}$, $\mathbf{c} = \mathbf{a} - \mathbf{M}_{n-1}\mathbf{d}$, and

$$\mathbf{b}^{\mathrm{T}} = \begin{cases} \mathbf{c}^+ & \text{if } \mathbf{c} \neq \mathbf{0} \\ (1 + \mathbf{d}^{\mathrm{T}}\mathbf{d})^{-1}\mathbf{d}^{\mathrm{T}}\mathbf{M}_{n-1}^+ & \text{if } \mathbf{c} = \mathbf{0} \end{cases} \tag{16}$$

with $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and $\mathbf{d}$ being column vectors.

In our special case, $\mathbf{M}_{n-1} = \widehat{\mathbf{L}}$ is $(n-1) \times (n-1)$, and since we must obtain $\mathbf{Le} = \mathbf{0}$ ($\mathbf{L}$ is doubly centered), the appended column $\mathbf{a}$ is minus the sum of the columns of $\widehat{\mathbf{L}}$; that is, $\mathbf{a} = -\widehat{\mathbf{L}}\widehat{\mathbf{e}}$. We thus have $\mathbf{d} = \widehat{\mathbf{L}}^+\mathbf{a} = -\widehat{\mathbf{L}}^{-1}\widehat{\mathbf{L}}\widehat{\mathbf{e}} = -\widehat{\mathbf{e}}$.

We will show that we need not to explicitly compute $\mathbf{b}$; indeed, we obtain from Equation (15)

$$\mathbf{M}_n^+ = \begin{bmatrix} \widehat{\mathbf{L}}^+ + \widehat{\mathbf{e}}\mathbf{b}^{\mathrm{T}} \\ \mathbf{b}^{\mathrm{T}} \end{bmatrix} \tag{17}$$

By looking carefully at (17), we observe that $\widehat{\mathbf{L}}^+$ can be obtained from $\mathbf{M}_n^+$ by subtracting the nth row of $\mathbf{M}_n^+$ (that is, $\mathbf{b}^{\mathrm{T}}$) from all the rows of $\mathbf{M}_n^+$. Indeed,

$\widehat{\mathbf{e}}\mathbf{b}^{\mathrm{T}}$ is a matrix repeating $\mathbf{b}^{\mathrm{T}}$ on all its rows:

$$\widehat{\mathbf{e}}\mathbf{b}^{\mathrm{T}} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \mathbf{b}^{\mathrm{T}} = \begin{bmatrix} \mathbf{b}^{\mathrm{T}} \\ \mathbf{b}^{\mathrm{T}} \\ \vdots \\ \mathbf{b}^{\mathrm{T}} \end{bmatrix}$$

In other words,

$$\mathbf{M}_n^+ = \begin{bmatrix} \widehat{\mathbf{L}}^+ \\ \mathbf{0}^{\mathrm{T}} \end{bmatrix} + \begin{bmatrix} \mathbf{b}^{\mathrm{T}} \\ \mathbf{b}^{\mathrm{T}} \\ \vdots \\ \mathbf{b}^{\mathrm{T}} \end{bmatrix}$$

This means that $[\widehat{\mathbf{L}}^+]_{ij} = \widehat{l}_{ij}^+ = [\mathbf{M}_n^+]_{ij} - [\mathbf{M}_n^+]_{nj}$.

Exactly the same reasoning holds when we append a $1 \times n$ row vector $\mathbf{a}'^{\mathrm{T}}$ to $\mathbf{M}_n$ in order to obtain $\mathbf{L} = \begin{bmatrix} \mathbf{M}_n \\ \mathbf{a}'^{\mathrm{T}} \end{bmatrix}$. It suffices to transpose $\mathbf{M}_n$ and add a column which verifies $\mathbf{a}' = -\mathbf{M}_n^{\mathrm{T}}\widehat{\mathbf{e}}$. Hence, $\mathbf{d} = (\mathbf{M}_n^{\mathrm{T}})^+\mathbf{a} = -(\mathbf{M}_n^{\mathrm{T}})^+\mathbf{M}_n^{\mathrm{T}}\widehat{\mathbf{e}} = -\widehat{\mathbf{e}}$ since the $n \times (n-1)$ matrix $\mathbf{M}_n^{\mathrm{T}}$ has rank $n-1$ and therefore $(\mathbf{M}_n^{\mathrm{T}})^+\mathbf{M}_n^{\mathrm{T}} = \mathbf{I}$ (this can be shown easily by computing the SVD form of the pseudoinverse matrix (see Theorem 6.2.16 of [27])). By using the same trick as before, we obtain $[\mathbf{M}_n^+]_{ij} = [\mathbf{L}^+]_{ij} - [\mathbf{L}^+]_{in}$.

