



Similarity on Graphs & Hypergraphs

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Abstract

Samenvatting

Deze thesis bespreekt similariteit op grafen & hypergrafen. De notie van similariteit op grafen vindt zijn oorsprong in het HITS-algoritme: dit algoritme werd eind jaren negentig ontdekt om zoekresultaten van een internetzoekmachine op een betekenisvolle manier te sorteren. Het algoritme onderzoekt de relaties tussen de hyperlinks van een verzameling webpagina's: sommige webpagina's worden bestempeld als goede doorverwijzers, andere webpagina's worden dan weer als een gezaghebbende bron beschouwd voor de zoekterm. Uiteraard is deze tweedeling sterk verwant: pagina's die goede doorverwijzers zijn zullen veel links naar pagina's bevatten die als een gezaghebbende bron gezien worden en omgekeerd, zullen pagina's als gezaghebbende bron worden beschouwd als ze veel inkomende links krijgen van goede doorverwijzers. Dit algoritme was erg vernieuwend in die tijd, vermits tot dan toe zoekresultaten enkel gesorteerd werden op het aantal inkomende links (zonder daarbij de bronpagina na te gaan) of het aantal keren dat een zoekterm voorkwam.

Deze methode werd rond 2005 veralgemeend naar een notie van similariteit tussen grafen. Een verzameling webpagina's die onderling gelinkt zijn zoals die in het HITS-algoritme gebruikt worden, kan immers beschouwd worden als een graf. Deze veralgemening leidt tot een methode waarbij we een soort score kunnen klevan op hoe twee toppen van twee verschillende grafen op elkaar lijken. Deze 'similariteitscore' zal hoger zijn als de adjacente toppen van deze twee toppen ook gelijkaardig zijn.

Eens we similariteit op de toppen van grafen hebben ingevoerd, gaan we deze methode verder uitbreiden tot similariteit op toppen en bogen van grafen en tot similariteit tussen gekleurde grafen. We hebben zo een compleet overzicht van de meest recente studies over het onderwerp. Opvallend is dat de convergentie van de resulterende algoritmes van al deze uitbreidingen met dezelfde convergentiestelling kunnen bewezen worden.

Een belangrijke opmerking is hier wel dat deze verschillende uitbreidingen lichtjes andere resultaten opleveren. Er bestaat niet zoiets als 'de' similariteitsscore tussen twee toppen van twee grafen, eenvoudigweg omdat elke uitbreiding een licht verschillend resultaat zal opleveren. Daarom zijn deze similariteitscores vooral in verhouding tot de andere scores interessant: we kunnen bv. gemakkelijk bepalen welke top van de ene graf, het meest lijkt op de top van een andere graf simpelweg door de grootste similariteitsscore te bekijken. Dit zal ook blijken uit het korte overzicht van toepassingen dat op het einde van deze masterproef is toegevoegd, ook daar wordt een similariteitsscore enkel in verhouding tot de andere similariteitscores bekeken.

In het voorlaatste hoofdstuk ontdekken we tot slot nieuw terrein: we proberen via tensoren het concept van similariteit over te brengen op de meer algemene structuur van hypergrafen. Een generalizatie die wonderwel slaagt door de tensoren zo om te vormen dat we opnieuw dezelfde convergentiestelling als bij grafen toe te passen. Toch is er ook een grote maar, want net zoals bij de meeste andere uitbreidingen via tensoren, is ook hier de vloek van de

dimensionaliteit nooit ver weg.

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Chapter 1

Preliminaries and notations

The Perron-Frobenius theorem states that a real square matrix with nonnegative entries has a unique largest real eigenvalue with an eigenvector that has only positive entries. The theorem was proved by Oskar Perron (1880-1975) in 1907 for strictly positive entries and extended by Ferdinand Georg Frobenius (1849-1917) to irreducible matrices with nonnegative entries.

1.1 Some families of matrices

In this section, we first introduce different kinds of matrices. Note that all matrices in this master thesis have real entries, unless otherwise stated. We start with permutation matrices and their uses. With permutation matrices, we can introduce irreducible matrices. Also nonnegative and primitive square matrices are presented. After defining those, we look at the Perron-Frobenius theorem.

1.1.1 Permutation matrices

Definition 1.1.1. *Given a permutation π of n elements:*

$$\pi : \{1, \dots, n\} \rightarrow \{1, \dots, n\},$$

with:

$$\pi = \begin{pmatrix} 1 & 2 & \cdots & n \\ \pi(1) & \pi(2) & \cdots & \pi(n) \end{pmatrix}$$

*the associated **permutation matrix** P_π is the $n \times n$ -matrix obtained by permuting the rows of the identity matrix I_n according to π . So:*

$$P_\pi = \begin{bmatrix} e_{\pi(1)}^T \\ e_{\pi(2)}^T \\ \vdots \\ e_{\pi(n)}^T \end{bmatrix}.$$

where e_j is the j -th column of I_n .

Example 1.1.2. The permutation matrix P_π corresponding to the permutation

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 2 & 3 \end{pmatrix}$$

is:

$$P_\pi = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Note that $p_{ij} = 1$ if and only if $\pi(i) = j$.

Property 1.1.3. A permutation matrix P satisfies:

$$PP^T = I_n,$$

where P^T is the transpose and I_n is the identity matrix.

Proof. By direct computation, we get:

$$(PP^T)_{ij} = \sum_{k=1}^n P_{ik}P_{kj}^T = \sum_{k=1}^n P_{ik}P_{jk}$$

Assume $i \neq j$. Then for each k , $P_{ik}P_{jk} = 0$ since there is only one nonzero entry in the k -th row and $i \neq j$, P_{ik} and P_{jk} can't be both the nonzero entry. So, $(PP^T)_{ij} = 0$ when $i \neq j$.

When $i = j$, then there exists a $k' \in \{1, \dots, n\}$ with $P_{ik'}P_{jk'} = 1$, since there is only one nonzero entry in the k -th row, this k' is unique, which results in $\sum_{k=1}^n P_{ik}P_{jk} = (PP^T)_{ij} = 1$.

In other words,

$$(PP^T)_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases},$$

this is exactly the formula for the entries of the identity matrix. □

Corollary 1.1.4. The transpose of a permutation matrix P is its inverse:

$$P^T = P^{-1}.$$

This can also more easily be concluded by the fact that a permutation matrix is clearly an orthogonal matrix (a real $n \times n$ -matrix with orthonormal entries).

1.1.2 Nonnegative and primitive matrices

Definition 1.1.5. Let A and B be two real $n \times r$ -matrices. Then, $A \geq B$ (respectively $A > B$) if $a_{ij} \geq b_{ij}$ (respectively $a_{ij} > b_{ij}$) for all $1 \leq i \leq n, 1 \leq j \leq r$.

Definition 1.1.6. A real $n \times r$ -matrix A is **nonnegative** if $A \geq 0$, with 0 the $n \times r$ -null matrix.

Definition 1.1.7. A real $n \times r$ -matrix A is **positive** if $A > 0$, with 0 the $n \times r$ -null matrix.

Since row vectors are $1 \times n$ -matrices, we shall use the terms nonnegative and positive vector throughout.

Notation 1.1.8. Let B be an arbitrary complex $n \times r$ -matrix, then $|B|$ denotes the matrix with entries $|b_{ij}|$. This is not to be confused with the determinant of a square matrix B , which we denote by $\det(B)$.

Definition 1.1.9. A nonnegative square matrix A is called **primitive** if there is a $k \in \mathbb{N}_0$ such that all entries of A^k are positive.

1.1.3 Irreducible nonnegative matrices

In developing the Perron-Frobenius theory, we shall first establish a series of theorems and lemmas on nonnegative irreducible square matrices.

Definition 1.1.10. A square matrix A is called **reducible** if there is a permutation matrix P such that

$$PAP^T = \begin{pmatrix} B & 0 \\ C & D \end{pmatrix}$$

where B , and D are square matrices, each of size at least one and 0 is a zero matrix. A square matrix A is called **irreducible** if it is not reducible.

It follows immediately that a 1×1 -matrix is always irreducible by definition. We now show a useful property to identify a reducible matrix.

Property 1.1.11. Let A be an $n \times n$ -matrix with $n \geq 2$. Consider a nonempty, proper subset S of $\{1, \dots, n\}$ with $a_{ij} = 0$ for $i \in S$, $j \notin S$. Then A is reducible.

Proof. Let $S = \{i_1, i_2, \dots, i_k\}$, where we assume, without loss of generality, that $i_1 < i_2 < \dots < i_{k-1} < i_k$. Let S^c be the complement of S , consisting of the ordered set of elements $j_1 < j_3 < \dots < j_{n-k}$. Consider the permutation σ of $\{1, 2, \dots, n\}$ given by

$$\sigma = \begin{pmatrix} 1 & 2 & \dots & k & k+1 & k+2 & \dots & n \\ i_1 & i_2 & \dots & i_k & j_1 & j_2 & \dots & j_{n-k} \end{pmatrix}$$

σ can be represented by the permutation matrix $P_\sigma = (p_{ij})$, where $p_{rs} = 1$ if $\sigma(r) = s$. We prove that

$$PAP^T = \begin{pmatrix} B & 0 \\ C & D \end{pmatrix}$$

where B and D are square matrices and 0 is a $k \times (n - k)$ zero matrix. Consider row c and column d , where $1 \leq c \leq k$ and $k + 1 \leq d \leq n$:

$$(PAP^T)_{cd} = \sum_i \sum_j p_{ci} a_{ij} p_{dj}. \quad (1.1)$$

It is enough to show that each term in the summation is zero. Suppose $p_{ci} = p_{dj} = 1$. Thus $\sigma(c) = i$ and $\sigma(d) = j$. Since $1 \leq c \leq k$, then $i \in \{i_1, i_2, \dots, i_k\}$; similarly, since $k + 1 \leq d \leq n$, we have $j \in \{j_1, j_2, \dots, j_{n-k}\}$. By assumption, for such a pair i, j , we have $a_{ij} = 0$. That completes the proof. \square

We now prove some equivalent definitions for a nonnegative, irreducible square matrix.

Theorem 1.1.12. *Let $A \geq 0$ be a nonnegative $n \times n$ -matrix. Then the following conditions are equivalent:*

- (1) A is irreducible.
- (2) $(I + A)^{n-1} > 0$
- (3) For any pair (i, j) , with $1 \leq i, j \leq n$, there is a positive integer $k = k(i, j) \leq n$ such that $(A^k)_{ij} > 0$.

Proof. (1) \Rightarrow (2): Let $\mathbf{x} \geq 0, \mathbf{x} \neq \mathbf{0}$ be an arbitrary vector in \mathbb{R}^n . If a coordinate of \mathbf{x} is positive, the same coordinate is positive in $\mathbf{x} + A\mathbf{x} = (I + A)\mathbf{x}$ as well. We claim that $(I + A)\mathbf{x}$ has fewer zero coordinates than \mathbf{x} as long as \mathbf{x} has a zero coordinate. If this claim is not true, then the number of zero coordinates must be at least equal, this means that for each coordinate j with $x_j = 0$ we would have that $x_j + (A\mathbf{x})_j = 0$. Let $J = \{j : x_j > 0\}$. For any $j \notin J, r \in J$, we have $(A\mathbf{x})_j = \sum_k a_{jk}x_k = 0$ and $x_r > 0$. It must be that $a_{jr} = 0$. It follows from Property 1.1.11 that A is reducible, which is a contradiction and the claim is proved. Thus $(I + A)\mathbf{x}$ has at most $n - 2$ zero coordinates. Continuing in this manner we conclude that $(I + A)^{n-1}\mathbf{x} > 0$. Let $\mathbf{x} = \mathbf{e}_i$, then the corresponding column of $(I + A)^{n-1}$ must be positive. Thus (2) holds.

(2) \Rightarrow (3): We have $(I + A)^{n-1} > 0, A \geq 0$, so $A \neq 0$ and

$$A(I + A)^{n-1} = \sum_{k=1}^n \binom{n-1}{k-1} A^k > 0.$$

Thus for any i, j at least one of the matrices A, A^2, \dots, A^n has its (i, j) -th element entry positive.

(3) \Rightarrow (1): Suppose A is reducible. Then for some permutation matrix P ,

$$PAP^T = \begin{pmatrix} B_1 & 0 \\ C_1 & D_1 \end{pmatrix}$$

where B_1 and D_1 are square matrices. Furthermore, we know from Property 1.1.3 that $PAP^T PAP^T = PA^2P^T$, whence for some square matrices B_2, C_2 we have:

$$PA^2P^T = \begin{pmatrix} B_2 & 0 \\ C_2 & D_2 \end{pmatrix}$$

More generally, for some matrix C_t and square matrices B_t and D_t ,

$$PA^tP^T = \begin{pmatrix} B_t & 0 \\ C_t & D_t \end{pmatrix}$$

Thus $(PA^tP^T)_{rs} = 0$ for $t = 1, 2, \dots$ and for any r, s corresponding to an entry of the zero submatrix in PAP^T . Now, for $t = 1, \dots, n$:

$$0 = (PA^tP^T)_{rs} = \sum_k \sum_l p_{rk} a_{kl}^{(t)} p_{st}$$

By using the same reasoning as in 1.1, choose k, l so that $p_{rk} = p_{st} = 1$. Then $a_{kl}^{(t)} = 0$ for all t , contradicting the hypothesis. This completes the proof. \square

Corollary 1.1.13. *If A is irreducible then $I + A$ is primitive.*

Corollary 1.1.14. *A^T is irreducible whenever A is irreducible.*

Property 1.1.15. *No row or column of an irreducible matrix A can vanish. This means that A cannot have a row or a column of zeros.*

Proof. Suppose that A has a zero row, then it could be permuted to

$$PAP^T = \begin{pmatrix} 0 & 0 \dots 0 \\ c_1 & \\ \vdots & D \\ c_n & \end{pmatrix}$$

by some permutation matrix P . It follows from Definition 1.1.10 that A is reducible. Similarly, if A has zero column, it can be permuted to

$$PAP^T = \begin{pmatrix} & 0 \\ B & \vdots \\ & 0 \\ c_1 \dots c_n & 0 \end{pmatrix}$$

again from Definition 1.1.10 we conclude that A is reducible. □

1.2 Perron-Frobenius Theorem

1.2.1 Spectral radii of nonnegative matrices

Definition 1.2.1. *Let A be an $n \times n$ -matrix with complex entries and eigenvalues λ_i , $1 \leq i \leq n$. Then:*

$$\rho(A) = \max_{1 \leq i \leq n} |\lambda_i|$$

*is called the **spectral radius** of the matrix A .*

Geometrically, if all the eigenvalues λ_i of A are plotted in the complex plane, then $\rho(A)$ is the radius of the smallest disk $|z| \leq R$, with center at the origin, which includes all the eigenvalues of the matrix A .

We now establish a series of lemmas on nonnegative irreducible square matrices. These lemmas will allow us to prove the Perron-Frobenius at the end of this section.

If $A \geq 0$ is an irreducible $n \times n$ -matrix and \mathbf{x} , a vector of size n with $\mathbf{0} \neq \mathbf{x} \geq 0$, let

$$r_{\mathbf{x}} = \min \left\{ \frac{\sum_{j=1}^n a_{ij}x_j}{x_i} \right\} \quad (1.2)$$

where the minimum is taken over all i for which $x_i > 0$. Clearly, $r_{\mathbf{x}}$ is a nonnegative real number and is the supremum of all $p \geq 0$ for which

$$A\mathbf{x} \geq p\mathbf{x} \quad (1.3)$$

We now consider the nonnegative quantity r defined by

$$r = \sup_{\substack{\mathbf{x} \geq 0 \\ \mathbf{x} \neq 0}} \{r_{\mathbf{x}}\} \quad (1.4)$$

As $r_{\mathbf{x}}$ and $r_{\alpha\mathbf{x}}$ have the same value for any scalar $\alpha > 0$, we need consider only the set B of vectors $\mathbf{x} \geq 0$ with $\|\mathbf{x}\| = 1$, and we correspondingly let Q be the set of all vectors $\mathbf{y} = (I + A)^{n-1}\mathbf{x}$ where $\mathbf{x} \in B$. From Theorem 1.1.12, Q consists only of positive vectors. Multiplying both sides of the inequality $A\mathbf{x} \geq r_{\mathbf{x}}\mathbf{x}$ by $(I + A)^{n-1}$, we obtain:

$$\forall \mathbf{y} \in Q : A\mathbf{y} \geq r_{\mathbf{x}}\mathbf{y},$$

and we conclude from (1.3) that $r_{\mathbf{y}} \geq r_{\mathbf{x}}$. Therefore, the quantity r of (1.4) can be defined equivalently as:

$$r = \sup_{\mathbf{y} \in Q} \{r_{\mathbf{y}}\} \quad (1.5)$$

As B is a compact set (in the usual topology) of vectors, so is Q , and as $r_{\mathbf{y}}$ is a continuous function on Q , we know from the extreme value theorem that there necessarily exists a positive vector \mathbf{z} for which:

$$A\mathbf{z} \geq r\mathbf{z}, \quad (1.6)$$

and no vector $\mathbf{w} \geq 0$ exists for which $A\mathbf{w} > r\mathbf{w}$.

Definition 1.2.2. We call all nonnegative, nonzero vectors \mathbf{z} satisfying (1.6) **extremal vectors** of the matrix A .

Lemma 1.2.3. If $A \geq 0$ is an irreducible $n \times n$ -matrix, the quantity r of (1.4) is positive.

Proof. If \mathbf{x} is the positive vector whose coordinates are all unity, then since the matrix A is irreducible, we know from Property 1.1.15 that no row of A can vanish, and consequently no component of $A\mathbf{x}$ can vanish. Thus, $r_{\mathbf{x}} > 0$, proving that $r > 0$. \square

Lemma 1.2.4. If $A \geq 0$ is an irreducible $n \times n$ -matrix, each extremal vector \mathbf{z} is a positive eigenvector of A with corresponding eigenvalue r of (1.4), i.e., $A\mathbf{z} = r\mathbf{z}$ and $\mathbf{z} > 0$.

Proof. Let \mathbf{z} be an extremal vector with $A\mathbf{z} - r\mathbf{z} = \mathbf{t}$. If $\mathbf{t} \neq 0$, then some coordinate of \mathbf{t} is positive; multiplying through by the matrix $(I + A)^{n-1}$, we have:

$$A\mathbf{w} - r\mathbf{w} > 0, \text{ with } \mathbf{w} = (I + A)^{n-1}\mathbf{z}$$

from Theorem 1.1.12 we know that $\mathbf{w} > 0$. It would then follow that $r_{\mathbf{w}} > r$, contradicting the definition of r in (1.5). Thus $A\mathbf{z} = r\mathbf{z}$, and since $\mathbf{w} > 0$ and $\mathbf{w} = (I + A)^{n-1}\mathbf{z}$, then we have $\mathbf{z} > 0$, completing the proof. \square

Lemma 1.2.5. Let $A \geq 0$ be an irreducible $n \times n$ -matrix, and let B be an $n \times n$ - complex matrix with $|B| \leq A$. If β is any eigenvalue of B , then

$$|\beta| \leq r, \quad (1.7)$$

where r is the positive quantity of (1.4). Moreover, equality is valid in (1.7), i.e., $\beta = re^{i\phi}$, if and only if $|B| = A$, and where B has the form:

$$B = e^{i\phi} D A D^{-1}, \quad (1.8)$$

and D is a diagonal matrix whose diagonal entries have modulus unity.

Proof. If $\beta \mathbf{y} = B\mathbf{y}$ where $\mathbf{y} \neq \mathbf{0}$, then

$$\beta y_i = \sum_{j=1}^n b_{ij} y_j, \text{ with } 1 \leq i \leq n.$$

Using the hypotheses of the lemma and the notation of Definition 1.1.8, it follows that:

$$|\beta| |\mathbf{y}| \leq |B| |\mathbf{y}| \leq A |\mathbf{y}|, \quad (1.9)$$

which implies that $|\beta| \leq r_{|\mathbf{y}|} \leq r$, proving (1.7). If $|\beta| = r$, then $|\mathbf{y}|$ is an extremal vector of A . Therefore, from Lemma 1.2.4, $|\mathbf{y}|$ is a positive eigenvector of A corresponding to the positive eigenvalue r . Thus,

$$r |\mathbf{y}| = |B| |\mathbf{y}| = A |\mathbf{y}|, \quad (1.10)$$

and since $|\mathbf{y}| > 0$, we conclude from (1.10) and the hypothesis $|B| \leq A$ that

$$|B| = A \quad (1.11)$$

For the vector \mathbf{y} , where $|\mathbf{y}| > 0$, let

$$D = \text{diag} \left\{ \frac{y_1}{|y_1|}, \dots, \frac{y_n}{|y_n|} \right\}.$$

It is clear that the diagonal entries of D have modulus unity, and

$$\mathbf{y} = D |\mathbf{y}|. \quad (1.12)$$

Setting $\beta = re^{i\phi}$, then $B\mathbf{y} = \beta \mathbf{y}$ can be written as:

$$C |\mathbf{y}| = r |\mathbf{y}|, \quad (1.13)$$

where

$$C = e^{-i\phi} D^{-1} B D. \quad (1.14)$$

From (1.10) and (1.13), equating terms equal to $r |\mathbf{y}|$ we have

$$C |\mathbf{y}| = |B| |\mathbf{y}| = A |\mathbf{y}|. \quad (1.15)$$

From the definition of the matrix C in (1.14), $|C| = |B|$. Combining with (1.11), we have:

$$|C| = |B| = A. \quad (1.16)$$

Thus, from (1.15) we conclude that $C |\mathbf{y}| = |C| |\mathbf{y}|$, and as $|\mathbf{y}| > 0$, it follows that $C = |C|$ and thus $C = A$ from (1.16). Combining this result with (1.14), gives the desired result that $B = e^{i\phi} D A D^{-1}$. Conversely, it is obvious that if B has the form in (1.8), then $|B| = A$, and B has an eigenvalue β with $|\beta| = r$, which completes the proof. \square

Corollary 1.2.6. *If $A \geq 0$ is an irreducible $n \times n$ -matrix, then the positive eigenvalue r of Lemma 1.2.4 equals the spectral radius $\rho(A)$ of A*

Proof. Setting $B = A$ in Lemma 1.2.5 immediately gives us this result. \square

In other words, if $A \geq 0$ is an irreducible $n \times n$ -matrix, its spectral radius $\rho(A)$ is positive, and the intersection in the complex plane of the circle $|z| = \rho(A)$ with the positive real axis is an eigenvalue of A .

Definition 1.2.7. A **principal square submatrix** of an $n \times n$ -matrix A is any matrix obtained by crossing out any j rows and the corresponding j columns of A , with $1 \leq j \leq n$.

Lemma 1.2.8. *If $A \geq 0$ is an irreducible $n \times n$ -matrix, and B is any principal square submatrix of A , then $\rho(B) < \rho(A)$.*

Proof. If B is any principal submatrix of A , then there is an $n \times n$ -permutation matrix P such that $B = A_{11}$ where

$$C = \begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix}; PAP^T = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad (1.17)$$

Here, A_{11} and A_{22} are, respectively, $m \times m$ and $(n-m) \times (n-m)$ principal square submatrices of PAP^T , $1 \leq m \leq n$. Clearly, $0 \leq C \leq PAP^T$, and $\rho(C) = \rho(B) = \rho(A_{11})$, but as $C = |C| \neq PAP^T$, the conclusion follows immediately from Lemma 1.2.5 and Corollary 1.2.6. \square

The following lemma is used to prove that $\rho(A)$ is a simple eigenvalue of A in the Perron-Frobenius theorem. The proof uses the extension of the product rule of derivation for multilinear functions $M(a_1, \dots, a_k)$. Suppose x_1, \dots, x_k are differentiable vector functions, then $M(x_1, \dots, x_k)$ is differentiable and:

$$\frac{d}{dt} M(x_1, \dots, x_k) = M\left(\frac{d}{dt} x_1, x_2, \dots, x_k\right) + M\left(x_1, \frac{d}{dt} x_2, \dots, x_k\right) + \dots + M\left(x_1, x_2, \dots, \frac{d}{dt} x_k\right)$$

The most important application of this rule is for the derivative of the determinant:

$$\frac{d}{dt} \det(x_1, \dots, x_k) = \det\left(\frac{d}{dt} x_1, x_2, \dots, x_k\right) + \det\left(x_1, \frac{d}{dt} x_2, \dots, x_k\right) + \dots + \det\left(x_1, x_2, \dots, \frac{d}{dt} x_k\right)$$

Lemma 1.2.9. *Let A be an $n \times n$ -matrix over the complex numbers and let $\phi(A, \lambda) = \det(\lambda I_n - A)$ be the characteristic polynomial of A . Let B_i be the principal submatrix of A formed by deleting the i -th row and column of A and let $\phi(B_i, \lambda)$ be the characteristic polynomial of B_i . Then:*

$$\phi'(A, \lambda) = \frac{d\phi(A, \lambda)}{d\lambda} = \sum_i \phi(B_i, \lambda)$$

Proof. The proof is immediately done by direct computation:

$$\phi(A, \lambda) = \det \begin{bmatrix} \lambda - a_{1,1} & -a_{1,2} & \dots & -a_{1,n} \\ -a_{2,1} & \lambda - a_{2,2} & \dots & -a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n,1} & -a_{n,2} & \dots & \lambda - a_{n,n} \end{bmatrix}.$$

Using the extension of the product rule of derivation for multilinear functions

$$\begin{aligned} \phi'(A, \lambda) = \det \begin{bmatrix} 1 & 0 & \dots & 0 \\ -a_{2,1} & \lambda - a_{2,2} & \dots & -a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n,1} & -a_{n,2} & \dots & \lambda - a_{n,n} \end{bmatrix} + \det \begin{bmatrix} \lambda - a_{1,1} & -a_{1,2} & \dots & -a_{1,n} \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -a_{n,1} & -a_{n,2} & \dots & \lambda - a_{n,n} \end{bmatrix} + \dots \\ + \det \begin{bmatrix} \lambda - a_{1,1} & -a_{1,2} & \dots & -a_{1,n} \\ -a_{2,1} & \lambda - a_{2,2} & \dots & -a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix} = \sum_i \phi(B_i, \lambda). \end{aligned}$$

□

1.2.2 Proof

We now collect the above results into the following main theorem: we finally arrived at the Perron-Frobenius Theorem:

Theorem 1.2.10. (Perron-Frobenius theorem) *Let $A \geq 0$ be an irreducible $n \times n$ -matrix. Then,*

1. *A has a positive real eigenvalue equal to its spectral radius.*
2. *To $\rho(A)$ there corresponds an eigenvector $\mathbf{x} > 0$.*
3. *$\rho(A)$ increases when any entry of A increases.*
4. *$\rho(A)$ is a simple eigenvalue of A .*
5. *If $A\mathbf{x} = \rho(A)\mathbf{x}$ where $\mathbf{x} > 0$ and \mathbf{x} is a normalized vector, then \mathbf{x} is unique.*

Proof. (1) and (2) follow immediately from Lemma 1.2.4 and Corollary 1.2.6.

(3) Suppose we increase some entry of the matrix A , giving us a new irreducible matrix \tilde{A} where $\tilde{A} \geq A$ and $\tilde{A} \neq A$. Applying Lemma 1.2.5, we conclude that $\rho(\tilde{A}) > \rho(A)$.

(4) $\rho(A)$ is a simple eigenvalue of A , i.e., $\rho(A)$ is a zero of multiplicity one of the characteristic polynomial $\phi(\lambda) = \det(\lambda I_n - A)$, we make use of Lemma 1.2.9 by using the fact that $\phi'(\lambda)$ is the sum of the determinants of the principal $(n-1) \times (n-1)$ submatrices of $\lambda I - A$. If A_i is any principal submatrix of A , then from Lemma 1.2.8, $\det(\lambda I - A_i)$ (with I the identity matrix with the same size as the principal submatrix A_i) cannot vanish for any $\lambda \geq \rho(A)$. From this it follows that:

$$\det(\rho(A)I - A_i) > 0,$$

and thus

$$\phi'(\rho(A)) > 0.$$

Consequently, $\rho(A)$ cannot be a zero of $\phi(\lambda)$ of multiplicity greater than one and thus $\rho(A)$ is a simple eigenvalue of A .

(5) If $A\mathbf{x} = \rho(A)\mathbf{x}$ where $\mathbf{x} > 0$ and $\|\mathbf{x}\| = 1$ ($\|\mathbf{x}\|$ denotes the standard Euclidean norm), we cannot find another eigenvector $\mathbf{y} \neq s\mathbf{x}$, with s a scalar, of A with $A\mathbf{y} = \rho(A)\mathbf{y}$, so that the eigenvector \mathbf{x} , meaning that the normalized eigenvector \mathbf{x} is uniquely determined. □

With the previous proof in mind, the following definition comes not unexpected:

Definition 1.2.11. *If a matrix A has an eigenvalue equal to the spectral radius $\rho(A)$, this eigenvalue is called the **Perron root**, the corresponding eigenvector \mathbf{x} such that:*

$$A\mathbf{x} = \rho(A)\mathbf{x} \quad \text{and} \quad \|\mathbf{x}\|_1 = 1$$

*s called the **Perron vector**.*

1.2.3 Example

To check whether a matrix with nonnegative entries is primitive, irreducible or neither, we just have to replace all nonzero entries by 1 since this does not affect the classification. The matrix

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

is strictly positive and thus primitive. The matrices

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

both have 1 as a double eigenvalue hence can not be irreducible. The matrix $\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$ satisfies:

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$$

and hence is primitive. The same goes for

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix},$$

this matrix is irreducible but not primitive. Its eigenvalues are 1 and -1 .

1.3 Norms

If one has several vectors in \mathbb{R}^n or several matrices in $\mathbb{R}^{n \times m}$, how do we measure that some of them are ‘large’ and some of them are ‘small’? One way to answer this question is to study norms, which are basically functions that assign a positive ‘size’ to a vector in a vector space. The norms that we define in this master thesis are limited to \mathbb{R}^n and $\mathbb{R}^{n \times m}$ and we call them respectively *vector norms* (norms on \mathbb{R}^n) and *matrix norms* (norms on $\mathbb{R}^{n \times m}$). This section is mainly based on chapter 2 from [GOLUB] and chapter 5 from [HORN].

1.3.1 Vector norms

Definition 1.3.1. *A **vector norm** on \mathbb{R}^n is a function $\|\cdot\| : \mathbb{R}^n \rightarrow \mathbb{R}$ with the following properties:*

1. $\|\mathbf{x}\| \geq 0$, for all $\mathbf{x} \in \mathbb{R}^n$ with equality if and only if $\mathbf{x} = \mathbf{0}$.

2. $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.
3. $\|\alpha\mathbf{x}\| = |\alpha|\|\mathbf{x}\|$ for all $\alpha \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^n$.

We now give some well known vector norms:

***p*-norms**

Definition 1.3.2. *The Hölder or p-norms are defined by:*

$$\|\mathbf{x}\|_p = (\|x_1\|^p + \cdots + \|x_n\|^p)^{\frac{1}{p}} = \left(\sum_{i=1}^n |\mathbf{x}_i|^p \right)^{\frac{1}{p}},$$

for $\mathbf{x} \in \mathbb{R}^n$.

The 1-norm is also known as the *Manhattan* norm:

$$\|\mathbf{x}\|_1 = |x_1| + \cdots + |x_n|$$

The 2-norm is also known as the standard *Euclidean* norm:

$$\|\mathbf{x}\|_2 = (|x_1|^2 + \cdots + |x_n|^2)^{\frac{1}{2}} = (\text{trace}(\mathbf{x}^T \mathbf{x}))^{\frac{1}{2}}$$

Notice that the 2-norm is invariant under orthogonal transformation, for if $Q^T Q = I$ with $Q \in \mathbb{R}^{n \times n}$ and $\mathbf{x} \in \mathbb{R}^n$:

$$\|Q\mathbf{x}\|_2^2 = \text{trace}(\mathbf{x}^T Q^T Q \mathbf{x}) = \text{trace}(\mathbf{x}^T \mathbf{x}) = \|\mathbf{x}\|_2^2$$

Maximum norm

Finally, when $p \rightarrow \infty$ we get the *maximum* norm:

$$\|\mathbf{x}\|_\infty = \max(|x_1|, \dots, |x_n|)$$

We will prove this:

Theorem 1.3.3. *Let $\mathbf{x} \in \mathbb{R}^n$ then:*

$$\lim_{p \rightarrow \infty} \|\mathbf{x}\|_p = \|\mathbf{x}\|_\infty = \max(|x_1|, \dots, |x_n|)$$

Proof. Rewrite $\|\mathbf{x}\|_p$ as:

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{\frac{1}{p}} = \|\mathbf{x}\|_\infty \left(\sum_{i=1}^n \left(\frac{|x_i|}{\|\mathbf{x}\|_\infty} \right)^p \right)^{\frac{1}{p}}$$

Note that $\left(\frac{|x_i|}{\|\mathbf{x}\|_\infty} \right) \leq 1$ for every i , with equality at least once and at most n times, then:

$$\|\mathbf{x}\|_\infty \leq \|\mathbf{x}\|_p \leq \|\mathbf{x}\|_\infty n^{\frac{1}{p}}$$

because $n > 0$, we get $\lim_{p \rightarrow \infty} n^{\frac{1}{p}} = 1$, then:

$$\lim_{p \rightarrow \infty} \|\mathbf{x}\|_p = \|\mathbf{x}\|_\infty.$$

□

Norm equivalence

One very import property of all the norms of \mathbb{R}^n is that they are all *equivalent*, meaning that when two vectors have about the same size according to one vector norm, they also will have more or less the same size according to another vector norm.

Theorem 1.3.4. *All norms on \mathbb{R}^n are equivalent, i.e., if $\|\cdot\|_\alpha$ and $\|\cdot\|_\beta$ are norms on \mathbb{R}^n , then there exist positive constants $c_1, c_2 \in \mathbb{R}^+$ such that:*

$$c_1 \|\mathbf{x}\|_\alpha \leq \|\mathbf{x}\|_\beta \leq c_2 \|\mathbf{x}\|_\alpha$$

Proof. We demonstrate that any norm $\|\cdot\|_\alpha$ on \mathbb{R}^n is equivalent to the Euclidean norm. Let $\{\mathbf{e}_1, \dots, \mathbf{e}_n\}$ be the canonical basis for \mathbb{R}^n , so any $\mathbf{x} \in \mathbb{R}^n$ can be written as $x = \sum_{i=1}^n x_i \mathbf{e}_i$. For all pairs of vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ we check that $\|\cdot\|_\alpha$ is continuous with respect to the Euclidean norm and we get using the Cauchy-Schwarz inequality:

$$\begin{aligned} \|\mathbf{x} - \mathbf{y}\|_\alpha &= \left\| \sum_{i=1}^n (x_i - y_i) \mathbf{e}_i \right\|_\alpha \\ &\leq \sum_{i=1}^n (x_i - y_i) \|\mathbf{e}_i\|_\alpha \\ &\leq \max_{1 \leq i \leq n} (\|\mathbf{e}_i\|_\alpha) \sum_{i=1}^n (x_i - y_i) \\ &\leq M \left(\sum_{i=1}^n (x_i - y_i)^2 \right)^{\frac{1}{2}} \\ &= M \|\mathbf{x} - \mathbf{y}\|_2, \end{aligned}$$

with $M = \max_{1 \leq i \leq n} (\|\mathbf{e}_i\|_\alpha)$. This means that when two vectors are nearby with respect to the Euclidean norm, they are also nearby with respect to any other norm. Now consider the unit sphere with respect to the Euclidean norm $S = \{\mathbf{x} \in \mathbb{R}^n : \|\mathbf{x}\|_2 = 1\}$. This set is closed and bounded in the Euclidean topology, so the theorem of Heine-Borel (see Theorem 3.5.2 in [CAENEPEEL]) shows that it is compact. Therefore, the continuous function $\|\cdot\|_\alpha$ attains it's maximum and minimum values on S , say c'_1 and c'_2 . That is,

$$c'_1 \|\mathbf{x}\|_2 \leq \|\mathbf{x}\|_\alpha \leq c'_2 \|\mathbf{x}\|_2$$

for any \mathbf{x} with on the Euclidean unit sphere. But every vector $\mathbf{y} \in \mathbb{R}^n$ can be expressed as $\mathbf{y} = \alpha \mathbf{x}$ for some \mathbf{x} on the Euclidean unit sphere. If we multiply the foregoing inequality by $|\alpha|$ and draw the scalar into the norms, we get:

$$c'_1 \|\mathbf{y}\|_2 \leq \|\mathbf{y}\|_\alpha \leq c'_2 \|\mathbf{y}\|_2$$

for any vector \mathbf{y} . We must check that the constants c'_1 and c'_2 are positive. They are clearly nonnegative since $\|\cdot\|_\alpha$ is nonnegative and $c'_1 \leq c'_2$ by definition. Assume that $c'_1 = 0$, which implies the existence of a point \mathbf{x} on the Euclidean unit sphere for which $\|\mathbf{x}\|_\alpha = 0$, but then $x = 0$, a contradiction. So, we have proved that we can find c'_1, c'_2, c''_1, c''_2 such that:

$$\begin{aligned} c'_1 \|\mathbf{y}\|_2 &\leq \|\mathbf{y}\|_\alpha \leq c'_2 \|\mathbf{y}\|_2 \\ c''_1 \|\mathbf{y}\|_2 &\leq \|\mathbf{y}\|_\beta \leq c''_2 \|\mathbf{y}\|_2 \end{aligned}$$

so we get:

$$\frac{1}{c_2'} \|\mathbf{y}\|_\alpha \leq \|\mathbf{y}\|_2 \leq \frac{1}{c_1''} \|\mathbf{y}\|_\beta$$

and:

$$\frac{1}{c_2''} \|\mathbf{y}\|_\beta \leq \|\mathbf{y}\|_2 \leq \frac{1}{c_1'} \|\mathbf{y}\|_\alpha$$

Take $c_1 = \frac{c_1''}{c_2'}$ and $c_2 = \frac{c_2''}{c_1'}$.

□

For example, for any $\mathbf{x} \in \mathbb{R}^n$ we have:

$$\begin{aligned} \|\mathbf{x}\|_2 &\leq \|\mathbf{x}\|_1 \leq \sqrt{n} \|\mathbf{x}\|_2 \\ \|\mathbf{x}\|_\infty &\leq \|\mathbf{x}\|_2 \leq \sqrt{n} \|\mathbf{x}\|_\infty \\ \|\mathbf{x}\|_\infty &\leq \|\mathbf{x}\|_1 \leq n \|\mathbf{x}\|_\infty \end{aligned}$$

1.3.2 Matrix norms

The analysis of matrix algorithms requires that we be able to assess the size of matrices. We introduce therefore *matrix norms*, off course, this definition is completely analogous:

Definition 1.3.5. A *matrix norm* on $\mathbb{R}^{n \times m}$ is a function $\|\cdot\| : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}$ with the following properties:

1. $\|A\| \geq 0$, for all $A \in \mathbb{R}^{n \times m}$ with equality if and only if A is a matrix with only zero entries.
2. $\|A + B\| \leq \|A\| + \|B\|$ for all $A, B \in \mathbb{R}^{n \times m}$.
3. $\|\alpha A\| = |\alpha| \|A\|$ for all $\alpha \in \mathbb{R}$, $A \in \mathbb{R}^{n \times m}$.

Frobenius norm

One of the most frequently used matrix norms is the so called *Frobenius norm*:

$$\|A\|_F = \left(\sum_{i=1}^n \sum_{j=1}^m |a_{ij}|^2 \right)^{\frac{1}{2}} = \text{trace}(A^T A)^{\frac{1}{2}},$$

If $A \in \mathbb{R}^{1 \times m}$, then the Frobenius norm equals the 2-norm.

p -norms

We can also define p -norms on matrices:

$$\|A\|_p = \sup_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}$$

Again, we can show that all matrix norms are equivalent with the same reasoning as in Theorem 1.3.4.

1.4 Numerical analysis

1.4.1 Bachmann-Landau notations

For comparing the computational cost of algorithms, it's important to know the *Bachmann-Landau notations*. These notations are used to describe the limiting behavior of a function in terms of simpler functions. These notations are used a lot in computer science to classify algorithms by how their number of steps depends on changes in input size. We are only interested in the effects on the number of steps for really large input sizes, so constants don't play any role in the classification.

Big Oh

Definition 1.4.1. (*Big Oh*)

Big Oh is the set of all functions f that are bounded above by g asymptotically (up to constant factor).

$$O(g(n)) = \{f | \exists c, n_0 \geq 0 : \forall n \geq n_0 : 0 \leq f(n) \leq cg(n)\}$$

We now proof a very simple lemma to show that indeed constant factors doesn't matter for Big Oh:

Lemma 1.4.2. $\forall k > 0 : O(k.g(n)) = O(g(n))$

Proof.

$$\begin{aligned} O(k.g(n)) &= \{f | \exists c, n_0 \geq 0 : \forall n \geq n_0 : 0 \leq f(n) \leq k.c.g(n)\} \\ &= \{f | \exists c, n_0 \geq 0 : \forall n \geq n_0 : 0 \leq f(n) \leq (k.c).g(n)\} \\ \text{let } c' &= k.c \\ &= \{f | \exists c', n_0 \geq 0 : \forall n \geq n_0 : 0 \leq f(n) \leq c'.g(n)\} \\ &= O(g(n)) \end{aligned}$$

□

Small Oh

Definition 1.4.3. (*Small Oh*)

Small Oh is the set of all functions f that are dominated by g asymptotically.

$$o(g(n)) = \{f | \forall \varepsilon > 0, \exists n_0 \forall n \geq n_0 : f(n) \leq \varepsilon.g(n)\}$$

Note that the small oh-notation is a much stronger statement than the corresponding big oh-notation: every function that is in the small oh of g is also in big oh, but the inverse isn't necessarily true. Intuitively, $f(x) \in o(g(x))$ means that $g(x)$ grows much faster than $f(x)$.

Asymptotical Equality

Definition 1.4.4. (*Asymptotically Equal*)

Let f and g real functions, then f is asymptotically equal to $g \Leftrightarrow \lim_{x \rightarrow +\infty} \frac{f(x)}{g(x)} = 1$. Notation: $f \sim g$.

In fact asymptotical equality, can also be defined as an equivalency relation: $f \sim g \Leftrightarrow (f - g) \in o(g)$. It's trivially clear that as $f \sim g \Rightarrow f \in O(g)$.