This allows us to express the elements of $\widehat{\mathbf{L}}^+$ in terms of those of $\mathbf{L}^+$:

$$\begin{aligned} \widehat{l}_{ij}^+ &= [\mathbf{M}_n^+]_{ij} - [\mathbf{M}_n^+]_{nj} = [\mathbf{L}^+]_{ij} - [\mathbf{L}^+]_{in} - [\mathbf{L}^+]_{nj} + [\mathbf{L}^+]_{nn} & (18) \\ &= l_{ij}^+ - l_{in}^+ - l_{nj}^+ + l_{nn}^+ & (19) \end{aligned}$$

By substituting (18) in (14), we obtain

$$o(n|i) = \sum_{j=1}^{n-1} \widehat{l}_{ij}^{-1} b_j = \sum_{j=1}^{n-1} \left(l_{ij}^+ - l_{in}^+ - l_{nj}^+ + l_{nn}^+ \right) b_j = \sum_{j=1}^{n} \left(l_{ij}^+ - l_{in}^+ - l_{nj}^+ + l_{nn}^+ \right) b_j$$

since $\mathbf{L}^+$ is symmetric.

Now, remember that we renumbered the states in order to put state k at the nth row/column. For any arbitrary state, we thus have

$$o(k|i) = \sum_{j=1}^{n} \left(l_{ij}^+ - l_{ik}^+ - l_{kj}^+ + l_{kk}^+ \right) b_j \qquad (20)$$

where $b_i = \sum_{j=1}^{n} a_{ij} c(j|i)$. Notice that in the case of the average first-passage time, $c(j|i) = 1$, and $b_i = \sum_{j=1}^{n} a_{ij} c(j|i) = a_{i.} = d_{ii}$, the sum of the weights reaching node i. Therefore,

$$m(k|i) = \sum_{j=1}^{n} \left(l_{ij}^+ - l_{ik}^+ - l_{kj}^+ + l_{kk}^+ \right) d_{jj} \qquad (21)$$

C   Computation of the average commute time in terms of $\mathbf{L}^+$

Since we already have the formula for the average first-passage time (Equation (21)), computing the average commute time is trivial:

$$
\begin{aligned}
n(i,j) &= m(j|i) + m(i|j) \\
&= \sum_{k=1}^{n} \left(l_{ik}^+ - l_{ij}^+ - l_{jk}^+ + l_{jj}^+ \right) d_{kk} + \sum_{k=1}^{n} \left(l_{jk}^+ - l_{ji}^+ - l_{ik}^+ + l_{ii}^+ \right) d_{kk} \quad (22) \\
&= \sum_{k=1}^{n} \left(l_{ii}^+ + l_{jj}^+ - 2l_{ij}^+ \right) d_{kk} = \left(l_{ii}^+ + l_{jj}^+ - 2l_{ij}^+ \right) \sum_{k=1}^{n} d_{kk} \quad (23) \\
&= V_G \left(l_{ii}^+ + l_{jj}^+ - 2l_{ij}^+ \right) \quad (24)
\end{aligned}
$$

Notice that Equation (23) can be put in matrix form:

$$
n(i,j) = V_G \, (\mathbf{e}_i - \mathbf{e}_j)^{\mathrm{T}} \mathbf{L}^+ (\mathbf{e}_i - \mathbf{e}_j) \quad (25)
$$

and we easily observe that $[n(i,j)]^{1/2}$ is a distance measure in the node space since $\mathbf{L}^+$ is positive semidefinite.

D   Mapping to a space preserving the ECTD

Let us show that the node vectors $\mathbf{e}_i$ can be mapped into a new Euclidean space that preserves the commute time distances. Indeed, every positive semidefinite matrix can be transformed to a diagonal matrix, $\mathbf{\Lambda} = \mathbf{U}^{\mathrm{T}} \mathbf{L}^+ \mathbf{U}$, where $\mathbf{U}$ is an orthonormal matrix made of the eigenvectors of $\mathbf{L}^+$, $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_{n-1}, \mathbf{0}]$: the column vectors $\mathbf{u}_k$ are the orthonormal eigenvectors of $\mathbf{L}^+$, $\mathbf{u}_i^{\mathrm{T}} \mathbf{u}_j = \delta_{ij}$ or $\mathbf{U}^{\mathrm{T}} \mathbf{U} = \mathbf{I}$ (see for instance [46]). Hence we have