1.4.2 The Power Method

We now introduce the *classical power method*, also called the *Von Mises iteration* ([GOLUB]) because adaptations of this iterative method will appear in the following chapters of this master thesis. The power method is an eigenvalue algorithm that, given a diagonalizable matrix A , finds the eigenvalue λ with the greatest magnitude and a corresponding eigenvector \mathbf{v} such that:

$$A\mathbf{v} = \lambda\mathbf{v}.$$

The power method is special because it doesn't use any matrix decomposition technique for obtaining results, making it suitable for very large matrices. At the other hand, it only finds one eigenvalue with a corresponding eigenvector and the iterative process might converge very slowly.

There are plenty of variations of the power method available that overcome all these difficulties (finding only 1 eigenvalue/eigenvector, slow convergence, A must be diagonalizable, ...) but we limit our discussion here to the very basic method, therefore we call it the *classical power method*.

We first introduce some needed definitions, theorems and notations.

Definition 1.4.5. Consider a real $n \times n$ -matrix A with (not necessarily different) eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$. When

$$|\lambda_1| > |\lambda_2| \leq |\lambda_3| \leq \dots \leq |\lambda_n|,$$

λ_1 is called the **dominant eigenvalue**.

Corollary 1.4.6. The dominant eigenvalue λ_1 of a $n \times n$ -matrix A is real.

Proof. This is trivial, if λ_1 would be complex, the complex conjugate of λ_1 would also be an eigenvalue with the same modulus. \square

Theorem 1.4.7. A $n \times n$ matrix A is diagonalizable if and only if it has an eigenbasis (a basis containing only linear independent eigenvectors).

Proof. \Leftarrow Consider $A \in \mathbb{R}^{n \times n}$ with (not necessarily different) eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ and the eigenbasis $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$. Let:

$$X = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n]$$

Because the columns of X are linearly independent, X is invertible. Since:

$$AX_i = \lambda_i X_i$$

we also have:

$$AX = X\Lambda$$

with $\Lambda = (\lambda_1, \lambda_2, \dots, \lambda_n)$, thus:

$$X^{-1}AX = \Lambda.$$

\Rightarrow When $A \in \mathbb{R}^{n \times n}$ is diagonalizable, then there exist an invertible matrix T so:

$$TAT^{-1} = D$$

with D diagonal. Let $Y = T^{-1}$, then:

$$AY = YD.$$

This means that the columns of Y are eigenvectors where the corresponding eigenvalues are noted in the diagonal matrix D . Because T and Y are invertible, the columns of Y are linear independent. This means that A has n linear independent eigenvectors, forming an eigenbasis. \square

Notation 1.4.8. Let $\mathbf{x}^{(i)}$ denote vector \mathbf{x} at iteration step i .

The algorithm

Let $A \in \mathbb{R}^{n \times n}$ be a diagonalizable matrix with dominant eigenvalue λ_1 . We know that A has eigenbasis $V = \{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$. Every vector $\mathbf{x}^{(0)} \in \mathbb{R}^n$ can be written as a linear combination of elements in V , because V spans the space \mathbb{R}^n . So:

$$\mathbf{x}^{(0)} = \sum_{i=1}^n \xi_i \mathbf{v}_i.$$

Now construct the sequence of vectors $\mathbf{x}^{(k)}$:

$$\mathbf{x}^{(k)} = A\mathbf{x}^{(k-1)} = A^k \mathbf{x}^{(0)}$$

Now:

$$\begin{aligned} A^k \mathbf{x}^{(0)} &= \sum_{i=1}^n \xi_i A^k \mathbf{v}_i \\ &= \sum_{i=1}^n \xi_i \lambda_i^k \mathbf{v}_i \\ &= \lambda_1^k \left\{ \xi_1 \mathbf{v}_1 + \xi_2 \left(\frac{\lambda_2}{\lambda_1} \right)^k \mathbf{v}_2 + \dots + \xi_n \left(\frac{\lambda_n}{\lambda_1} \right)^k \mathbf{v}_n \right\} \end{aligned}$$

Because $|\lambda_i| < |\lambda_1|$ for $i > 1$, we have that

$$\left(\frac{\lambda_i}{\lambda_1} \right)^k \rightarrow 0 \text{ for } k \rightarrow \infty$$

so:

$$\mathbf{x}^{(k)} = \lambda_1^k \xi_1 \mathbf{v}_1 + o(1) \text{ for } k \rightarrow \infty \quad (1.18)$$

This means that for k large enough $\mathbf{x}^{(k+1)}$ is equal to λ_1 times $\mathbf{x}^{(k)}$. So when, the ratio between the corresponding vector entries in $\mathbf{x}^{(k+1)}$ and $\mathbf{x}^{(k)}$ becomes constant after k iteration steps, then this ratio will be equal to the dominant eigenvalue λ_1 . $\mathbf{x}^{(k)}$ will be a corresponding eigenvector because it's proportional to \mathbf{v}_1 .

The start value $\mathbf{x}^{(0)}$ must only satisfy the condition that $\xi_1 \neq 0$, in other words: $\mathbf{x}^{(0)}$ must have a non-zero component belonging to the dominant eigenvector. In general, each randomly chosen option for $\mathbf{x}^{(0)}$ will normally fulfill this requirement. Even if we are so unlucky to pick

a starting vector which doesn't, subsequent $\mathbf{x}^{(k)}$ will again fulfill the requirement because rounding errors sustained during the iteration will have a component in this direction.

A practical problem arises now when one of the components of $\mathbf{x}^{(k)}$ is equal to zero. If we want to take the ratio between the corresponding components of $\mathbf{x}^{(k)}$ and $\mathbf{x}^{(k+1)}$ we get a division by zero. We can solve this by a property that any norm function has:

$$\|\lambda_1 \mathbf{x}^{(k)}\| = |\lambda_1| \|\mathbf{x}^{(k+1)}\|.$$

Because $\mathbf{x}^{(k)} \neq 0$ we have that $\|\mathbf{x}^{(k+1)}\| \approx \|\lambda_1 \mathbf{x}^{(k+1)}\|$, so we calculate λ_1 in the power method by:

$$|\lambda_1| = \lim_{k \rightarrow \infty} \frac{\|\mathbf{x}^{(k+1)}\|}{\|\mathbf{x}^{(k)}\|}$$

To decide on the sign of λ_1 , just divide two non-zero components of $\mathbf{x}^{(k+1)}$ and $\mathbf{x}^{(k)}$.

Another issue to address is that the components of $\mathbf{x}^{(k)} = A^k \mathbf{x}^{(0)}$ can become very high or very low, which can cause an overflow or underflow in the real number representation of computers. To avoid this, we use normed versions of the $\mathbf{x}^{(k)}$ -vectors: we start with a vector $\mathbf{y}^{(0)}$ with $\|\mathbf{y}^{(0)}\| = 1$. Subsequently, we calculate for $k = 0, 1, \dots$:

$$\mathbf{z}^{(k+1)} = A\mathbf{y}^{(k)}, \quad \mu_{k+1} = \|\mathbf{z}^{(k+1)}\|, \quad \mathbf{y}^{(k+1)} = \frac{\mathbf{z}^{(k+1)}}{\mu_{k+1}}.$$

The vectors $\mathbf{y}^{(k)}$ have all magnitude 1 and the components of $\mathbf{z}^{(k)}$ are restricted because:

$$\|\mathbf{z}^{(k)}\| = \|A\mathbf{y}^{(k-1)}\| \leq \|A\| \|\mathbf{y}^{(k-1)}\| = \|A\|$$

and when A is invertible we have $\|\mathbf{y}^{(k-1)}\| = 1 \leq \|A^{-1}\| \|\mathbf{z}^{(k)}\|$. Thus $\|\mathbf{z}^{(k)}\| \geq \frac{1}{\|A^{-1}\|}$. If we want to calculate the eigenvalue we can use:

$$\begin{aligned} A^k \mathbf{y}^{(0)} &= A^{k-1} A \mathbf{y}^{(0)} = A^{k-1} \mathbf{z}^{(1)} = A^{k-1} \mu_1 \mathbf{y}^{(1)} \\ &= A^{k-2} \mu_1 A \mathbf{y}^{(1)} = A^{k-2} \mu_1 \mathbf{z}^{(2)} = A^{k-2} \mu_1 \mu_2 \mathbf{y}^{(2)} \\ &= \dots \\ &= \mu_1 \mu_2 \dots \mu_k \mathbf{y}^{(k)} \end{aligned}$$

So:

$$|\lambda_1| = \lim_{k \rightarrow \infty} \frac{\|A^{k+1} \mathbf{y}^{(0)}\|}{\|A^k \mathbf{y}^{(0)}\|} = \lim_{k \rightarrow \infty} \frac{\mu_1 \mu_2 \dots \mu_{k+1} \|\mathbf{y}^{(k+1)}\|}{\mu_1 \mu_2 \dots \mu_k \|\mathbf{y}^{(k)}\|} = \lim_{k \rightarrow \infty} \mu_{k+1}$$

Because μ_{k+1} converges, a good choice for a stop condition for our numerical algorithm could be

$$|\mu_k - \mu_{k-1}| < Tol,$$

which guarantees an estimation error of at most Tol (usually $Tol = 10^{-5}$) for the approximation of the dominant eigenvalue. With all this information, we construct algorithm 5. Just to give an understandable algorithm, we used the Euclidean norm in this algorithm¹.

¹ $\|\cdot\|_2$ is the Euclidean vector norm.

Data:

$\mathbf{y}^{(0)}$: a start vector with $\|\mathbf{y}^{(0)}\|_2 = 1$,

Tol : Tolerance for the estimation error.

Result:

$\mathbf{y}^{(k)}$: an estimation of a dominant eigenvector,

μ_k : an estimation of the dominant eigenvalue.

begin power_method($\mathbf{y}^{(0)}, k$)

$k = 1$;

repeat

$\mathbf{z}^{(k)} = A\mathbf{y}^{(k-1)}$;

$\mu_k = \|\mathbf{z}^{(k)}\|_2$;

$\mathbf{y}^{(k)} = \frac{\mathbf{z}^{(k)}}{\mu_k}$;

$k = k + 1$

until $k > 2$ and $|\mu_k - \mu_{k-1}| < Tol$;

if the components $\mathbf{y}^{(k)}$ and $\mathbf{y}^{(k-1)}$ have a different sign **then**

$\mu_k = -\mu_k$;

end

return $\mathbf{y}^{(k)}, \mu_k$;

end

Algorithm 1: The Power method

Computational cost & Usage

The computational cost of the algorithm is determined by the speed at which the $o(1)$ terms in 1.18 go to zero. This is indicated by the slowest converging term $(\lambda_2/\lambda_1)^k$. This means that the algorithm converges slowly when there is an eigenvalue close in magnitude to the dominant eigenvalue. We get following expression for approximation μ_k of λ_1 :

$$|\mu^k - \lambda_1| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$$

In our algorithm we accepted an estimation error of 10^{-5} , so the number of steps n can be computed as:

$$\left|\frac{\lambda_2}{\lambda_1}\right|^n \approx Tol$$

So, for example, for $Tol = 10^{-5}$ we get $n = -5/\log \lambda_1/\lambda_2$, we become:

$$\text{power_method} \in O\left(\frac{-1}{\log \lambda_1 - \lambda_2}\right)$$

Note that this O holds for any estimation error Tol of the form 10^{-e} with $e \in \mathbb{N}$.

When $\lambda_2 \approx \lambda_1$ we see that the power method (almost) has infinitely many steps. Since we do not know the eigenvalues of A , this means we cannot know in advance whether the power method will work or not. Recall that the eigenvalues of a real matrix A are in general complex, and occur in conjugate pairs. This means, when the dominant eigenvalue of A is not real, the power method will certainly fail. Therefore, it is a good idea to apply the power method only to matrix whose eigenvalues are known to be real. The only thing that can

go wrong with those matrices is that the dominant eigenvalue has an algebraic multiplicity larger than 1.

From the Perron-Frobenius theorem in 1.2.10, we also get another good choice: namely the irreducible matrices or any matrix with strictly positive entries. Indeed, The Perron-Frobenius theorem tells us that they have a unique dominant eigenvalue.

Example

Example 1.4.9. Consider the matrix:

$$A = \begin{pmatrix} 1 & -3 & 5 \\ -1 & -7 & 11 \\ -1 & -9 & 13 \end{pmatrix}$$

A has a dominant eigenvalue 3 and a double eigenvalue 2. A corresponding dominant eigenvector is $(1, 1, 1)$. Now we use the classical power method with start vector $\mathbf{y}^{(0)} = (1, 0, 0)$, $Tol = 10^{-5}$ and we become the values in Table 1.4.9. Because we know the eigenvalues

k	μ_k	k	μ_k
0	1.00000	15	3.00459
1	1.73205	16	3.00305
2	4.12311	17	3.00204
3	4.06564	18	3.00136
4	3.58774	19	3.00090
5	3.34047	20	3.00060
6	3.20743	21	3.00040
7	3.13055	22	3.00026
8	3.08385	23	3.00017
9	3.05457	24	3.00011
10	3.03582	25	3.00008
11	3.02363	26	3.00005
12	3.01564	27	3.00003
13	3.01037	28	3.00002
14	3.00689	29	3.00001

Table 1.1: The iteration values μ_k of Example 1.4.9.

of A , we can predict the number of steps $n = -5/\log \lambda_2/\lambda_1 = -5/(\log 2/3) \approx 28$. Because $\lambda_2/\lambda_1 = 2/3$ is not that small, the convergence here is also not that fast. We have for the approximation of a corresponding eigenvector

$$\mathbf{y}^{(29)} = (-0.577348, -0.577352, -0.577351)$$

which is (more or less) in proportion with $(1, 1, 1)$.

1.5 Graphs

After introducing different kinds of matrices and proving the Perron-Frobenius theorem, we now take a closer look at graphs. Here too, we'll look at different families of graphs and prove

some relevant properties about them. We also link the concept of graphs with different kinds of matrices, deepening our insight of some theorems of the previous section.

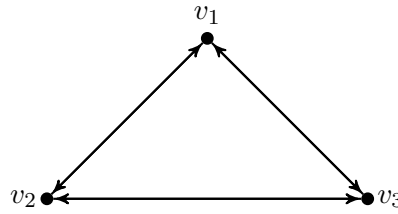
The definitions and results in this section are mainly based on the course ‘Discrete Mathematics’ by P. Cara [CARA].

1.5.1 General definitions

Definition 1.5.1. A **graph** is an ordered pair (V, \rightarrow) where V is a set and \rightarrow is a relation. The elements of V are called **vertices** and \rightarrow is called the **adjacency relation**. Let $u, v \in V$, then the ordered pair (u, v) belonging to \rightarrow is called an **arc** or **edge** and we write $u \rightarrow v$. We also say that u is **adjacent** to v . When $v \rightarrow v$ (with $v \in V$) we say that the graph has a **loop** at v . A graph (V, \rightarrow) is most of the time denoted by calligraphic letters $\mathcal{G}, \mathcal{H}, \dots$

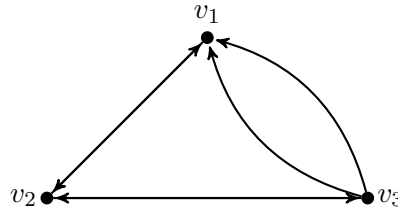
When the relation \rightarrow is symmetric, we call the graph **undirected**, in this case we often write E instead of \rightarrow .

Example 1.5.2. The graph



is an undirected graph with vertices v_1, v_2, v_3 . The adjacency relation \rightarrow equals $\{(v_1, v_2), (v_2, v_1), (v_2, v_3), (v_3, v_2), (v_3, v_1), (v_1, v_3)\}$.

There is a small problem with our definition, because not all graphs are taken into account, for example the graph below is not a graph following our definition because you can not define multiple edges between vertices in a relation.



Therefore we define multisets and make a remark that introduces the concept of multiplicity of an edge using these multisets. Multisets are a generalization of the notion of a set in which elements are allowed to appear more than once.

Definition 1.5.3. A **multiset** $A = (S, \mu)$ is an ordered pair with S a set and $\mu : S \rightarrow \mathbb{N}_0$ a function that gives the **multiplicity** of an element of S . A multiset can be written as a set in the following way:

$$A = (S, \mu) = \{(s, \mu(s)) : s \in S\}$$

The **cardinality** of a multiset is defined as

$$|A| = \sum_{s \in S} \mu(s).$$

Consider as an example the multiset $\{a, a, b, b, bc\}$ (with a, b, c different elements), which can be denoted as a set as $\{(a, 2), (b, 3), (c, 1)\}$

We now introduce the following important remark using multisets:

Remark 1.5.4. *Although we will stay writing a graph as $\mathcal{G} = (V, \rightarrow)$, this definition doesn't allow for repeated edges. A graph that can have multiple edges between two vertices is often called a **multigraph**, but in this master thesis we call a multigraph just a graph. To define this in a mathematical correct way, you define \mathcal{G} as an ordered pair (V, \rightarrow) where V is a finite set and \rightarrow is a multiset consisting of elements of the cartesian product $V \times V$.*

Definition 1.5.5. *The **neighbourhood** of a vertex v of a graph $\mathcal{G} = (V, \rightarrow)$ is the induced subgraph \mathcal{G}_v with vertex set V' consisting of all vertices adjacent to v without v itself and with the multiplicity function μ' , which is the restriction of μ to the vertices in V' . A vertex with a neighbourhood equal to the empty graph (a graph with an empty set of vertices) is called isolated.*

Definition 1.5.6. *Let $\mathcal{G} = (V, \rightarrow)$ be a graph with vertices $v_1, v_2, \dots, v_n \in V$ and edges (defined as ordered pairs) $e_1, \dots, e_m \in \rightarrow$. Let $u \rightarrow v$ be an edge between $u, v \in V$. We call u the **source node** and v the **terminal node** of the edge. $s_{\mathcal{G}}(i)$ denotes the source node u_i of edge i , $t_{\mathcal{G}}(i)$ denotes the terminal node w_i of edge i .*

Definition 1.5.7. *The **order of a finite graph** \mathcal{G} is the number of vertices of \mathcal{G} and is denoted by $|\mathcal{G}|$.*

Definition 1.5.8. *The **indegree of a vertex** v in a graph \mathcal{G} is the number of times v is a terminal node of an edge.*

Definition 1.5.9. *The **outdegree of a vertex** v in a graph \mathcal{G} is the number of times v is a source node of an edge.*

Definition 1.5.10. *The **degree of a vertex** v in a graph \mathcal{G} is the sum of the indegree and outdegree of vertex v .*

Definition 1.5.11. *A **walk** in a graph \mathcal{G} is a sequence of vertices*

$$v_0, v_1, \dots, v_k$$

*such that $v_{i-1} \rightarrow v_i$ for each $i \in \{1, \dots, k\}$. The **length** of the walk is k , one less than the number of vertices.*

Definition 1.5.12. *If all edges are distinct in a walk in a graph \mathcal{G} , we call the walk a **path**.*

Definition 1.5.13. *A **cycle** is a walk from v_0 to v_0 in which all vertices except v_0 are distinct.*

Definition 1.5.14. *A **simple graph** is an undirected graph $\mathcal{G} = (V, \rightarrow)$ containing no loops and for all vertices $v_i, v_j \in V$, there is at most one edge.*

Product graphs

Definition 1.5.15. *Take two graphs $\mathcal{G} = (U, \rightarrow)$, $\mathcal{H} = (V, \rightarrow')$, the **product graph** $\mathcal{G} \times \mathcal{H}$ is the graph with $|\mathcal{G}| \cdot |\mathcal{H}|$ vertices and that has an edge between vertices (u_i, v_j) and (u_k, v_l) if there is an edge between u_i and u_k in \mathcal{G} and there is an edge between v_j and v_l in \mathcal{H} .*

Colored graphs

Definition 1.5.16. A **node colored graph** \mathcal{G} is quadruple (V, \rightarrow, C, a) with V a set of vertices, \rightarrow an adjacency relation, C a set of colors and a a surjective function $a : V \rightarrow C$ that assigns to each vertex one color.

Definition 1.5.17. In a node colored graph $\mathcal{G} = (V, \rightarrow, C, a)$, $c_{\mathcal{G}}(i)$ denotes the number of vertices of color i . So:

$$c_{\mathcal{G}}(i) = |\{(i, v_j) \in C \times V | a(v_j) = i\}|$$

Adjacency matrices

We now represent a finite graph in the form of an adjacency matrix. This matrix gives a lot of useful information about the graph and vice versa.

Definition 1.5.18. Let $\mathcal{G} = (V, \mu)$ be a graph of order n and define a numbering on the vertices v_1, \dots, v_n . Then the **adjacency matrix** $A_{\mathcal{G}}$ of \mathcal{G} is the real $n \times n$ -matrix with a_{ij} equal to $\mu(v_i, v_j)$.

Corollary 1.5.19. The adjacency matrix of an undirected graph $\mathcal{G} = (V, \sim)$ is a symmetric matrix.

Proof. This is trivial by the definition of an undirected graph. □

Theorem 1.5.20. Let $k > 0$. The element on place (i, j) in $A_{\mathcal{G}}^k$ contains the number of walks of length k from i to j in the graph $\mathcal{G} = (V, \mu)$.

Proof. By induction on k .

For $k = 1$ we count the walks of length 1. These are edges and the result follows immediately from the definition of $A_{\mathcal{G}}$.

Let v_l be a vertex of \mathcal{G} . If there are b_{il} walks of length k from i to l and a_{lj} walks of length 1 (edges) from v_l to v_j , then there are $b_{il}a_{lj}$ walks of length $k + 1$ from v_i to v_j passing vertex v_l . Therefore, the number of walks of length $k + 1$ between v_i and v_j is equal to:

$$\sum_{l \in V} b_{il}a_{lj} =: c_{ij}.$$

By the induction hypothesis we now that b_{il} equals the element on place (i, l) in $A_{\mathcal{G}}^k$ so c_{ij} is exactly the element on place (i, j) in the matrix product

$$A_{\mathcal{G}}^k A_{\mathcal{G}} = A_{\mathcal{G}}^{k+1}.$$

□

Example 1.5.21. The adjacency matrix of the graph in Example 1.5.2 is:

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

1.5.2 Strong connectivity

In this section, we take a closer look at *directed graphs* and introduce the concept of connectivity.

Definition 1.5.22. An undirected graph \mathcal{G} is **connected** if it possible to establish a path from any vertex to any other vertex.

Definition 1.5.23. A directed graph $\mathcal{G}(V, \rightarrow)$ is **connected** if the underlying undirected graph (remove all arrows on the edges) is connected, the directed graph \mathcal{G} is **strongly connected** if there is a path in each direction between each pair of vertices of the graph.

In the next proof, we study the equivalence of the matrix property of irreducibility of Definition 1.1.10 with the concept of the strongly connected directed graphs of a matrix:

Theorem 1.5.24. Let \mathcal{G} be a (directed) graph with adjacency matrix A . Then \mathcal{G} is strongly connected if and only if A is irreducible.

Proof. From Theorem 1.5.20 we know that a graph is strongly connected if and only if for every pair of indices i and j there is an integer k such that $(A^k)_{ij} > 0$, from Theorem 1.1.12 we know this means that A is irreducible and vice versa. □

1.6 Hypergraphs

After introducing graphs, we now introduce hypergraphs. Intuitively, a hypergraph is a generalization of a graph in which an edge can connect to any number of vertices.

In contrast to the section about graphs, the representation of a hypergraph as a (multi-dimensional) adjacency matrix is not yet introduced here. This representation is not trivial and needs an introduction in basic tensor theory. It's not our goal to introduce this whole theory in this master thesis (in fact, this would be a master thesis on it's own), but it will only be clear to the reader after reading chapter 2 on similarity on graphs why certain topics are introduced and others are left out. Therefore, the representation of a hypergraph as an adjacency tensor is discussed in chapter 3 on similarity on hypergraphs.

The reason why we separate both subjects is that hypergraphs are not as known as graphs, and so we think it's interesting to the reader to discover the most important definitions about hypergraphs already in this stage of the thesis, as it gives the reader an idea of all the mathematical objects we will be discussing. The definitions presented are mainly from [BERGE] and [PEARSON].

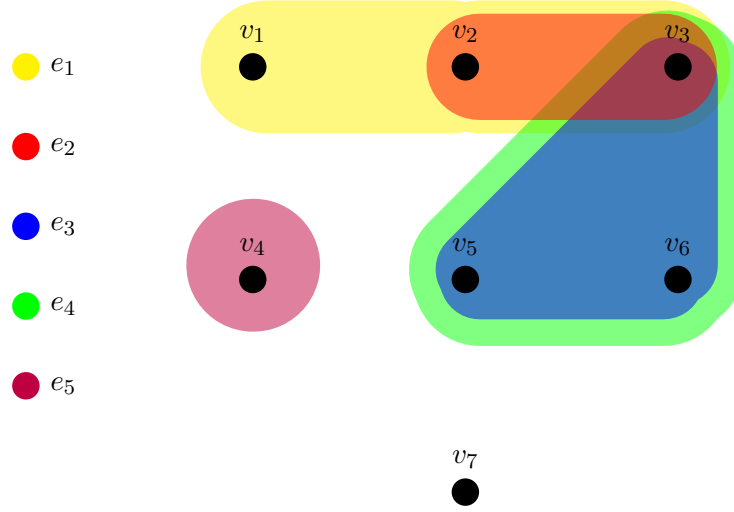
1.6.1 General definitions

Definition 1.6.1. A **hypergraph** is an ordered pair (V, E) with V a finite set of and $E \subseteq 2^V$, the power set of V . The elements of V are called the **vertices** and the elements of E are called the **edges**. An hypergraph (V, E) will be denoted by calligraphic letters $\mathcal{G}, \mathcal{H}, \dots$

Remark 1.6.2. As in graphs, the classic definitions of a hypergraphs doesn't allow to have multiple edges that cover the same vertices. Also repeated vertices within an edge, often called **hyperloops** are not allowed by the above definition. A hypergraph that can have multiple

edges connecting the same vertices, and hyperloops is called a **multi-hypergraph**, but in this master thesis we call a multi-hypergraph just a hypergraph. To define this in mathematical correct way, a hypergraph \mathcal{G} is an ordered pair (V, E) where V a finite set and E is a multi-set consisting of multi-subsets of V (a multi-subset is just a subset of a set where the elements are allowed to appeared more than once).

Example 1.6.3. The hypergraph $\mathcal{G} = (V, E)$ consist of 7 vertices and 4 edges. The edges are equal to the multiset $\{\{v_1, v_2, v_3\}, \{v_2, v_3\}, \{v_3, v_5, v_6\}, \{v_3, v_5, v_6\}, \{v_4\}\}$. Note that the colors don't have any meaning to the hypergraph (the hypergraph is not an edge colored hypergraph), but only serve to clarify the drawing.



Definition 1.6.4. In a hypergraph $\mathcal{G} = (V, E)$, two vertices $v_i, v_j \in V$ are called **adjacent** if there is an edge $e \in E$ that contains both vertices. Two edges e_k, e_l are called adjacent if there intersection is not empty.

Definition 1.6.5. The **order of a finite graph G** is the number of vertices of \mathcal{G} and is denoted by $|\mathcal{G}|$.

We define now the degree of a vertex in a hypergraph. Note that we don't define the indegree and outdegree of vertex as the hypergraphs we consider are undirected.

Definition 1.6.6. The **degree of a vertex v** in a hypergraph \mathcal{G} is the number of times v is contained in an edge.

k -hypergraphs

In most applications, the edges of an hypergraph connect a fixed number of vertices. This is called a uniform hypergraph:

Definition 1.6.7. A **k -uniform hypergraph** with $k \geq 2 \in \mathbb{N}$ if for all $e \in E$, the cardinality $|e|$ is equal to k . The cardinality of multisets is defined in Definition 1.5.3. The term **k -graph** is often used instead of a k -uniform hypergraph. The edges in a k -graph are sometimes called **k -edges**.

Notice that the 2-hypergraphs are just the undirected graphs we defined in the previous section.

Directed hypergraphs

An important difference with the previous section is that all hypergraphs we have defined are **undirected**: there is no specific order in which an edge connects different vertices. In a graph, directed edges arise naturally as some vertex can be the source node and some vertex can be the terminal node, no other nodes are connected by an edge of a graph. For edges of hypergraphs this concept is not straightforward to generalize: one option is to see edges as paths connecting vertices in a specific order, another option is to split the vertices connected by an edge in a set of source nodes and a set of terminal nodes. This last notion is studied in [GALLO]. We will not discuss this topic in detail, all the hypergraphs in this master thesis are undirected.

1.6.2 Incidence matrix

A hypergraph can be represented as an incidence matrix by numbering the vertices and the edges. The resulting incidence matrix will be a boolean matrix with only 1 and 0 entries. An alternative way to represent a hypergraph is by using adjacency tensors. As said in this introduction, these are discussed in chapter 3.

Definition 1.6.8. *The **incidence matrix** of a hypergraph $\mathcal{G} = (V, E)$ with vertices $v_1, \dots, v_n \in V$ and edges $e_1, \dots, e_m \in E$ is a $n \times m$ -matrix A where rows represent the vertices and the columns represent the edges, such that:*

$$(A)_{ij} = \begin{cases} 1 & \text{if } v_i \in e_j \\ 0 & \text{if } v_i \notin e_j \end{cases}$$

Example 1.6.9. The corresponding incidence matrix of the hypergraph of Example 1.6.3 is:

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Chapter 2

Similarity on graphs

In the previous chapter all the basic terminology and results were introduced, now we take an extensive look at the concept of similarity on graphs. Similarity on graphs is a fairly new concept to compare the nodes of two graphs. The concept arose from the research on algorithms for web searching engines (like *Google*, *Yahoo*,...) in the late nineties. More specifically, Jon M. Kleinberg introduced in his paper ‘Authoritative Sources in a Hyperlinked Environment’ [KLEINBERG] the famous ‘HITS algorithm’ for extracting information from the link structure of websites. The method leads to an iterative algorithm where graphs represent the link structure of a collection of websites on a specific topic. Because this paper formed the basis of later research on similarity on graphs, the whole idea and algorithm of Kleinberg is introduced in the first section of this chapter. In 2004, V.D. Blondel et al. [BLONDEL] generalized the algorithm of Kleinberg, introducing the notion of similarity on directed graphs. This similarity is covered in the second section. With this similarity on directed graphs, there is a much wider scope of applications than just search algorithms. Next, we extend the notion of similarity on directed graphs: the method of Blondel only returns the concept of node similarity which is in fact a measurement of how similar two nodes of two graphs are to each other.

2.1 The HITS algorithm of Kleinberg

2.1.1 History

Back in the nineties, internet became more and more popular by the public. The popular search engines back then were Altavista and Yahoo, but they weren’t as advanced as search engines today. The main pitfall of the first search engines was that the search results were purely based on the number of occurrences of a word in a webpage. This was a pitfall for many reasons. The first reason was the growing popularity of the internet: as more and more webpages were put online, simply getting the relevant pages to a search query in this text-based manner, was a process that could possibly return millions of relevant pages. Also *content similarity* was an issue: a website owner can easily cheat in a text-based search system by just adding and repeating some very popular search words, making his website appear in the results of a large number of search queries. Two possible solutions were simultaneously invented in 1997 and 1998. The first one was the *PageRank*-system developed by Larry Page and Sergey Brin ([PAGE]). The PageRank system led to the foundation of the immensely popular Google search engine. Meanwhile, also Jon Kleinberg came up with his own solution,

the *HITS algorithm* (hyperlink-induced topic search). At that time, he was both a professor in the Computer Science Department at the Cornell University and researcher for IBM. The algorithm is used inter alia today by the Ask search engine (www.ask.com). Both these algorithms use the hyperlinks between webpages to rank search results. Because this master thesis is about similarity and this concept is introduced on graphs as a generalization of the HITS algorithm, we don't go into further detail about the PageRank-algorithm. In the following paragraphs, the HITS algorithm is extensively explained.

2.1.2 Motivation

Kleinberg's work originates in the problems that arise with text-based searching the WWW. Text-based searching just counts all the occurrences of a given search query on webpages and returns a set of webpages ordered by decreasing occurrence. When a user supplies a search query, we probably face an *abundance problem* with this method: the number of pages that could reasonably be returned as relevant is far too large for a human user to digest. To provide effective search results under these conditions, we need to filter the 'authoritative' ones. We face some complications when we want to filter the 'authoritative' webpages in a text-based system. For example, if we search for 'job offers in Flanders' the most authoritative page and expected first result in a search engine would be www.vdab.be. Unfortunately, the query 'job offers' is used in over a million pages on the internet and www.vdab.be is not the one using the term most often. Therefore, there is no way to favor www.vdab.be in a text-based ranking function. This is a recurring phenomenon, as another example if you search for the query 'computer brands', there is no reason at all to be sure that the website of Apple or Toshiba even contain this search term.

The HITS algorithm solves these difficulties by analyzing the hyperlink structure among webpages. The idea is that hyperlinks encode a sort of human judgment and that this judgement is crucial to formulate a notion of authority. Specifically, when a page p includes a link to page q , it means that p gives a *conferred authority* on q . Again we face difficulties, because this conferred authority doesn't hold for every link. Links are created for a wide variety of reasons, for example, a large number of links are created for navigation within a website (e.g. "Return to homepage") and these have of course nothing to do with a notion of authority.

The HITS method is based on the relationship between the *authorities* for a topic and those pages that link to many related authorities, called *hubs*. Page p is called an *authority* for the query "smartphone brand" if it contains valuable information on the subject. In our example websites of smartphone manufacturers such as "www.apple.com", "www.samsung.com",... would be good authorities for this search query and these are the results a user expects from a search engine.

A hub is a second category of pages needed to find good authorities. Their role is to advertise authoritative pages. Hubs contain useful links toward these authorities. In our example, consumer websites with reviews on smartphones, websites of smartphone shops,... would be good hubs. In fact, hubs point the search process in the 'right direction'.

To really grasp the idea, we make an analogy with everyday life. If you tell a friend that you think of buying a new smartphone, he might tell you his experiences with smartphones and he will probably share some opinions he got from other friends. He might suggest you some good models and good brands. Now, you are more inclined to buy a smartphone that your friend suggested. Well, this idea is used in the HITS-method: your friend served as hub,

Data: σ : a query string. \mathcal{E} : a text-based search engine. t : natural number (usually initiated to 200) d : natural number (usually initiated to 50).**Result:** A page set S_σ satisfying all the properties of our wish list.

```

begin create_graph( $\sigma, \mathcal{E}, t, d$ )
  Let  $R_\sigma$  denote the top  $t$  results of  $\mathcal{E}$  on  $\sigma$ ;
  Set  $S_\sigma := R_\sigma$ ;
  for each page  $p \in R_\sigma$  do
    Let  $\Gamma^+(p)$  denote the set of all pages  $p$  points to;
    Let  $\Gamma^-(p)$  denote the set of all pages pointing to  $p$ ;
    Add all pages in  $\Gamma^+(p)$  to  $S_\sigma$ ;
    if  $|\Gamma^-(p)| \leq d$  then
      | Add all pages in  $\Gamma^-(p)$  to  $S_\sigma$ ;
    else
      | Add an arbitrary set of  $d$  pages from  $\Gamma^-(p)$  to  $S_\sigma$ ;
    end
  end
  return  $S_\sigma$ ;
end

```

Algorithm 2: Algorithm to construct S_σ .

the brands and models he suggested are good authorities.

2.1.3 Constructing relevant graphs of webpages

Any collection of hyperlinked pages can be transformed to a directed graph $\mathcal{G} = (V, \rightarrow)$: the nodes correspond to the pages, and if there is a link from page p to page q , there is an arc $p \rightarrow q$. Suppose a search query is performed, specified by a query σ . We wish to determine the authoritative pages by an analysis of the link structure. But first we have to construct a subgraph of the internet on which our algorithm will operate. We want to make the computational effort as efficient as possible, so we restrict the subgraph to the set Q_σ of all pages where the query σ occurs. For this, we could use any already existing text-based search engine. But, for our algorithm Q_σ is possibly much too big: it may contain millions of pages making it impossible for any computer to preform the algorithm. Moreover it is, as explained in the motivation in 2.1.2, possible that Q_σ does not contain some of the most important authorities because they never use the query string σ on their website.

Therefore, we wish to transform the set Q_σ to a set S_σ of pages following this ‘wish list’ of properties:

1. S_σ is relatively small,
2. S_σ is rich in relevant pages,
3. S_σ contains most of the strongest authorities.

By keeping S_σ small, the computational cost of performing non-trivial algorithms can be kept under control. By the property of being rich in relevant pages, it will be easier to find good authorities.

To construct S_σ , we first construct a *root set* R_σ with the t highest-ranked pages for σ using a text-based search engine (they sort results based on the occurrence of σ). Typically, t is set about 200. R_σ complies with properties 1 and 2 of our wish list, but because $R_\sigma \subset Q_\sigma$, it may fail from satisfying property 3. Now we use the root set R_σ to create the set S_σ satisfying our complete wish list. When a strong authority is not in R_σ , it is very likely that at least one of the pages in R_σ points to this authority. Hence, by using the pages in R_σ , we can expand it to S_σ by looking at the links that enter and leave R_σ . We get algorithm 2.

Thus, we obtain S_σ by expanding R_σ to include any page pointed to by a page in R_σ . We also add d pages that point to a page in R_σ . d is usually initiated to 50. The parameter d is crucial to stay in accordance with property 1 of our wish list. Indeed, a webpage can be pointed to by several thousands and thousands of other webpages, and we don't want to include them all if we want to keep S_σ relatively small. Some experiments in [KLEINBERG] showed that this algorithm resulted in a S_σ with a size in the range of 1000 to 5000 web pages. Property 3 of our wish list is usually met because a strong authority need only be reference once in the t pages of the root set R_σ to be added to S_σ .

Denote the resulting graph of the page set S_σ by $\mathcal{G}[S_\sigma]$. Note that $\mathcal{G}[S_\sigma]$ will contain a lot of links serving only navigational purposes within a website. As mentioned before, these links have nothing to do with the the notion of authority and they must be removed from our final graph if we want a good determination of the authoritative pages by an analysis of the link structure. A very simple heuristic can be used to derive a subgraph of $\mathcal{G}[S_\sigma]$ leaving out all the navigational links: we make a distinction between *transverse* links and *intrinsic* links. Transverse links are links between different domain names (e.g. a link between `www.vub.ac.be` and `www.ua.ac.be`) and intrinsic links are links between the same domain name (e.g. a link between `www.vub.ac.be` and `dwis.vub.ac.be`). Intrinsic links exist to allow navigation within a website and they tell us very little about the authority of the pages they point to. Therefore, we delete all intrinsic links from $\mathcal{G}[S_\sigma]$, keeping only the arcs corresponding to transverse links.

Our graph still contains some meaningless links in the context of page authority. Suppose a large number of pages from the same domain name have a transverse link to the same page p . Most of the time, this means a form of advertisement (by example 'Website created by...' at the bottom of each page). It is useful to only allow m pages (m is usually initiated to 6) from the same domain name to have a transverse link to the same page. If m is exceeded, all the transverse links must be deleted from the graph. Note, however, that not all links to advertisements will be erased because on most web pages, advertisements change on every page which avoids the exceedance of m .

Applying the two described heuristics above on $\mathcal{G}[S_\sigma]$, we get a new graph \mathcal{G}'_σ which is exactly what we need to perform our link analysis.

2.1.4 Hubs and Authorities

A very simple approach would now be to order the pages in \mathcal{G}'_σ by their indegree. Although this approach can sometimes return good search results, this heuristic is often too simple because S_σ will probably contain some web pages with a lot of incoming links without being very relevant to the search query σ (e.g. advertisements). With these incoming links, those

web pages are ranked high in the final search result, which we want to avoid.

Do we have to return to a text-based approach to avoid irrelevant web pages being on top of the search results? No, the link structure of \mathcal{G}'_σ can tell us a lot more than it may seem at first glance. Authoritative pages relevant to query σ should indeed have a large in-degree, but there should also be a considerable overlap in the sets of pages that point to authoritative pages. This set of pages that point to authoritative pages are called *hubs*. Hubs have links to several authoritative pages and they sort of “concentrate” all the authorities on query σ . Figure 2.1.1 shows what this means conceptually.

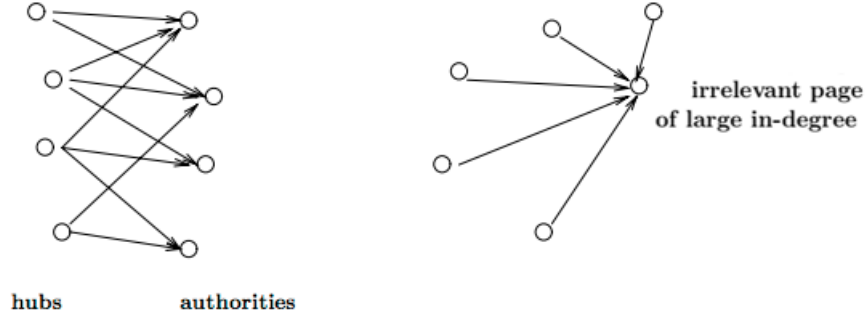


Figure 2.1.1: The concept of hubs and authorities (Source: [KLEINBERG])

So, for each page j we assign two scores, an *authority score* which estimates the value of the content of the page and a *hub score* which estimates the value of the outgoing links to other pages. We get now a *mutually reinforcing relation*: a good hub is a page pointing to many good authorities, a good authority is a page that is pointed to by many good hubs. This leads us to a *mutually reinforcing relation* resulting in an iterative method to break this circularity.