$$
\begin{aligned}
n(i,j) &= V_G \, (\mathbf{e}_i - \mathbf{e}_j)^{\mathrm{T}} \mathbf{L}^+ (\mathbf{e}_i - \mathbf{e}_j) = V_G \, (\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}} \mathbf{U}^{\mathrm{T}} \mathbf{L}^+ \mathbf{U} (\mathbf{x}_i - \mathbf{x}_j) \\
&= V_G \, (\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}} \mathbf{\Lambda} (\mathbf{x}_i - \mathbf{x}_j) = V_G \, (\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}} \mathbf{\Lambda}^{1/2} \, \mathbf{\Lambda}^{1/2} (\mathbf{x}_i - \mathbf{x}_j) \\
&= V_G \, (\mathbf{x}_i - \mathbf{x}_j)^{\mathrm{T}} (\mathbf{\Lambda}^{1/2})^{\mathrm{T}} \mathbf{\Lambda}^{1/2} (\mathbf{x}_i - \mathbf{x}_j) = V_G \, (\mathbf{x}_i' - \mathbf{x}_j')^{\mathrm{T}} (\mathbf{x}_i' - \mathbf{x}_j')
\end{aligned}
$$

where we made the transformations

$$
\begin{cases}
\mathbf{e}_i = \mathbf{U} \mathbf{x}_i \\
\mathbf{x}_i' = \mathbf{\Lambda}_i^{1/2} \mathbf{x}
\end{cases}
\quad (26)
$$

So, in this n-dimensional Euclidean space, the transformed node vectors, $\mathbf{x}_i'$, are exactly separated by Euclidean commute time distances.

Now, we easily observe from (26) that if u_i^k is coordinate i of eigenvector $\mathbf{u}_k$ ($[\mathbf{u}_k]_i = u_i^k$) corresponding to eigenvalue λ_k of $\mathbf{L}^+$, and if x_k^i is coordinate k of vector $\mathbf{x}_i$ ($[\mathbf{x}_i]_k = x_k^i$), we obtain $x_k^i = u_i^k$. We thus have $x_k'^i = \sqrt{\lambda_k} u_i^k$ where $x_k'^i$ is coordinate k of vector $\mathbf{x}_i'$ ($[\mathbf{x}_i']_k = x_k'^i$).

In other words, the first coordinate of the n node vectors, $\mathbf{x}_i'$, $i = 1 \ldots n$, corresponding to the *first axis* ($k = 1$) of the transformed space, are $x_1'^1, x_1'^2, \ldots, x_1'^n$,

or $\sqrt{\lambda_1}u_1^1, \sqrt{\lambda_1}u_2^1, \ldots, \sqrt{\lambda_1}u_n^1$, and correspond to the principal eigenvector of $\mathbf{L}^+$ multiplied by $\sqrt{\lambda_1}$. Thus, the first coordinate of these n node vectors is simply the projection of the original node vectors, $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$, on the first eigenvector, $\mathbf{u}_1$, weighted by $\sqrt{\lambda_1}$. More generally, coordinate k of the node vectors in the transformed space is simply the projection of the original node vectors, $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$, on $\mathbf{u}_k$, weighted by $\sqrt{\lambda_k}$. The idea developed in Section 5 is thus to discard the axes (eigenvectors) corresponding to the smallest eigenvalues of $\mathbf{L}^+$.

E $\mathbf{L}^+$ is a kernel

In this section, we show that $\mathbf{L}^+$ is a valid kernel a Gram matrix (see for instance [57, 58]). Indeed, $\mathbf{L}^+$ is the matrix containing the inner products of the transformed vectors $\mathbf{x}'_i$:

$$\mathbf{x}'^{\mathrm{T}}_i \mathbf{x}'_j = (\mathbf{\Lambda}^{1/2}_i \mathbf{x}_i)^{\mathrm{T}} \mathbf{\Lambda}^{1/2}_j \mathbf{x}_j = \mathbf{x}^{\mathrm{T}}_i \mathbf{\Lambda} \mathbf{x}_j = \mathbf{e}^{\mathrm{T}}_i \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{\mathrm{T}} \mathbf{e}_j = \mathbf{e}^{\mathrm{T}}_i \mathbf{L}^+ \mathbf{e}_j = l^+_{ij}$$

Let us also show that the vectors $\mathbf{x}'_i$ are centered (their center of gravity is $\mathbf{0}$):

$$\sum_{i=1}^{n} \mathbf{x}'_i = \mathbf{\Lambda}^{1/2} \sum_{i=1}^{n} \mathbf{x}_i = \mathbf{\Lambda}^{1/2} \mathbf{U}^{\mathrm{T}} \sum_{i=1}^{n} \mathbf{e}_i = \mathbf{\Lambda}^{1/2} \mathbf{U}^{\mathrm{T}} \mathbf{e} \qquad (27)$$