So let $\mathcal{G}'_\sigma = (V, \rightarrow)$ and let h_j and a_j be the hub and authority scores of vertex v_j (corresponding with page j). These scores must be initialized by some positive start values and then updated simultaneously for all vertices. This leads to a *mutually reinforcing relation* in which the hub score of v_j is set equal to the sum of the authority scores of all vertices pointed to by v_j and in an equal manner the authority score of v_j is set equal to the sum of the hub scores of all vertices pointing to v_j .

$$\begin{cases} h_j := \sum_{i: (v_j, v_i) \in \rightarrow} a_i, \\ a_j := \sum_{i: (v_i, v_j) \in \rightarrow} h_i. \end{cases}$$

The basic operations in which hubs and authorities reinforce one another are depicted in Figure 2.1.2. deze tekening wordt nog herwerkt

Let B be the adjacency matrix of \mathcal{G}'_σ and denote \mathbf{a} as the authority vector with coordinates (a_1, a_2, \dots, a_n) (with $n = |\mathcal{G}'_\sigma|$, the number of pages) and \mathbf{h} as the hub vector. The mutually reinforcing relation can now be rewritten as:

$$\begin{pmatrix} \mathbf{h} \\ \mathbf{a} \end{pmatrix}^{(k+1)} = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{h} \\ \mathbf{a} \end{pmatrix}^{(k)}, \quad k = 0, 1, \dots,$$

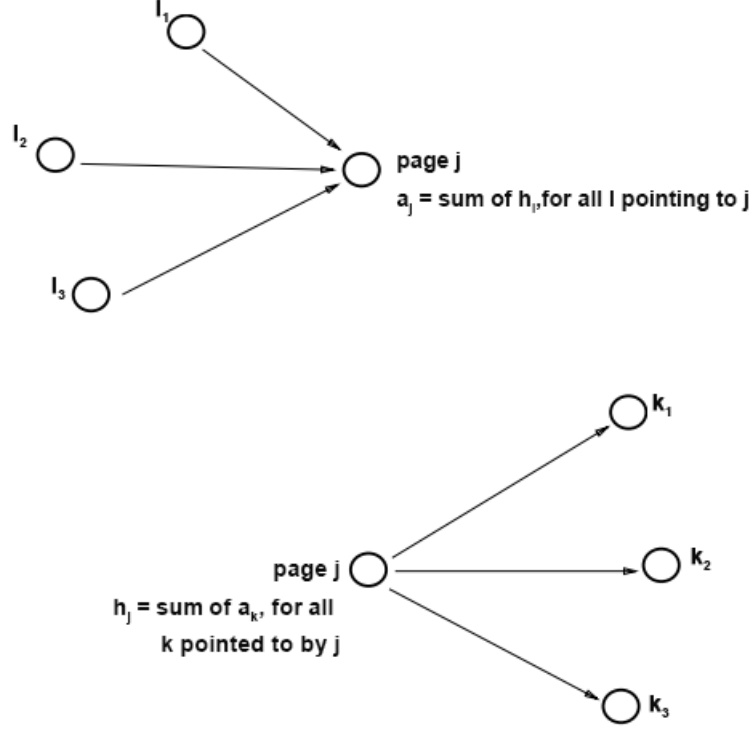


Figure 2.1.2: The basic operations in the reinforcing relation between hubs and authorities (Source: [KLEINBERG])

In compact form, we denote

$$\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)}, \quad k = 0, 1, \dots, \quad (2.1)$$

where

$$\mathbf{x}^{(k)} = \begin{pmatrix} \mathbf{h} \\ \mathbf{a} \end{pmatrix}^{(k)}, \quad M = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

After each iteration, we have to normalize h_j and a_j . Indeed, we want to get the authority and hub weights for each page and in order to compare these after each iteration step, they must be normalized because only the relative differences do matter, otherwise the whole procedure would be meaningless. Pages with larger a_j -scores are viewed as being better authorities, pages with larger h_j -scores are better hubs.

We get the following sequence (with $z^{(0)}$ some positive start value) of normalized vectors:

$$\mathbf{z}^{(0)} = \mathbf{x}^{(0)} > 0, \quad \mathbf{z}^{(k+1)} = \frac{M\mathbf{z}^{(k)}}{\|M\mathbf{z}^{(k)}\|_2}, \quad k = 0, 1, \dots, \quad (2.2)$$

How do we decide on $\mathbf{x}^{(0)}$? We will see that any positive vector in \mathbb{R}^{2n} is a good choice, but for the sake of simplicity, we make the natural choice¹ $\mathbf{1} \in \mathbb{R}^{2n}$. The limit to which the

¹ $\mathbf{1}$ is a matrix, or vector, whose entries are all equal to 1.

Data:

\mathcal{G} : a graph of n linked pages.

k : natural number.

Result: A vector (\mathbf{h}, \mathbf{a}) containing the hub and authority scores after k steps.

begin hits(\mathcal{G}, k)

 Set $\mathbf{a}^{(0)} = (1, 1, \dots, 1) \in \mathbb{R}^n$;

 Set $\mathbf{h}^{(0)} = (1, 1, \dots, 1) \in \mathbb{R}^n$;

for $i = 1, 2, \dots, k$ **do**

 Calculate

$\mathbf{h}'^{(i)} = \left(\sum_{m:(v_1, v_m) \in \rightarrow} \mathbf{a}_m^{(i-1)}, \sum_{m:(v_2, v_m) \in \rightarrow} \mathbf{a}_m^{(i-1)}, \dots, \sum_{m:(v_n, v_m) \in \rightarrow} \mathbf{a}_m^{(i-1)} \right)$;

 Normalize $\mathbf{h}'^{(i)}$ obtaining $\mathbf{h}^{(i)}$;

 Calculate $\mathbf{a}'^{(i)} = \left(\sum_{m:(v_m, v_1) \in \rightarrow} \mathbf{h}_m^{(i)}, \sum_{m:(v_m, v_2) \in \rightarrow} \mathbf{h}_m^{(i)}, \dots, \sum_{m:(v_m, v_n) \in \rightarrow} \mathbf{h}_m^{(i)} \right)$;

 Normalize $\mathbf{a}'^{(i)}$ obtaining $\mathbf{a}^{(i)}$;

end

return $(\mathbf{h}^{(k)}, \mathbf{a}^{(k)})$;

end

Algorithm 3: The iterative HITS-algorithm.

Data:

\mathcal{G} : a graph of n linked pages.

k : natural number.

c : natural number.

Result: A vector $((\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_c), (\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_c))$ containing exactly the nodes of the c top hubs and c top authorities.

begin filter(\mathcal{G}, k, c)

$(\mathbf{h}, \mathbf{a}) = \text{hits}(\mathcal{G}, k)$;

 Sort the pages with the c largest values in \mathbf{h} , resulting in a vector of nodes

$(\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_c)$;

 Sort the pages with the c largest values in \mathbf{a} , resulting in a vector of nodes

$(\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_c)$;

return $((\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_c), (\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_c))$;

end

Algorithm 4: Returning the top c hubs and authorities

sequence converges results in ‘definitive’ hub and authority scores for each page in the graph \mathcal{G}'_σ .

To compute the iterative algorithm, we update the hub and authority scores in an alternating form (by each step we have to normalize the scores). Because we will prove that the sequence converges, theoretically we can keep on iterating until a fixed point is approximated. But in most practical settings, we choose a fixed number of steps k to reduce the computational cost because we can not know beforehand how large k has to be to reach the limit. But of course, it is extremely important to know that method converges anyway. Let $\mathbf{x}^{(i)}$ denote vector \mathbf{x} at iteration step i as in Notation 1.4.8, and we get Algorithm 3.

To filter the top c hubs and the top c authorities, you can use the trivial Algorithm 4.

How do we decide on the values of k and c ? It’s immediately clear that c and k must be

proportional: for low c values, a lower value for the number of iteration steps k is appropriate and vice versa. Experiments in [KLEINBERG] showed that k set to 20 is sufficient to become stable for finding the 5 best hubs and authorities, thus for $c = 5$.

2.1.5 Convergence of the algorithm

We now want to prove that for arbitrarily large values of k , the sequence $Z^{(k)}$ converge to a limit $(\mathbf{h}', \mathbf{a}')$. Before prove the convergence, note that adjacency matrices are nonnegative by definition, and thus the matrix M is nonnegative too. M is also clearly a symmetric $n' \times n'$ -matrix with nonnegative, real entries. We prove that such matrices have n' (not necessarily different) real eigenvalues and that we can diagonalize M . This is the first condition of the power method we introduced in section 1.4.2. If we can also prove the second condition (having a unique dominant eigenvalue), convergence is immediately shown by the power method.

However, there is a problem here: we can not prove that nonnegative symmetric matrices have a unique dominant eigenvalue (a unique dominant eigenvalue means the largest eigenvalue with multiplicity 1), simply because this is not true in general.² In the original paper of Kleinberg [KLEINBERG] he solves this issue by simply imposing that the matrix M has a unique dominant eigenvalue and he doesn't pay any further attention to this problem. He presents it as 'a small, technical assumption for the sake of simplicity'.

Is this justified in practice? Actually it is, because you can prove with probability theory that a random matrix C_n , with a probability tending to 1, has no repeated eigenvalues as the size of the matrix goes to infinity (See for example Theorem 2.2.3 in [DEIFT]). You can also defend this differently: the only reason why we can't use the Perron-Frobenius theorem (see 1.2.10) here, is because M will have zero entries (not all pages in S_σ will be linked to each other, the graph \mathcal{G}'_σ is not strongly connected in general). But, it is intuitively clear that by adding 1 to each entry of M , the final results of the algorithm (a sorted vector with the best hubs and authorities) will not be changed at all, because pages with larger indegrees and outdegrees will continue to get better hub and authority scores (note, however, that the relative hub and authority scores can fluctuate a bit and the algorithm will converge slower because of the lack of zero entries). So, by adding 1 to each entry of M , the matrix becomes a positive, real matrix and we know from the Perron-Frobenius that these matrices have a unique dominant eigenvalue. So yes, the 'small, technical assumption' in the paper of Kleinberg is justified.

Now that this problem is solved, we present the relevant theorems below. We also impose on the matrix M that it has a unique dominant eigenvalue with the preceding explanations in mind. Remember that we will generalize the idea of the HITS algorithm to introduce similarity on graphs. Therefore, we will reconsider the convergence of the (generalized) algorithm again in the following section, and there we prove that there exists also a limit even when the matrix M has no unique dominant eigenvalue. The reason why we don't present this result immediately, is because we want to present the results as authentic possible and we want to show the evolution of the ideas in the successive papers.

Theorem 2.1.1. *If A is a symmetric, real $n \times n$ -matrix, then it has n (not necessarily*

²The matrix $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is a simple counterexample of a symmetric, nonnegative, real matrix that has no unique dominant eigenvalue.

different) real eigenvalues corresponding to real eigenvectors.

Proof. First, treat A as complex matrix. The characteristic polynomial $\det(A - \lambda I)$ has n roots in \mathbb{C} and each root is an eigenvalue for A . Let $\lambda \in \mathbb{C}$ be any eigenvalue and $\mathbf{v} \in \mathbb{C}^n$ be a corresponding eigenvector for A . We have:

$$A\mathbf{v} = \lambda\mathbf{v}.$$

As $A = A^t$, we also get:

$$\mathbf{v}^t A = \lambda \mathbf{v}^t.$$

Taking the complex conjugate of both sides we get (A is a real matrix):

$$\bar{\mathbf{v}}^t A = \bar{\lambda} \bar{\mathbf{v}}^t$$

We get:

$$\bar{\mathbf{v}}^t A \mathbf{v} = (\bar{\mathbf{v}}^t A) \mathbf{v} = (\bar{\lambda} \bar{\mathbf{v}}^t) \mathbf{v} = \bar{\lambda} \bar{\mathbf{v}}^t \mathbf{v}.$$

We also have:

$$\bar{\mathbf{v}}^t A \mathbf{v} = \bar{\mathbf{v}}^t (A \mathbf{v}) = \lambda \bar{\mathbf{v}}^t \mathbf{v}.$$

Hence:

$$\bar{\lambda} \bar{\mathbf{v}}^t \mathbf{v} = \lambda \bar{\mathbf{v}}^t \mathbf{v}.$$

We conclude that $\lambda = \bar{\lambda}$ for $\mathbf{v} \neq 0$. We proved that every eigenvalue of A is real. If λ is an eigenvalue of A , then the matrix $(A - \lambda I)$ is not invertible so a vector $\mathbf{s} \in \mathbb{R}^n$ exists with

$$(A - \lambda I)\mathbf{s} = 0,$$

proving that also the corresponding eigenvector is real. □

Theorem 2.1.2. (Symmetric Schur Decomposition) *Let A be a real symmetric matrix, then there exist an orthogonal matrix P such that:*

- (i) $P^{-1}AP = D$, a diagonal matrix,
- (ii) The diagonal entries of D are the eigenvalues of A ,
- (iii) The column vectors of P are the eigenvectors of the eigenvalues of A .

Proof. By induction on the order of the matrix. For $n = 1$ the theorem is trivial. Let A be a symmetric $n \times n$ -matrix. A has at least one eigenvalue λ_1 by the previous theorem. Let \mathbf{x}_1 be a corresponding eigenvector with $\|\mathbf{x}_1\| = 1$ and $A\mathbf{x}_1 = \lambda_1\mathbf{x}_1$. By the Gram-Schmidt procedure, we construct an orthonormal basis $V_1 = \{\mathbf{x}_1, \mathbf{v}_2, \dots, \mathbf{v}_n\}$ of \mathbb{R}^n . Let:

$$S_1 = [\mathbf{x}_1, \mathbf{v}_2, \dots, \mathbf{v}_n],$$

since S_1 is orthonormal, we get $S_1^t = S_1^{-1}$. Consider the matrix: $S_1^{-1}AS_1$. We have:

$$(S_1^{-1}AS_1)^t = (S_1^tAS_1)^t = S_1^tA^tS_1 = S_1^{-1}AS_1$$

Thus $S_1^{-1}AS_1$ is a symmetric matrix. Since $S_1\mathbf{e}_1 = \mathbf{x}_1$, we get:

$$\begin{aligned} S_1^{-1}AS_1\mathbf{e}_1 &= (S_1^{-1}A)(\mathbf{x}_1) \\ &= S_1^{-1}(\lambda_1\mathbf{x}_1) \\ &= \lambda_1(S_1^{-1}\mathbf{x}_1) \\ &= \lambda_1\mathbf{e}_1 \end{aligned}$$

So we get:

$$S_1^{-1}AS_1 = \left(\begin{array}{c|c} \lambda_1 & \mathbf{0} \\ \hline \mathbf{0}^t & A_1 \end{array} \right),$$

with $\mathbf{0}$ a vector of zero entries of size $n-1$ and A_1 an $(n-1) \times (n-1)$ symmetric matrix. We know by induction that there exist a $(n-1) \times (n-1)$ orthogonal matrix S_2 such that $S_2^{-1}A_1S_2 = D'$ with D' an $(n-1) \times (n-1)$ diagonal matrix. Let:

$$S'_2 = \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2 \end{array} \right),$$

and also S'_2 is an orthogonal matrix, we get:

$$\begin{aligned} (S'_2)^{-1}S_1^{-1}AS_1S'_2 &= \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2^t \end{array} \right) (S_1^{-1}AS_1) \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2 \end{array} \right) \\ &= \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2^t \end{array} \right) \left(\begin{array}{c|c} \lambda_1 & \mathbf{0} \\ \hline \mathbf{0}^t & A_1 \end{array} \right) \left(\begin{array}{c|c} 1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2 \end{array} \right) \\ &= \left(\begin{array}{c|c} \lambda_1 & \mathbf{0} \\ \hline \mathbf{0}^t & S_2^t A_1 S_2 \end{array} \right) \\ &= \left(\begin{array}{c|c} \lambda_1 & \mathbf{0} \\ \hline \mathbf{0}^t & D' \end{array} \right) \end{aligned}$$

Thus, if we put

$$\begin{aligned} P &= S_1S'_2 \\ D &= \left(\begin{array}{c|c} \lambda_1 & \mathbf{0} \\ \hline \mathbf{0}^t & D' \end{array} \right), \end{aligned}$$

we have proved (1). From the definition of diagonalizable matrices and Theorem 1.4.7 (ii) and (iii) immediately follow. \square

Theorem 2.1.3. *Giving a graph \mathcal{G} with n linked pages, the sequence as defined in the previous paragraph:*

$$\mathbf{z}^{(0)} = \mathbf{1} \in \mathbb{R}^n, \mathbf{z}^{(k+1)} = \frac{M\mathbf{z}^{(k)}}{\|M\mathbf{z}^{(k)}\|_2}, \quad k = 0, 1, \dots,$$

converges when M has a unique dominant eigenvalue.

Proof. Since 1) M is diagonalizable as symmetric matrix by Theorem 2.1.2 and 2) M has a unique dominant eigenvalue, it follows from the power method that the sequence will converge to a corresponding dominating eigenvector $(\mathbf{h}', \mathbf{a}')$. This eigenvector contains the hub and authority scores. \square

We conclude with a nice corollary.

Corollary 2.1.4. *The second power of the matrix M has the form:*

$$M^2 = \begin{pmatrix} BB^T & 0 \\ 0 & B^T B \end{pmatrix},$$

and the normalized hub and authority scores are given by the dominant eigenvectors of BB^T and $B^T B$.

Proof. By the compact form given in equation 2.1, we see that $\mathbf{h}_k \leftarrow (BB^T)^{k-1} B \mathbf{a}_0$ and $\mathbf{a}_k \leftarrow (B^T B)^k \mathbf{a}_0$. Let \mathbf{a}_0 be $\mathbf{1} \in \mathbb{R}^n$. From the previous theorem we also know that:

$$\lim_{k \rightarrow \infty} \mathbf{h}_k = \mathbf{h} \quad \text{and} \quad \lim_{k \rightarrow \infty} \mathbf{a}_k = \mathbf{a},$$

and also from the previous proof we know that (\mathbf{h}, \mathbf{a}) is the dominant eigenvector of M . It follows immediately that also \mathbf{h} is the dominant eigenvector of BB^T and \mathbf{a} is the dominant eigenvector of $B^T B$. \square

2.1.6 Examples

Searching for math professors at the VUB

Example 2.1.5. We conclude this section with a fictitious example of the HITS-algorithm. Suppose you are looking for `math professors vub` with a text-based search engine and you get the following results:

- The website of the mathematics department of the VUB,
- The website of the faculty of science of the VUB,
- The websites of 4 math professors,
- The website of 10 PhD students at the the mathematics department of the VUB.

Lets take a look at the link structure of these web pages (remember that it is a fictitious example):

- The website of the mathematics department at the VUB links to the websites of all the 4 professors, the 10 PhD students and the faculty of science,
- The website of the faculty of science of the VUB links to the websites of all the 4 math professors and the mathematics department,
- The websites of the 4 math professors link to the website of the Mathematics department and the faculty of science,
- The websites of the 10 PhD students at the the VUB link to the the website of their promotor. 1 professor has 4 PhD students, the other 3 professors have 2 PhD students.

We can now construct the graph \mathcal{G}_σ (of course this graph is not completely made according to Algorithm 2) and we have the following adjacency matrix of \mathcal{G}_σ :

- **Row 1:** website of the mathematics department,
- **Row 2:** website of the faculty of science,
- **Row 3:** website of the professor with the 4 PhD students,
- **Row 4, 5, 6:** websites of the professors with the 2 PhD students,
- **Row 7, 8, 9, 10:** websites of the 4 PhD students of the professor on row 3,
- **Row 11, 12:** websites of the 2 PhD students of the professor on row 4,
- **Row 12, 14:** websites of the 2 PhD students of the professor on row 5,
- **Row 14, 16:** websites of the 2 PhD students of the professor on row 6,

Leads to:

$$B = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

Intuitively, we expect that the professor with his 4 PhD student will have the largest authority score, immediately followed by the other 3 professors. The website of the mathematics department is clearly the best hub in this example and should get the largest hub score. Also the website of the faculty of science should get a high hub score.

We now apply the HITS-method by calculating the dominant eigenvector of BB^T (this returns the hub scores) and the dominant eigenvector of B^TB (this returns the authority scores) with the power method (see 1.4.2). We get:

$$\mathbf{a} = \begin{pmatrix} 0.1979 \\ 0.3162 \\ \mathbf{0.3688} \\ 0.3231 \\ 0.3231 \\ 0.3231 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \\ 0.2029 \end{pmatrix} \quad \text{and} \quad \mathbf{h} = \begin{pmatrix} \mathbf{0.8645} \\ 0.3605 \\ 0.1207 \\ 0.1207 \\ 0.1207 \\ 0.1207 \\ 0.0866 \\ 0.0866 \\ 0.0866 \\ 0.0866 \\ 0.0758 \\ 0.0758 \\ 0.0758 \\ 0.0758 \\ 0.0758 \\ 0.0758 \\ 0.0758 \end{pmatrix}$$

We see that the websites of the 4 math professors are indeed the best authorities for the search query **math professors vub** and that the website of the mathematics department is an extremely good hub (this is very logic because it links to all the other relevant websites). The professor with his 4 PhD students would be ranked first in the search results (he has the highest authority score), the other professors would appear just underneath him. Obviously, a hub score of 0.8645 is so high that it would be quite exceptional in a graph containing a lot more websites (it's very unlikely that you find a website containing links to all the other pages/nodes in the graph). Nevertheless, we conclude that the HITS-algorithm returns the results we wanted intuitively.

Predictors in the Eurovision Song Contest 2009-2014

The Eurovision Song Contest is an annual competition between countries whose public broadcaster is part of the EBU-network. The contest is the biggest music competition in the world, reaching about 200 million annually.

The contest consists of three shows: 2 semi-finals and 1 grand final. From each semi-final, 10 countries proceed to the grand final. Italy, Germany, Spain, United Kingdom and France are always qualified for the grand final because they are the main funders of the event. Also the winner of last year participates automatically in the final. Each country, also those who dropped out during the semi-finals, gives points during the voting of the grand final. The voting during the grand final takes place after all the countries have performed their song. Each country is called and awards 12 points to their favorite song, 10 points to their second favorite, and then points from 8 down to 1 to eight other songs. Countries can not vote for themselves.

The voting system is in fact a positional voting system that is very similar to the Borda count method (see [SAARI] for a scientific explanation of Borda count): the list of points of a country represents the ranking of the 10 best countries in the voting of that country. So the points are values on an ordinal scale.

The complete voting procedure during the Eurovision Song Contest can be seen as a directed graph: all the participating countries are the nodes and the edges represent the

points between the countries (when country a assigns 3 points to country b , then there are 3 edges from a to b).

Let A be the adjacency matrix of the voting during a song contest (A will in fact be just a points table). If we take A as input for the HITS-algorithm, we expect that the country with the highest authority score will be the winner of the competition. Actually we expect a lot more: when we order the countries based on their authority score, we expect that this ordering will be practically equal to the final ranking of the contest. This is based on the simple fact that Borda count just sums up points, and we only expect very small differences when the difference in points is low between two countries. This small differences are then be caused by the algorithm: remember that the HITS-algorithm does not simply give a high authority score to nodes with a large indegree, but also takes the hub scores into account, but we will see that the hub scores will be low so their influence will indeed be limited.

But what is very interesting now, is the role that the hub scores are playing. In fact these scores can be seen as a kind of ‘predictive value’ of a country: a country with a high hub score will have assigned points in such way that it is seen as a reliable source, meaning that the points of that country will match well with the final result of the contest.

Let’s take the Eurovision Song Contest 2014 as an example.

The final results of the contest where (the complete result table can be found in Appendix B):

1. Austria (290 points)
2. The Netherlands (238 points)
3. Sweden (218 points)
4. Armenia (174 points)
5. Hungary (143 points)
6. Ukraine (113 points)
7. Russia (89 points)
8. Norway (88 points)
9. Denmark (74 points)
10. Spain (74 points)
11. Finland (72 points)
12. Romania (72 points)
13. Switzerland (64 points)
14. Poland (62 points)
15. Iceland (58 points)
16. Belarus (43 points)
17. United Kingdom (40 points)
18. Germany (39 points)
19. Montenegro (37 points)
20. Greece (35 points)
21. Italy (33 points)

- 22. Azerbaijan (33 points)
- 23. Malta (32 points)
- 24. San Marino (14 points)
- 25. Slovenia (9 points)
- 26. France (2 points)

Now we calculate the hub and authority scores, based on the full scoreboard and the results are presented in Table 2.1.6.

Notice that ordering the countries by their authority scores indeed returns the final ranking of the contest. The countries who have an authority score equal to 0 are the countries that didn't make it to the final and couldn't therefore receive any points. When looking at the hub scores, it appears that Portugal 'predicted' the final ranking the best. When we look at the points awarded by Portugal during the final, this is indeed true:

- **12 points:** Austria
- **10 points:** The Netherlands
- **8 points:** Sweden
- **7 points:** Switzerland
- **6 points:** Hungary
- **5 points:** Denmark
- **4 points:** Armenia
- **3 points:** Norway
- **2 points:** Russia
- **1 point:** Romania

No less than 7 countries in the points of Portugal have achieved the final top 10, the top 3 results of Portugal are even equal to the final top 3! Russia, Romania and Switzerland are the 3 countries where Portugal awarded points to but didn't achieve the top 10, but still they are placed 11, 12 and 13 in the final ranking. So it is absolutely not surprising that Portugal is the country with the highest hub score.

Note that countries who scored very well during the final, usually have a moderate hub score: this is due to the fact that countries can not vote for themselves. The average hub score is, in general, also lower than the average authority score, this is because countries can award points to only 10 countries, but (qualified) countries can receive points from every country, except themselves. The 'predictive value' of a country is therefore limited to only 10 countries, while the voting produces a complete final ranking of 26 countries.

Of course, it's tempting to research the predictive value of countries during a couple of years. We opted for the period 2009-2014 because during the last five years the voting procedure remained unchanged: the points awarded by each country are based on 50% televoting and 50% jury vote. So we take the average of the hub scores of the last five years of each country. We only put one condition on these countries: they should have participated at 4 out of 5 times, more than 1 absence would possibly make the average misleading. The result is presented in Table 2.1.6. The complete results of each year can be found in Appendix B.

Participant	Authority Score	Participant	Hub Score
Austria	0.285110029	Portugal	0.173610946
The Netherlands	0.235720093	Finland	0.172574335
Sweden	0.212949392	Belgium	0.169584694
Armenia	0.156091783	Latvia	0.166295198
Hungary	0.124453384	Spain	0.165764986
Ukraine	0.095410297	Hungary	0.165699760
Norway	0.086504385	Iceland	0.165062483
Denmark	0.074474911	Estonia	0.162056401
Finland	0.070675128	Denmark	0.160549539
Spain	0.068432379	Lithuania	0.159920120
Russia	0.065352465	Greece	0.159278464
Romania	0.062560768	Norway	0.156676045
Switzerland	0.055868228	Slovenia	0.156533823
Iceland	0.053973263	Sweden	0.155725338
Poland	0.052246035	Romania	0.155212094
United Kingdom	0.037978889	France	0.153993935
Germany	0.029958317	Switzerland	0.153864143
Belarus	0.027945852	Israel	0.153059334
Malta	0.026911408	Ireland	0.147584917
Italy	0.023817428	The Netherlands	0.145211066
Montenegro	0.023425296	United Kingdom	0.144342619
Azerbaijan	0.022613716	Austria	0.137956312
Greece	0.021816155	Germany	0.136869443
San Marino	0.009315756	Ukraine	0.135769452
Slovenia	0.005843162	Italy	0.121638547
France	0.002167387	Malta	0.119063784
Albania	0	Georgia	0.117423087
Belgium	0	Moldova	0.115874904
Estonia	0	Poland	0.112296570
FYR Macedonia	0	FYR Macedonia	0.107531180
Georgia	0	Russia	0.102149330
Ireland	0	San Marino	0.098204303
Israel	0	Montenegro	0.097193444
Latvia	0	Albania	0.091897617
Lithuania	0	Belarus	0.089227164
Moldova	0	Azerbaijan	0.068005452
Portugal	0	Armenia	0.050899422

Table 2.1: The authority and hub scores of the countries during the Final of the Eurovision Song Contest 2014

We see that Hungary, Cyprus and Belgium are the best predictors during the last five years. The bottom is also not very surprising: in 2010, 2012 and 2013 Albania did not receive enough televotes so the jury decided their points (see [EUROVISION] for more information), making their judging process vary from one year to another. Azerbaijan and Armenia scored

very high in the last five years, (e.g. Azerbaijan reached the top 5 every year except 2014, won in 2011 and became second in 2013) but due to their dispute about the Nagorno-Karabakh region, they never exchanged a single point during the last five years. Also cultural differences are probably an explanation: Georgia, Azerbaijan and Armenia are located in the Caucasus, a remote corner of Europe, with many Asian influences (the region is sometimes referred to as Eurasia).

2.1.7 Final reflection

The HITS-algorithm is one of the few algorithms that has the ability to rank pages according to a specific search query. Also the computational cost of the HITS-algorithm, which equals the cost of the power method (see 1.4.2), is not excessive and feasible for most servers. The result of the HITS-algorithm for popular queries will also be cached by most search engines, which reduces the computational cost even more because the saved results can be served directly to the user without any new calculations.

The biggest disadvantage of the HITS-algorithm is that it suffers from *topic drift*: the graph \mathcal{G}'_σ could contain nodes which have high authority scores for the query but are completely irrelevant. E.g. Facebook is nowadays a universally popular website, almost every website contains a ‘like’ or ‘share’ button linking to Facebook, and Facebook itself contains tons of posts linking to other webpages. This means that Facebook has a great chance to appear in almost any \mathcal{G}'_σ and receive a high authority score because the original HITS-algorithm as presented here cannot detect such ‘universally popular’ websites. The same goes for other social media websites and some advertisements.

Nowadays, we know that Ask.com uses this algorithm. In fact, most search engines are very secretive about their search algorithm (e.g. Google) to make profit and avoid cheating by webmasters. Still, the chances are that other search engines use some variant of the algorithm as well, in combination with a lot of other procedures.

2.2 Node similarity

This section provides a detailed overview of the paper ‘*A Measure of Similarity between Graph Vertices: Applications to Synonym Extraction and Web Searching*’[BLONDEL] of V. D. Blondel and others. The paper generalizes the HITS-algorithm leading to the concept of similarity on directed graphs. This concept is explained in detail and far more mathematically rigorously than in the previous section. Recall our assumption in the previous section stating that the matrix M has to have a unique dominant eigenvalue. Although this is satisfactory in practical examples, we want to construct a concept that works for all types of directed graphs, also the ones leading to matrices with dominant eigenvalues with multiplicity greater than 1 and therefore we will develop a method to work around this situation.

From Hubs and Authorities to structure graphs

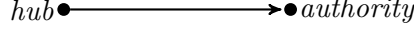
We start with an introduction on how we generalize the construction of the previous section. We don’t present any proofs in this subsection, the results are shown in the next subsections.

Remember from the previous section we constructed a graph \mathcal{G}'_σ and calculated hub and authorities scores for each vertex. Now, for any directed graph \mathcal{G} , the authority score of

Participant	2014	2013	2012	2011	2010	2009	Average
Hungary	0.165700	0.150320	0.151291	0.130650	-	0.158260	0.151244
Cyprus	-	0.161413	0.140385	0.145691	0.144175	0.146567	0.147646
Belgium	0.169585	0.159189	0.153462	0.118487	0.147362	0.122234	0.145053
Lithuania	0.159920	0.141552	0.144121	0.127425	0.144634	0.152601	0.145042
The Netherlands	0.145211	0.133926	0.147638	0.137637	0.139085	0.163395	0.144482
Israel	0.153059	0.157744	0.139948	0.131677	0.118970	0.157031	0.143072
Spain	0.165765	0.153609	0.133174	0.114255	0.162626	0.122739	0.142028
Latvia	0.166295	0.134627	0.138436	0.121329	0.142837	0.143788	0.141219
Estonia	0.162056	0.141096	0.131495	0.143254	0.136098	0.131401	0.140900
Slovenia	0.156534	0.141375	0.148665	0.118682	0.137277	0.133178	0.139285
Malta	0.119064	0.146482	0.122804	0.162192	0.138073	0.139682	0.138049
Iceland	0.165062	0.149906	0.129060	0.130358	0.137492	0.113493	0.137562
Denmark	0.160550	0.112496	0.139704	0.104782	0.144174	0.156365	0.136345
Greece	0.159278	0.144943	0.124054	0.145912	0.095629	0.148054	0.136312
Austria	0.137956	0.127058	0.153796	0.129429	-	0.132217	0.136091
Croatia	-	0.169310	0.132023	0.129980	0.114014	0.134540	0.135974
France	0.153994	0.135187	0.151435	0.137268	0.118194	0.109034	0.134185
Russia	0.102149	0.130277	0.129907	0.143360	0.141861	0.152992	0.133424
Sweden	0.155725	0.122816	0.099063	0.106864	0.153858	0.160329	0.133109
Ireland	0.147585	0.137790	0.132864	0.103704	0.147411	0.128126	0.132913
Romania	0.155212	0.141742	0.119829	0.131675	0.128084	0.119466	0.132668
Germany	0.136869	0.126650	0.157167	0.103942	0.115909	0.155134	0.132612
Finland	0.172574	0.108008	0.141472	0.101891	0.133330	0.132773	0.131675
Bulgaria	-	0.136342	0.150772	0.110776	0.136208	0.122794	0.131378
Norway	0.156676	0.098933	0.154850	0.099012	0.155455	0.107546	0.128745
United Kingdom	0.144343	0.143615	0.121922	0.096917	0.136172	0.133630	0.128594
Portugal	0.173611	-	0.116836	0.130723	0.107674	0.105899	0.126949
Serbia	-	0.165969	0.113907	0.095025	0.132455	0.123080	0.126087
Ukraine	0.135769	0.106438	0.123998	0.120992	0.139278	0.142826	0.125295
FYR Macedonia	0.107531	0.138521	0.132612	0.116197	0.127626	0.124228	0.124453
Belarus	0.089227	0.143351	0.120914	0.138934	0.104108	0.149588	0.124354
Moldova	0.115875	0.139519	0.119439	0.126125	0.119696	0.119161	0.123302
Switzerland	0.153864	0.117585	0.125128	0.092621	0.127077	0.117733	0.122335
Georgia	0.117423	0.147386	0.123067	0.132744	0.086281	-	0.121380
Albania	0.091898	0.102282	0.098185	0.142108	0.140538	0.141493	0.119417
Azerbaijan	0.068005	0.109553	0.113396	0.119173	0.120818	0.109357	0.106717
Armenia	0.050899	0.125792	-	0.128531	0.101509	0.109782	0.103303

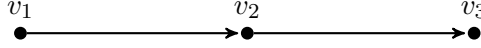
Table 2.2: The average of the hub scores between 2009-2014. Countries must have participated at least 4 times.

a vertex v_j of \mathcal{G} can be thought of as a *score* between v_j of \mathcal{G} and the vertex denoted as *authority* of the graph:



and, conversely, the hub score of vertex v_j of \mathcal{G} can be thought of as a score between v_j and the vertex denoted as *hub*. We call the hub-authority graph a *structure graph* and we already know the resulting iterative method from the previous section. We will call this scores *similarity scores*.

The central question is now: which *mutually reinforcing relation* (iterative method) do we get when using another structure graph, different from the hub-authority structure graph? We start with an example. In our example, we use as structure graph a path graph with three vertices v_1, v_2, v_3 .



Let $\mathcal{G}(W, \rightarrow)$ be a graph. With each vertex w_i of \mathcal{G} we now associate three scores x_{i1}, x_{i2} and x_{i3} , one for each vertex of the structure graph. We initialize these scores with a positive value and then update them according to the mutually reinforcing relation:

$$\begin{cases} x_{i1} := \sum_{j:(w_i, w_j) \in \rightarrow} x_{j2}, \\ x_{i2} := \sum_{j:(w_j, w_i) \in \rightarrow} x_{j1} + \sum_{j:(w_i, w_j) \in \rightarrow} x_{j3}, \\ x_{i3} := \sum_{j:(w_j, w_i) \in \rightarrow} x_{j2}, \end{cases}$$

or, in matrix form (\mathbf{x}_j denotes the column vector with entries x_{ij} , B is the adjacency matrix of graph \mathcal{G}),

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}^{(k+1)} = \begin{pmatrix} 0 & B & 0 \\ B^T & 0 & B \\ 0 & B^T & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}^{(k)}$$

which we, again, can denote by

$$\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)}. \quad (2.3)$$

The principle is now exactly the same as the previous example with hubs and authorities. The matrix M is symmetric and nonnegative, and again the result is the limit of the normalized vector sequence:

$$\mathbf{z}^{(0)} = \mathbf{x}^{(0)} > 0, \mathbf{z}^{(k+1)} = \frac{M\mathbf{z}^{(k)}}{\|M\mathbf{z}^{(k)}\|_2}, \quad k = 0, 1, \dots, \quad (2.4)$$

Remember that the HITS-algorithm assumed that M has a unique dominant eigenvalue but we don't want to make this assumption in this section because we want a concept that can

be applied to all kinds of directed graphs. We will see that without this assumption, the sequence 2.4 does not always converge but oscillates between the limits:

$$\mathbf{z}_{\text{even}} = \lim_{k \rightarrow \infty} \mathbf{z}^{(2k)} \quad \text{and} \quad \mathbf{z}_{\text{odd}} = \lim_{k \rightarrow \infty} \mathbf{z}^{(2k+1)}$$

The limit vectors \mathbf{z}_{even} and \mathbf{z}_{odd} do in general depend on the initial vector $\mathbf{z}^{(0)}$. The set of all limit vectors obtained when starting from a positive initial vector is given by:

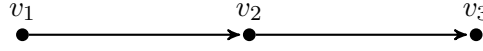
$$Z = \{\mathbf{z}_{\text{even}}(\mathbf{z}^{(0)}), \mathbf{z}_{\text{odd}}(\mathbf{z}^{(0)}) : \mathbf{z}^{(0)} > 0\},$$

and we would like to select a particular vector in that set. We will prove later on that the vector $\mathbf{z}^{(0)} = \mathbf{1}$ is a good choice because it's the unique vector with the largest possible Manhattan³ (we will prove this in Theorem 2.2.10) norm. We denote $\mathbf{z}_{\text{even}}(\mathbf{1})$.

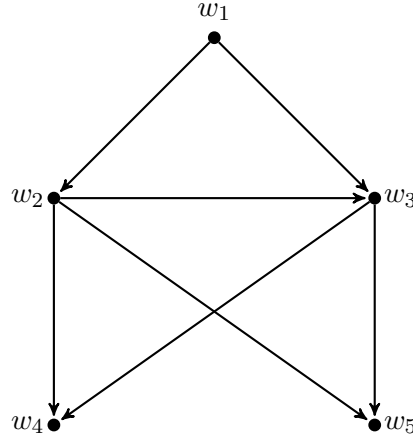
The extremal limit $\mathbf{z}_{\text{even}}(\mathbf{1})$ will be defined as the *similarity matrix*.

We now give a numerical example.

Example 2.2.1. Take as structure graph again the path graph with three vertices v_1, v_2, v_3 :



Let $\mathcal{G}(W, \rightarrow)$ be the following graph:



Then the adjacency matrix B is:

$$B = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

By using the described mutually reinforcing updating iteration we get the following similarity matrix (a numerical algorithm to calculate this is presented later on in this section):

$$S = \begin{pmatrix} 0.3557 & 0.1265 & 0 \\ 0.3102 & 0.3451 & 0.0557 \\ 0.2732 & 0.4619 & 0.4115 \\ 0 & 0.1579 & 0.3557 \\ 0 & 0.0840 & 0.1521 \end{pmatrix}$$

³ $\|\mathbf{x}\|_1 := \sum_{i=1}^n |x_i|$ for $\mathbf{x} \in \mathbb{R}^n$ is the Manhattan norm.

The similarity score of w_4 with v_2 of the structure graph is equal to 0.1579.

We now construct the general case. Take two directed graphs $\mathcal{G} = (U, \rightarrow)$ and $\mathcal{H} = (V, \rightarrow')$ with $n_{\mathcal{G}}$ and $n_{\mathcal{H}}$ the order of the graphs. We think of \mathcal{G} as the structure graph (such as the graphs hub \rightarrow authority and the graph $1 \rightarrow 2 \rightarrow 3$ in the previous paragraphs). We get the following mutually reinforcing updating iteration with as updating equations:

$$x_{ij}^{(k+1)} := \sum_{r:(v_r, v_i) \in \rightarrow', s:(u_s, u_j) \in \rightarrow} x_{rs}^{(k)} + \sum_{r:(v_i, v_r) \in \rightarrow', s:(u_j, u_s) \in \rightarrow} x_{rs}^{(k)} \quad (2.5)$$

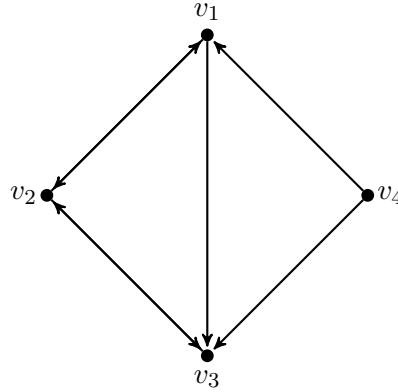
Consider the product graph $\mathcal{G} \times \mathcal{H}$ (see Definition 1.5.15). The above updating equation is equivalent to replacing the scores of all vertices of the product graph by the sum of the scores of the vertices linked by an incoming or outgoing edge.

Equation (2.4) can be rewritten in a more compact matrix form. Let X_k be the $n_{\mathcal{H}} \times n_{\mathcal{G}}$ matrix of entries x_{ij} at iteration k , and A and B are the adjacency matrices of \mathcal{G} and \mathcal{H} . Then the updating equations can be written as:

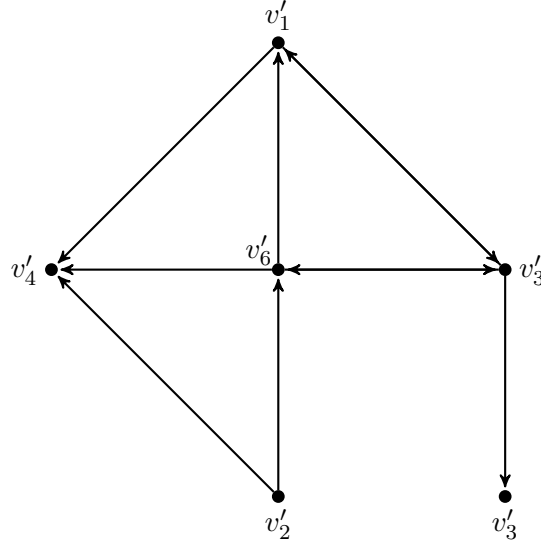
$$X^{(k+1)} = BX^{(k)}A^T + B^T X^{(k)}A, \quad k = 0, 1, \dots, \quad (2.6)$$

We'll prove that the normalized even and odd iterates of this updating equation converge and that the limit $\mathbf{z}_{\text{even}}(\mathbf{1})$ is the limit with the largest Manhattan norm. This limit is the definition of the similarity matrix. The following example shows a calculated similarity matrix of two directed graphs.