The columns of the orthonormal matrix $\mathbf{U}$ are made of the eigenvectors of $\mathbf{L}^+$ in decreasing order of corresponding eigenvalue. Since the smallest eigenvalue is $\lambda_n = 0$, and the corresponding (unnormalized) eigenvector is $\mathbf{e}$, all the columns of $\mathbf{U}$ are orthogonal to $\mathbf{e}$, except the nth one. Therefore, all the elements of the column vector $\mathbf{U}^{\mathrm{T}}\mathbf{e}$ are zero, except the last (nth) one. But since we further multiply $\mathbf{U}^{\mathrm{T}}\mathbf{e}$ by the diagonal matrix $\mathbf{\Lambda}^{1/2}$ in (27), and the last diagonal element of $\mathbf{\Lambda}$ is 0 (remember that $\lambda_n = 0$), the last (nth) element of $\sum_{i=1}^{n} \mathbf{x}'_i$ is also equal to zero. We therefore obtain $\sum_{i=1}^{n} \mathbf{x}'_i = \mathbf{0}$.

Another way of proving the same fact would be to notice that, from $\mathbf{\Lambda} = \mathbf{U}^{\mathrm{T}}\mathbf{L}^+\mathbf{U}$, we have $\mathbf{\Lambda}^{1/2}\mathbf{U}^{\mathrm{T}} = \mathbf{\Lambda}^{-1/2}\mathbf{U}^{\mathrm{T}}\mathbf{L}^+$. Therefore, $\sum_{i=1}^{n} \mathbf{x}'_i = (\mathbf{\Lambda}^{1/2}\mathbf{U}^{\mathrm{T}})\mathbf{e} = (\mathbf{\Lambda}^{-1/2}\mathbf{U}^{\mathrm{T}}\mathbf{L}^+)\mathbf{e} = \mathbf{0}$ since $\mathbf{L}^+\mathbf{e} = \mathbf{0}$.

Thus, if $\mathbf{X}'$ denotes the data matrix containing the coordinates of the nodes in the transformed space on each row:

$$\mathbf{X}' = [\mathbf{x}'_1, \mathbf{x}'_2, ..., \mathbf{x}'_n]^{\mathrm{T}}, \qquad (28)$$

we have $\mathbf{L}^+ = \mathbf{X}'(\mathbf{X}')^{\mathrm{T}}$ with elements $l^+_{ij} = \mathbf{x}'^{\mathrm{T}}_i \mathbf{x}'_j$.

F   Links with PCA

We will now show that this decomposition is similar to PCA in the sense that the projection has maximal variance among all the possible candidate projections. If $\mathbf{X}'$ denotes the data matrix containing the coordinates of the nodes in the transformed space, $\mathbf{x}'^{\mathrm{T}}_i$, on each row (see (28), in Appendix E), we easily deduce from (26) that $\mathbf{X}' = \mathbf{U}\mathbf{\Lambda}^{1/2}$.

It is well-known that the principal components analysis of a data matrix $\mathbf{X}'$ yields, as kth principal component, the eigenvector, $\mathbf{v}_k$, of $(\mathbf{X}')^{\mathrm{T}}\mathbf{X}'$ (which

is the variance-covariance matrix, since the $\mathbf{x}'_i$ are centered). But $(\mathbf{X}')^{\mathrm{T}}\mathbf{X}' = (\mathbf{U}\mathbf{\Lambda}^{1/2})^{\mathrm{T}}\mathbf{U}\mathbf{\Lambda}^{1/2} = \mathbf{\Lambda}$. Since $\mathbf{\Lambda}$ is a diagonal matrix, we deduce that the $\mathbf{x}'_i$ *are already expressed in the principal components coordinate system* – the eigenvectors of $(\mathbf{X}')^{\mathrm{T}}\mathbf{X}'$ are the basis vectors of the transformed space. Thus, if x'^i_k is coordinate k of vector $\mathbf{x}'_i$, it corresponds to the projection of node i on the kth principal component. The variance, in terms of ECTD, of the nodes cloud on each principal component k is therefore λ_k. An alternative proof of the same result is presented in [54].

We thus conclude that this projection can be viewed as a principal components analysis in the Euclidean space where the nodes are *exactly separated by ECTD*. This decomposition therefore defines the projection of the node vectors that has maximal variance (in terms of the ECTD) among all the possible candidate projections.