Example 2.2.2. Let $\mathcal{G}_A(V, \rightarrow)$ be the following graph:



Let $\mathcal{G}_B(V', \rightarrow')$ be the following graph:



We get the following similarity matrix (a numerical algorithm to calculate this matrix is introduced later in this section):

$$S = \begin{pmatrix} 0.2636 & 0.2786 & 0.2723 & 0.1289 \\ 0.1286 & 0.1286 & 0.0624 & 0.1268 \\ 0.2904 & 0.3115 & 0.2825 & 0.1667 \\ 0.1540 & 0.1701 & 0.2462 & 0 \\ 0.0634 & 0.0759 & 0.1018 & 0 \\ 0.3038 & 0.3011 & 0.2532 & 0.1999 \end{pmatrix}$$

We see for example, that vertex v_2 of \mathcal{G}_A is most similar to vertex v'_3 in \mathcal{G}_B because the similarity score s_{32} is the highest among the similarity scores in s_2 .

2.2.1 Convergence of the sequence $\mathbf{z}^{(k)}$

In the introduction, we mentioned already that the sequence in Equation (2.4) converges for even and odd iterates. We will prove this at the end of this subsection. But before we arrive there, we first need some results on the eigenvectors and eigenvalues of nonnegative matrices. The Perron-Frobenius applies only to nonnegative, *irreducible* matrices, but we will prove in Theorem 2.2.7 that also nonnegative matrices M have a Perron root (see Definition 1.2.11) that has an associated Perron vector. We will also investigate more specific results in the case M is not only nonnegative, but also symmetric.

The reason why we prove all this is clear: remember that in the previous chapter we assumed that M has a unique dominant eigenvalue and showed convergence by the Power Method. This approach is far too naive when introducing similarity on graph vertices, because graphs can lead to matrices where there is no unique dominant eigenvalue. To solve this, a more profound mathematical analysis of the concept is needed, which we present here.

We first want to prove the spectral radius formula. Next, two lemmas are presented which will also contribute to the proof of the spectral radius formula.

Before we prove the following lemma, remember the well known theorem about the Jordan canonical form of a square matrix A (see Theorem in [KIEBOOM2011]).

Theorem 2.2.3. *A square complex matrix A is similar to a block diagonal matrix*

$$J = \begin{pmatrix} J_1 & & \\ & \ddots & \\ & & J_p \end{pmatrix}$$

where each block J_i is a square matrix of the form:

$$J_i = \begin{pmatrix} \lambda_i & 1 & & \\ & \lambda_i & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_i \end{pmatrix}$$

So there exists an (invertible) matrix P such that

$$P^{-1}AP = J$$

J is called the **Jordan normal form** of A .

Lemma 2.2.4. *Let A be an $n \times n$ matrix and $\epsilon > 0$, there exist a matrix norm $\|\cdot\|$ such that:*

$$\|A\| \leq \rho(A) + \epsilon$$

Proof. The Jordan canonical form of A is:

$$A = S \begin{bmatrix} J_{n_1}(\lambda_1) & 0 & \dots & 0 \\ 0 & J_{n_2}(\lambda_2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & J_{n_k}(\lambda_k) \end{bmatrix} S^{-1},$$

where $S \in \mathbb{R}^{n \times n}$ is an invertible matrix, $\lambda_1, \dots, \lambda_k$ are the eigenvalues of A and $n_1 + \dots + n_k = n$. Let:

$$D(\eta) = \begin{bmatrix} D_{n_1}(\eta) & 0 & \dots & 0 \\ 0 & D_{n_2}(\eta) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & D_{n_k}(\eta) \end{bmatrix} \quad \text{with } D_m(\eta) = \begin{bmatrix} \eta & 0 & \dots & 0 \\ 0 & \eta^2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \eta^m \end{bmatrix}$$

Since the left multiplication by $D_m(1/\epsilon)$ multiplies the i th row by $1/\epsilon^i$ and the right multiplication on the right by $D_m(\eta)$ multiplies the j th column by ϵ^j , we calculate:

$$D(1/\epsilon)S^{-1}ASD(\epsilon) = \begin{bmatrix} B_{n_1}(\lambda_1, \epsilon) & 0 & \dots & 0 \\ 0 & B_{n_2}(\lambda_2, \epsilon) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & B_{n_k}(\lambda_k, \epsilon) \end{bmatrix}$$

with

$$B_m(\lambda, \epsilon) = D_m(1/\epsilon)J_m(\lambda)D_m(\epsilon) = \begin{bmatrix} \lambda & \epsilon & 0 & \dots & 0 \\ 0 & \lambda & \epsilon & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \lambda & \epsilon \\ 0 & \dots & 0 & 0 & \lambda \end{bmatrix}$$

We now define the matrix norm for $M \in \mathbb{R}^{n \times n}$ by:

$$\|M\| = \max_{\|\mathbf{x}\|_1=1} \|D(1/\epsilon)S^{-1}MSD(\epsilon)\mathbf{x}\|_1 \quad (2.7)$$

$$= \max_{l \in [1:n]} \sum_{k=1}^n |(D(1/\epsilon)S^{-1}MSD(\epsilon))_{k,l}|. \quad (2.8)$$

The conditions for being a matrix norm are trivially met because we know that $\max_{\|\mathbf{x}\|_1=1} \|A\mathbf{x}\|$ is a matrix norm for any A in $\mathbb{C}^{n \times n}$. \square

Theorem 2.2.5. Spectral radius formula Let a be an $n \times n$ matrix and let $\|\cdot\|$ be a matrix norm then:

$$\rho(A) = \lim_{k \rightarrow \infty} \|A^k\|^{1/k}$$

Proof. Given $k \geq 0$, we use Lemma ?? to write:

$$\rho(A)^k = \rho(A^k) \leq \|A^k\|,$$

so:

$$\rho(A) \leq \|A^k\|^{1/k}.$$

Taking the limit as $k \rightarrow \infty$ gives $\rho(A) \leq \lim_{k \rightarrow \infty} \|A^k\|^{1/k}$. To establish the reverse inequality, we need to prove that, for any $\epsilon > 0$, there exists a $K \geq 0$ such that $\|A^k\|^{1/k} \leq \rho(A) + \epsilon$ for all $k \geq K$. From Lemma 2.2.4, we know that there exists a matrix norm $\|\cdot\|$ so $\|A\| \leq \rho(A) + \epsilon/2$. Moreover, by the equivalence of the norms on $\mathbb{R}^{n \times n}$, we know that there exists some constant $C > 0$ such that $\|M\| \leq C\|M\|$ for all $M \in \mathbb{R}^{n \times n}$. Then, for any $k \geq 0$,

$$\begin{aligned} \|A^k\| &\leq C\|A^k\| \leq C\|A\|^k \leq C(\rho(A) + \epsilon/2)^k, \\ \|A^k\|^{1/k} &\leq C^{1/k}(\rho(A) + \epsilon/2) \rightarrow_{k \rightarrow \infty} \rho(A) + \epsilon/2 \end{aligned}$$

This implies the existence of $K \geq 0$ such that $\|A^k\|^{1/k} \leq \rho(A) + \epsilon$ for $k \geq K$, as desired. \square

Now we are ready for are first big result: since one is confronted in practice with non-negative matrices that are not necessary irreducible, we extend the Perron-Frobenius and see what remains without this assumption. We first start with a lemma and next we proof that the spectral radius $\rho(M)$ of a nonnegative matrix M is an eigenvalue of M , the Perron root. Moreover, there exists an associated nonnegative eigenvector $\mathbf{x} \geq 0$ ($\mathbf{x} \neq 0$), the Perron vector, such that $M\mathbf{x} = \rho\mathbf{x}$.

Lemma 2.2.6. Let A, B be $n \times n$ -matrices, if $|A| \leq B$, then $\rho(A) \leq \rho(|A|) \leq \rho(B)$. (See Definition 1.1.8 for the definition of $|\cdot|$).

Proof. For every $m = 1, 2, \dots$ we have

$$|A^m| \leq |A|^m \leq B^m$$

by using some trivial properties of the absolute value function. Let $\|\cdot\|_2$ be the matrix 2-norm induced by the Euclidean vector norm: for any matrix M , we have $\|M\|_2 = \max_{\|\mathbf{x}\|_2=1} \|M\mathbf{x}\|_2$. For this matrix norm it is trivial to see that if $|M| \leq |M'|$ (see Definition 1.1.5) it follows that $\|M\|_2 \leq \|M'\|_2$ and also $\|M\|_2 = \||M|\|_2$, we get:

$$\|A^m\|_2 \leq \||A|^m\|_2 \leq \|B^m\|_2$$

and

$$\|A^m\|_2^{1/m} \leq \||A|^m\|_2^{1/m} \leq \|B^m\|_2^{1/m}$$

for all $m = 1, 2, \dots$. If we now let $m \rightarrow \infty$ and apply the spectral radius formula from Theorem 2.2.5 we get:

$$\rho(A) \leq \rho(\|A\|) \leq \rho(B).$$

□

Theorem 2.2.7. *If $A \geq 0$ is an $n \times n$ -matrix, then $\rho(A)$ is an eigenvalue of A and there is a nonnegative vector $\mathbf{x} \geq 0, \mathbf{x} \neq 0$, such that $A\mathbf{x} = \rho(A)\mathbf{x}$.*

Proof. For any $\epsilon > 0$ define $A(\epsilon) = [a_{ij} + \epsilon] > 0$. Denote by $\mathbf{x}(\epsilon)$ the Perron vector of $A(\epsilon)$, so $\mathbf{x}(\epsilon) > 0$ and $\sum_{i=1}^n \mathbf{x}(\epsilon)_i = 1$. Since the set of vectors $\{\mathbf{x}(\epsilon) : \epsilon > 0\}$ is contained in the compact set $\{x : x \in \mathbb{C}^n, \|\mathbf{x}\|_1 \leq 1\}$, there is a monotone decreasing sequence $\epsilon_1 > \epsilon_2 > \dots$ with $\lim_{k \rightarrow \infty} \epsilon_k = 0$ such that $\lim_{k \rightarrow \infty} \mathbf{x}(\epsilon_k) = \mathbf{x}$ exists. Since $\mathbf{x}(\epsilon_k) > 0$ for all $k = 1, 2, \dots$, it must be that $\mathbf{x} = \lim_{k \rightarrow \infty} \mathbf{x}(\epsilon_k) \geq 0$; $\mathbf{x} = 0$ is impossible because:

$$\sum_{i=1}^n \mathbf{x}_i = \lim_{k \rightarrow \infty} \sum_{i=1}^n \mathbf{x}(\epsilon_k)_i = 1$$

By Lemma 2.2.6, $\rho(A(\epsilon_k)) \geq \rho(A(\epsilon_{k+1})) \geq \dots \geq \rho(A)$ for all $k = 1, 2, \dots$, so the sequence $\{\rho(A(\epsilon_k))\}_{k=1,2,\dots}$ is a monotone decreasing sequence. Thus, $\rho = \lim_{k \rightarrow \infty} \rho(A(\epsilon_k))$ exists and $\rho \geq \rho(A)$. From the fact that

$$\begin{aligned} A\mathbf{x} &= \lim_{k \rightarrow \infty} A(\epsilon_k)\mathbf{x}(\epsilon_k) \\ &= \lim_{k \rightarrow \infty} \rho(A(\epsilon_k))\mathbf{x}(\epsilon_k) \\ &= \lim_{k \rightarrow \infty} \rho(A(\epsilon_k)) \lim_{k \rightarrow \infty} \mathbf{x}(\epsilon_k) \\ &= \rho\mathbf{x}, \end{aligned}$$

and the fact that $\mathbf{x} \neq 0$ we conclude that ρ is an eigenvalue of A . But then $\rho \leq \rho(A)$ so it must be that $\rho = \rho(A)$. □

Now that we know that any nonnegative matrix M has its spectral radius as an eigenvalue and there exists an associated nonnegative eigenvector, we will see if we can get more specific results when handling nonnegative, symmetric matrices.

Theorem 2.2.8. *Let M be a symmetric nonnegative matrix with spectral radius ρ . Then the algebraic and geometric multiplicity of the Perron root ρ are equal; there is a nonnegative matrix X whose columns span the invariant subspace associated with the Perron root; and the elements of the orthogonal projector Π on the vector space associated with the Perron root of M are all nonnegative.*

Proof. We know that any symmetric nonnegative matrix M can be permuted to a Jordan cononical form with irreducible blocks M_i on the diagonal. We also know from the Perron-Frobenius theorem (see 1.2.10) that the algebraic multiplicity of the Perron root of an irreducible nonnegative matrix is equal to 1. It follows from both facts that the algebraic multiplicities and the geometric multiplicities of the Perron root ρ of M are equal. The corresponding eigenspace of M is obtained from the normalized Perron vectors of the M_i blocks padded with zeros. This normalized Perron vectors form a basis X which is nonnegative and orthonormal. \square

We are almost ready for the theorem about the convergence of $\mathbf{z}^{(k)}$, but we first need an easy result about the orthogonal projection.

Theorem 2.2.9. *Let \mathcal{V} be a linear subspace of \mathbb{R}^n with orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_m\}$. Arrange the column vectors \mathbf{v}_i in a matrix V and let $\mathbf{x} \in \mathbb{R}^n$. The **orthogonal projection** of \mathbf{x} on \mathcal{V} is then given by:*

$$\Pi \mathbf{x} = VV^T \mathbf{x},$$

the matrix $\Pi = VV^T$ is the **orthogonal projector**. Projectors have the property that $\Pi^2 = \Pi$

*Proof.*⁴ We use the connection between transposes and the standard inner product to find the matrix orthogonal projection on the subspace \mathcal{V} :

$$\begin{aligned} \text{proj}_{\mathcal{V}} \mathbf{x} &= \sum_{i=1}^m \frac{\langle \mathbf{v}_i, \mathbf{x} \rangle}{\|\mathbf{v}_i\|} \mathbf{v}_i \\ &= \sum_{i=1}^m \langle \mathbf{v}_i, \mathbf{x} \rangle \mathbf{v}_i \\ &= \sum_{i=1}^m \mathbf{v}_i \langle \mathbf{v}_i, \mathbf{x} \rangle \end{aligned}$$

Remember that $\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y}$ so:

$$\begin{aligned} &= \sum_{i=1}^m \mathbf{v}_i (\mathbf{v}_i^T \mathbf{x}) \\ &= \sum_{i=1}^m (\mathbf{v}_i \mathbf{v}_i^T) \mathbf{x} \\ &= VV^T \mathbf{x} \end{aligned}$$

⁴ $\langle \mathbf{x}, \mathbf{y} \rangle = \sum_{i=1}^n x_i y_i$ with $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ is the standard inner product of two vectors in \mathbb{R}^n .

Proving that $\Pi^2 = \Pi$ is also trivial, remember that for an orthogonal matrix A it holds that $A^T = A^{-1}$:

$$\begin{aligned}\Pi^2 &= (VV^T)^2 \\ &= VV^T VV^T \\ &= VV^{-1} VV^T \\ &= I_n VV^T \\ &= VV^T \\ &= \Pi\end{aligned}$$

□

Theorem 2.2.10. *Let M be a symmetric nonnegative, real matrix of spectral radius ρ . Let $Z^{(0)} > 0$ and consider the sequence*

$$\mathbf{z}^{(k+1)} = \frac{M\mathbf{z}^{(k)}}{\|M\mathbf{z}^{(k)}\|_2}, k = 0, 1, \dots$$

Two convergence cases can occur depending on whether or not $-\rho$ is an eigenvalue of M . When $-\rho$ is not an eigenvalue of M , then the sequence of $Z^{(k)}$ simply converges to $\frac{\Pi\mathbf{z}^{(0)}}{\|\Pi\mathbf{z}^{(0)}\|_2}$, where Π is the orthogonal projector on the eigenspace associated with the Perron root ρ . When $-\rho$ is an eigenvalue of M , then the subsequences $\mathbf{z}^{(2k)}$ and $\mathbf{z}^{(2k+1)}$ converge to the limits

$$\mathbf{z}_{\text{even}}(Z^{(0)}) = \lim_{k \rightarrow \infty} \mathbf{z}^{(2k)} = \frac{\Pi\mathbf{z}^{(0)}}{\|\Pi\mathbf{z}^{(0)}\|_2} \quad \text{and} \quad \mathbf{z}_{\text{odd}}(\mathbf{z}^{(0)}) = \lim_{k \rightarrow \infty} \mathbf{z}^{(2k+1)} = \frac{\Pi M\mathbf{z}^{(0)}}{\|\Pi M\mathbf{z}^{(0)}\|_2}.$$

where Π is the orthogonal projector on the sums of the invariant subspaces associated with ρ and $-\rho$. In both cases the set of all possible limits is given by:

$$\{\mathbf{z}_{\text{even}}(Z^{(0)}), \mathbf{z}_{\text{odd}}(Z^{(0)}) : \mathbf{z}^{(0)} > 0\} = \left\{ \frac{\Pi\mathbf{z}}{\|\Pi\mathbf{z}\|_2} : \mathbf{z} > 0 \right\}$$

and the vector $\mathbf{z}_{\text{even}}(\mathbf{1})$ is the unique vector of largest possible Manhattan norm in that set.

Proof. We prove only the case where $-\rho$ is an eigenvalue, the other case is an easy adaption. Denote the invariant subspaces of M corresponding to ρ , $-\rho$ and to the rest of the spectrum, respectively by \mathcal{V}_ρ , $\mathcal{V}_{-\rho}$ and \mathcal{V}_μ . From the previous theorem, we know that \mathcal{V}_ρ , $\mathcal{V}_{-\rho}$ are certainly nontrivial (ρ and $-\rho$ have at least multiplicity 1, so the eigenspace contains also at least 1 vector), also assume that \mathcal{V}_μ is nontrivial (if \mathcal{V}_μ would be trivial, the rest of the proof gets only easier). We have:

$$MV_\rho = \rho V_\rho, \quad MV_{-\rho} = -\rho V_{-\rho}, \quad MV_\mu = V_\mu M_\mu,$$

where M_μ is a square matrix (diagonal if V_μ is a basis of eigenvectors of the rest of the spectrum, see Theorem 2.1.2) with spectral radius μ strictly less than ρ .

Remember from Theorem 2.1.2 that $P^{-1}MP = D$, with D a diagonal matrix, this can be rewritten as $M = PDP^{-1}$ or $M = PDP^T$ (P is an orthogonal matrix), we can rewrite this in this case as (this is the so called *eigendecomposition* for symmetric matrices):

$$\begin{aligned}M &= \begin{bmatrix} V_\rho & V_{-\rho} & V_\mu \end{bmatrix} \begin{bmatrix} \rho I & & \\ & -\rho I & \\ & & M_\mu \end{bmatrix} \begin{bmatrix} V_\rho & V_{-\rho} & V_\mu \end{bmatrix}^T \\ &= \rho V_\rho V_\rho^T - \rho V_{-\rho} V_{-\rho}^T + V_\mu M_\mu V_\mu^T\end{aligned}$$

It then follows that:

$$M^2 = \rho^2 \Pi + V_\mu M_\mu^2 V_\mu^T,$$

where

$$\Pi = V_\rho V_\rho^T + V_{-\rho} V_{-\rho}^T$$

is the orthogonal projector onto the invariant subspace $\mathcal{V}_\rho \oplus \mathcal{V}_{-\rho}$ of M^2 corresponding to ρ^2 . We also have:

$$M^{2k} = \rho^{2k} \Pi + V_\mu M_\mu^{2k} V_\mu^T,$$

and since $\rho M_\mu = \mu < \rho$, it follows from multiplying this by $\mathbf{z}^{(0)}$ and $M\mathbf{z}^{(0)}$ that:

$$\mathbf{z}^{(2k)} = \frac{\Pi \mathbf{z}^{(0)}}{\|\Pi \mathbf{z}^{(0)}\|_2} + O\left(\frac{\mu}{\rho}\right)^{2k}$$

and

$$\mathbf{z}^{(2k+1)} = \frac{\Pi M \mathbf{z}^{(0)}}{\|\Pi M \mathbf{z}^{(0)}\|_2} + O\left(\frac{\mu}{\rho}\right)^{2k},$$

provided $\Pi \mathbf{z}^{(0)}$ and $\Pi M \mathbf{z}^{(0)}$ are nonzero, so the initial vectors $\mathbf{z}^{(0)}$ and $M\mathbf{z}^{(0)}$ must have a nonzero component. This is no problem, because the Euclidean norms of these vectors equal $\mathbf{z}^{(0)T} \Pi \mathbf{z}^{(0)}$ and $\mathbf{z}^{(0)T} M \Pi M \mathbf{z}^{(0)}$ since $\Pi^2 = \Pi$. These norms are both nonzero since $\mathbf{z}^{(0)} > 0$ and both Π and $M\Pi$ are nonnegative and nonzero.

From the fact that M is nonnegative and the formula for $\mathbf{z}_{\text{even}}(\mathbf{z}^{(0)})$ and $\mathbf{z}_{\text{odd}}(\mathbf{z}^{(0)})$ we conclude that both limits lie in $\{\Pi \mathbf{z} / \|\Pi \mathbf{z}\|_2 : \mathbf{z} > 0\}$. We now show that every element $\tilde{\mathbf{z}}^{(0)} \in \{\Pi \mathbf{z} / \|\Pi \mathbf{z}\|_2 : \mathbf{z} > 0\}$ can be obtained as $\mathbf{z}_{\text{even}}(\mathbf{z}^{(0)})$ for some $\mathbf{z}^{(0)} > 0$. Since the entries of Π are nonnegative, so are those of $\tilde{\mathbf{z}}^{(0)}$. This vector may have some zero entries. From $\tilde{\mathbf{z}}^{(0)}$ we construct $\mathbf{z}^{(0)}$ by adding $\epsilon > 0$ to all the zero entries of $\tilde{\mathbf{z}}^{(0)}$. The vector $\mathbf{z}^{(0)} - \tilde{\mathbf{z}}^{(0)}$ is clearly orthogonal to $\mathcal{V}_\rho \oplus \mathcal{V}_{-\rho}$ and will vanish in the iteration of M^2 . Thus we have $\mathbf{z}_{\text{even}}(\mathbf{z}^{(0)}) = \tilde{\mathbf{z}}^{(0)}$ for $\mathbf{z}^{(0)} > 0$, proving our statement.

We now prove the last statement. The matrix Π and all vectors are nonnegative and $\Pi^2 = \Pi$ and so:

$$\left\| \frac{\Pi \mathbf{1}}{\|\Pi \mathbf{1}\|_2} \right\|_1 = \sqrt{\mathbf{1}^T \Pi^2 \mathbf{1}}$$

and also:

$$\left\| \frac{\Pi \mathbf{z}^{(0)}}{\|\Pi \mathbf{z}^{(0)}\|_2} \right\|_1 = \frac{\mathbf{1}^T \Pi^2 \mathbf{z}^{(0)}}{\sqrt{\mathbf{z}^{(0)T} \Pi^2 \mathbf{z}^{(0)}}}$$

We apply the Cauchy-Schwarz inequality to $\Pi \mathbf{1}$ and $\Pi \mathbf{z}^{(0)}$, remember that $\Pi = WW^T$ for some W , so $\Pi^T = (WW^T)^T = (W^T)^T W^T = WW^T = \Pi$, that the matrix Π and all vectors are nonnegative and $\Pi^2 = \Pi$:

$$\begin{aligned} |\langle \Pi \mathbf{1}, \Pi \mathbf{z}^{(0)} \rangle| &\leq \|\Pi \mathbf{1}\| \cdot \|\Pi \mathbf{z}^{(0)}\| \\ \Leftrightarrow |(\Pi \mathbf{1})^T \Pi \mathbf{z}^{(0)}| &\leq \sqrt{\mathbf{1}^T \Pi^2 \mathbf{1}} \cdot \sqrt{\mathbf{z}^{(0)T} \Pi^2 \mathbf{z}^{(0)}} \\ \Leftrightarrow |\mathbf{1}^T \Pi^T \Pi \mathbf{z}^{(0)}| &\leq \sqrt{\mathbf{1}^T \Pi^2 \mathbf{1}} \cdot \sqrt{\mathbf{z}^{(0)T} \Pi^2 \mathbf{z}^{(0)}} \\ \Leftrightarrow |\mathbf{1}^T \Pi^2 \mathbf{z}^{(0)}| &\leq \sqrt{\mathbf{1}^T \Pi^2 \mathbf{1}} \cdot \sqrt{\mathbf{z}^{(0)T} \Pi^2 \mathbf{z}^{(0)}}, \end{aligned}$$

equality arises only when $\Pi \mathbf{z}^{(0)} = \lambda \Pi \mathbf{1}$ for some $\lambda \in \mathbb{C}$. But since $\Pi \mathbf{z}^{(0)}$ and $\Pi \mathbf{1}$ are both real nonnegative, the last statement is proved. \square

2.2.2 Compact form & Similarity matrices

We now come to the formal definition of the similarity matrix of two directed graphs $\mathcal{G}(U, \rightarrow)$ and $\mathcal{H}(V, \rightarrow')$, by proving that the mutually reinforcing relation is given by (A and B are the adjacency matrices of \mathcal{G} and \mathcal{H}):

$$X^{(k+1)} = BX^{(k)}A^T + B^TX^{(k)}A, \quad k = 0, 1, \dots, \quad (2.9)$$

which we already introduced in 2.6. To prove this relation, we take a detour via a nice property of the Kronecker product and the vec-operator. The vec-operator is a convenient way of stacking columns of a matrix left to right. With this operator we can rewrite 2.9 in $\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)}$ with M equal to a sum of Kronecker products. This will allow us to apply Theorem 2.2.10.

Definition 2.2.11. *With each $m \times n$ -matrix $A = [a_{ij}]$ we can associate the vector $\text{vec}(A) \in \mathbb{R}^{mn}$ defined by:*

$$\text{vec}(A) = \begin{pmatrix} a_{11} & \dots & a_{m1} & a_{12} & \dots & a_{m2} & a_{1n} & \dots & a_{mn} \end{pmatrix}^T$$

Definition 2.2.12. *The **Kronecker product** (or **tensor product**) of an $m \times n$ -matrix $A = (a_{ij})$ and a $p \times q$ -matrix $B = (b_{ij})$ is denoted by $A \otimes B$ and is defined by the matrix:*

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix} \in \mathbb{R}^{mp \times nq}$$

Lemma 2.2.13. *Consider a $m \times n$ -matrix $A = (a_{ij})$ and a $p \times q$ -matrix $B = (b_{ij})$, we have:*

$$A^T \otimes B^T = (A \otimes B)^T$$

Proof. By direct computation, we get:

$$\begin{aligned}
 (A \otimes B)^T &= \left(\begin{array}{ccc} a_{11} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1q} \\ \vdots & \ddots & \vdots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pq} \end{pmatrix} & \dots & a_{1n} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1q} \\ \vdots & \ddots & \vdots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pq} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ a_{m1} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1q} \\ \vdots & \ddots & \vdots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pq} \end{pmatrix} & \dots & a_{mn} \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1q} \\ \vdots & \ddots & \vdots & \vdots \\ b_{p1} & b_{p2} & \dots & b_{pq} \end{pmatrix} \end{array} \right)^T \\
 &= \left(\begin{array}{ccc} a_{11} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{p1} \\ \vdots & \ddots & \vdots & \vdots \\ b_{1q} & b_{2q} & \dots & b_{pq} \end{pmatrix} & \dots & a_{m1} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{p1} \\ \vdots & \ddots & \vdots & \vdots \\ b_{1q} & b_{2q} & \dots & b_{pq} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ a_{1n} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{p1} \\ \vdots & \ddots & \vdots & \vdots \\ b_{1q} & b_{2q} & \dots & b_{pq} \end{pmatrix} & \dots & a_{mn} \begin{pmatrix} b_{11} & b_{21} & \dots & b_{p1} \\ \vdots & \ddots & \vdots & \vdots \\ b_{1q} & b_{2q} & \dots & b_{pq} \end{pmatrix} \end{array} \right) \\
 &= \begin{pmatrix} a_{11}B^T & \dots & a_{m1}B^T \\ \vdots & \ddots & \vdots \\ a_{1n}B^T & \dots & a_{mn}B^T \end{pmatrix} \\
 &= A^T \otimes B^T
 \end{aligned}$$

□

Theorem 2.2.14. Let A a $m \times n$ -matrix, B a $p \times q$ -matrix and C a $m \times p$ matrix, the matrix equation:

$$AXB = C$$

with X an unknown $n \times p$ -matrix, is equivalent tot the system of qm equations and np unkonws given by:

$$(B^T \otimes A) \text{vec}(X) = \text{vec}(C)$$

so:

$$\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X)$$

Proof. Let Q_k be the k th column of a given matrix Q , we get:

$$\begin{aligned}
 (AXB)_k &= A(XB)_k \\
 &= AXB_k \\
 &= A \sum_{i=1}^p b_{ik} X_i \\
 &= Ab_{1k}X_1 + Ab_{2k}X_2 + \dots + Ab_{pk}X_p \\
 &= \begin{pmatrix} b_{1k}A & b_{2k}A & \dots & b_{pk}A \end{pmatrix} \text{vec}(X) \\
 &= (B_k^T \otimes A) \text{vec}(X)
 \end{aligned}$$

We get:

$$\text{vec}(AXB) = \begin{pmatrix} B_1^T \otimes A \\ \vdots \\ B_q^T \otimes A \end{pmatrix} \text{vec}(X)$$

But it follows immediately that:

$$\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X)$$

because the transpose of a column of B is a row of B^T . \square

Theorem 2.2.15. Let \mathcal{G} and \mathcal{H} be two directed graphs with adjacency matrices $A = [a_{ij}] \in \mathbb{R}^{n \times n}$ and $B = [b_{ij}] \in \mathbb{R}^{m \times m}$ and let $Z^{(0)} > 0$ be an initial positive matrix, and define⁵:

$$Z^{(k+1)} = \frac{BZ^{(k)}A^T + B^T Z^{(k)}A}{\|BZ^{(k)}A^T + B^T Z^{(k)}A\|_F}, \quad k = 0, 1, \dots$$

Then the matrix subsequences $Z^{(2k)}$ and $Z^{(2k+1)}$ converge to Z_{even} and Z_{odd} and among all the matrices in the set of all possible limits:

$$\{Z_{\text{even}}(Z^{(0)}), Z_{\text{odd}}(Z^{(0)}) : Z^{(0)} > 0\}$$

the matrix $Z_{\text{even}}(\mathbf{1})$ is the unique matrix of largest 1-norm⁶.

Proof. We first rewrite the compact form of 2.9:

$$\begin{aligned} X^{(k+1)} &= BX^{(k)}A^T + B^T X^{(k)}A \\ \Leftrightarrow \text{vec}(X^{(k+1)}) &= \text{vec}(BX^{(k)}A^T + B^T X^{(k)}A) \\ \Leftrightarrow \text{vec}(X^{(k+1)}) &= \text{vec}(BX^{(k)}A^T) + \text{vec}(B^T X^{(k)}A) \\ \Leftrightarrow \text{vec}(X^{(k+1)}) &= ((A^T)^T \otimes B) \text{vec}(X^{(k)}) + (A^T \otimes B^T) \text{vec}(X^{(k)}) \\ \Leftrightarrow \text{vec}(X^{(k+1)}) &= (A \otimes B + A^T \otimes B^T) \text{vec}(X^{(k)}) \end{aligned}$$

If we define $\mathbf{x}_k = \text{vec}(X^{(k)})$ and $M = A \otimes B + A^T \otimes B^T$ we get:

$$\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)},$$

exactly the same compact form as introduced in the beginning of this section in 2.3. If we can prove that M is symmetric and nonnegative, then we can apply Theorem 2.2.10 and the result follows. M is, of course, nonnegative because the adjacency matrices A and B are always nonnegative. To see that M is symmetric, first notice that M can be rewritten using Lemma 2.2.13 to:

$$M = A \otimes B + (A \otimes B)^T, \quad (2.10)$$

because $A \otimes B$ is a $nm \times nm$ square matrix, we know that M is symmetric because it's the sum of a square matrix and its transpose. In order to stay consistent with the vector norm appearing in Theorem 2.2.10, the matrix norm $\|\cdot\|_F$ or the *Frobenius* norm is the square root of the sum of all squared entries and the 1-norm $\|\cdot\|_1$ is the sum of all magnitudes of the entries. We can now apply Theorem 2.2.10 and the result follows. \square

⁵ $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n (a_{ij})^2}$ is the *Frobenius* norm for a $m \times n$ -matrix A .

⁶ $\|A\|_{1,1} = \sum_{i=1}^m \sum_{j=1}^n |a_{ij}|$ is the 1-norm for a $m \times n$ -matrix A

Definition 2.2.16. Let \mathcal{G}, \mathcal{H} be two directed graphs, then the unique matrix

$$S = Z_{\text{even}}(\mathbf{1}) = \lim_{k \rightarrow +\infty} Z^{(2k)}$$

(with the notations of the previous theorem) is the **similarity matrix** between \mathcal{G} and \mathcal{H} .

Notice that it follows from 2.9 that the similarity matrix between \mathcal{H} and \mathcal{G} is the transpose of the similarity matrix between \mathcal{G} and \mathcal{H} .

2.2.3 Algorithm & Computational cost

Data:

A : the $n \times n$ adjacency matrix of a directed graph \mathcal{G}

B : the $m \times m$ adjacency matrix of a directed graph \mathcal{H} .

TOL: tolerance for the estimation error.

Result:

S : the similarity matrix between \mathcal{G} and \mathcal{H} .

begin similarity_matrix(A, B, TOL)

$k = 1$;

$Z^{(0)} = \mathbf{1}$ ($n \times m$ -matrix with all entries equal to 1);

$\mu = n \times m$ -matrix with all entries equal to TOL;

repeat

$$Z^{(k)} = \frac{BZ^{(k-1)}A^T + B^T Z^{(k-1)}A}{\|BZ^{(k-1)}A^T + B^T Z^{(k-1)}A\|_F};$$

$k = k + 1$;

until k is even and $|Z - Z^{(k-2)}| < \mu$;

return $Z^{(k)}$;

end

Algorithm 5: Algorithm for calculating the similarity matrix between \mathcal{G} and \mathcal{H}

The compact form introduced in the previous section leads directly to the approximation algorithm 5. Note that the algorithm must iterate an even number of times and to check if the tolerance limit is reached, only the even iteration steps are considered. This is of course an obvious consequence of the definition of the similarity matrix. A Matlab implementation of the algorithm can be found in Listing A.2 in Appendix A.

To estimate the computational cost, we first notice that the algorithm is a matrix analogue to the power method introduced in section 1.4.2. We already showed in Theorem 2.2.10 that the convergence of the even iterates in the above recurrence relation is linear with ratio $(\mu/\rho)^{2n}$. With the accuracy level TOL, we become: **Ik weet dat ik \approx nog moet definiëren, maar ik weet niet goed hoe.**

$$\left| \frac{\mu}{\rho} \right|^{2n} \approx \text{TOL}$$

So, for example, for $\text{TOL} = 10^{-5}$ we get $n = -5/(2 \log \mu/\lambda)$, we become:

$$\text{similarity_matrix} \in O\left(\frac{-1}{\log \mu - \log \rho}\right)$$

Note that this O holds for any estimation error TOL of the form 10^{-e} with $e \in \mathbb{N}$. Also note that this is completely analogous to the computational cost of the power method, which

comes as no surprise since the algorithms are similar, but remember from Theorem 2.2.7 that we cannot encounter a situation in which $\mu = \rho$, since we know that ρ is the unique dominant eigenvalue (in contrast to the power method, where we don't know in general whether a matrix has a unique dominant eigenvalue or not).

2.2.4 Special cases

We now consider some special cases of similarity scores between two vertices of graphs.

HITS-algorithm

Remember that the HITS-algorithm assumed that

$$M = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix},$$

has a unique dominant eigenvalue to calculate the hub and authority scores of nodes in a graph \mathcal{G}_σ with adjacency matrix B . This assumption is a direct result of the power method, because it's one of the conditions to apply the algorithm. One of our goals of this section was to drop this assumption, making the concept of similarity more robust. We finally arrived at this result.

Theorem 2.2.17. *Let \mathcal{G} be a graph with adjacency matrix B . The normalized hub and authority scores of the vertices are given by the normalized dominant eigenvectors of the matrices BB^T and B^TB , provided the corresponding Perron root is of multiplicity 1. Otherwise, it is the normalized projection of the vector $\mathbf{1}$ on the eigenspace of the Perron root.*

Proof. The corresponding matrix M is:

$$M = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$$

so:

$$M^2 = \begin{pmatrix} BB^T & 0 \\ 0 & B^TB \end{pmatrix},$$

and the result follows from Theorem 2.2.10 under the condition that the matrix M^2 has a dominant root ρ^2 . This can be seen as follows: let V and U be orthonormal bases for the dominant eigenspaces of B :

$$BV = \rho U, \quad B^TU = \rho V$$

then clearly V and U are also bases for the dominant eigenspaces of B^TB and BB^T so:

$$B^TBV = \rho^2 V, \quad BB^TU = \rho^2 U.$$

The projectors associated with the dominant eigenvalues of BB^T and B^TB are, respectively:

$$\Pi_v = VV^T \quad \text{and} \quad \Pi_u = UU^T,$$

the projector of Π of M^2 is then:

$$\Pi = \text{diag}(\Pi_v, \Pi_u),$$

and hence the subvectors of $\Pi\mathbf{1}$ are the vectors $\Pi_v\mathbf{1}$ and $\Pi_u\mathbf{1}$, which can be computed with B^TB and BB^T . \square

Central scores

As for the hub and authority scores we can give an explicit expression for the similarity score with vertex 2, which we will call the *central score*.

Theorem 2.2.18. *Let \mathcal{G} be a graph with adjacency matrix B . The normalized similarity scores of vertex 2 of the path graph $1 \rightarrow 2 \rightarrow 3$ with the vertices of graph \mathcal{G} are called the central scores and are given by the normalized dominant eigenvector of the matrix $B^T B + B B^T$, provided the corresponding Perron root is of multiplicity 1. Otherwise, it is the normalized projection of the vector 1 on the dominant invariant subspace.*

Proof. Let

$$M = \begin{pmatrix} 0 & B & 0 \\ B^T & 0 & B \\ 0 & B^T & 0 \end{pmatrix}$$

so:

$$M^2 = \begin{pmatrix} B B^T & 0 & B B \\ 0 & B^T B + B B^T & 0 \\ B^T B^T & 0 & B^T B \end{pmatrix}$$

because M is nonnegative and symmetric, the result follows from Theorem 2.2.10 under the condition that the central matrix $B^T B + B B^T$ has a dominant root ρ^2 of M^2 . We can state this condition otherwise, because M can be permuted to:

$$M = P^T \begin{pmatrix} 0 & E \\ E^T & 0 \end{pmatrix} P, \quad \text{where } E = \begin{pmatrix} B \\ B^T \end{pmatrix}$$

Now let V and U be orthonormal bases for the dominant eigenspaces of $E^T E$ and $E E^T$, since:

$$E^T E V = \rho^2 V, \quad E E^T U = \rho^2 U.$$

Moreover,

$$P M^2 P^T = \begin{pmatrix} E E^T & 0 \\ 0 & E^T E \end{pmatrix},$$

and let

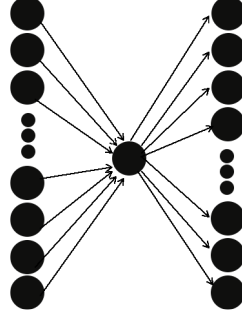
$$\Pi_v = V V^T \quad \text{and} \quad \Pi_u = U U^T$$

be the projectors associated with the dominant eigenvalues of $E E^T$ and $E^T E$. The project Π of M^2 is then equal to:

$$\Pi = P^T \text{diag}(\Pi_v, \Pi_u) P,$$

and it follows that the subvectors of $\Pi \mathbf{1}$ are the vectors $\Pi_v \mathbf{1}$ and $\Pi_u \mathbf{1}$, which can be computed from $E^T E$ or $E E^T$. Since $E^T E = B^T B + B B^T$, the central vector $\Pi_v \mathbf{1}$ is the central vector of $\Pi \mathbf{1}$. \square

Example 2.2.19. In order to illustrate the intuitive meaning of calculating a similarity matrix where the path graph $1 \rightarrow 2 \rightarrow 3$ is the structure graph, consider the following directed bow-tie graph:



Label the center vertex first, then the m left vertices and finally the n right vertices, then the adjacency matrix of the bow-tie graph becomes:

$$B = \left(\begin{array}{c|ccc|ccc} 0 & 0 & \dots & 0 & 1 & \dots & 1 \\ \hline 1 & & & & & & \\ \vdots & & \mathbf{0}_n & & & & \mathbf{0} \\ \hline 1 & & & & & & \\ \hline 0 & & & & & & \\ \vdots & & \mathbf{0} & & & \mathbf{0}_m & \\ \hline 0 & & & & & & \end{array} \right)$$

By direct computation, we get that the matrix $B^T B + B B^T$ is equal to:

$$B^T B + B B^T = \begin{pmatrix} m+n & 0 & 0 \\ 0 & \mathbf{1}_n & 0 \\ 0 & 0 & \mathbf{1}_m \end{pmatrix}$$

By Theorem 2.2.18, the Perron root of M is equal to $\rho = \sqrt{n+m}$ and the similarity matrix is the $(1+m+n) \times 3$ -matrix:

$$S = \frac{1}{\sqrt{m+n+1}} \left(\begin{array}{c|c|c} 0 & 1 & 0 \\ \hline 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ \hline 1 & 0 & 0 \\ \hline 0 & 0 & 1 \\ \vdots & \vdots & \vdots \\ \hline 0 & 0 & 1 \end{array} \right)$$

If we see vertex 2 of the path graph $1 \rightarrow 2 \rightarrow 3$ as the *center*, which can be seen as a vertex through which much information is passed, then it is not surprising that S indicates that vertex 1 of the directed bow-tie graph is the only one that looks like a center. The left vertices of the bow-tie graph look like vertex 1 of the path graph and the right vertices of the bow-tie graph look like vertex 3. This is a beautiful example because it confirms our intuition.

Self-similarity of a graph

When we compute the similarity matrix of two equal graphs $\mathcal{G} = \mathcal{H}$, the similarity matrix S is square matrix with as entries the similarity scores between vertices of \mathcal{G} , we call S the *self-similarity matrix* of \mathcal{G} in this case.

Intuitively, we expect that vertices have the highest similarity scores with themselves, which means that the largest entries are located on the diagonal of S . We prove in the next theorem that the largest entry of a self-similarity matrix appears always on the diagonal and that, except for some special cases, the diagonal elements of a self-similarity matrix are nonzero. This doesn't mean that the diagonal elements are always larger than the other elements on the same row or column and we conclude this paragraph with some easy examples the show this.

Theorem 2.2.20. *The self-similarity matrix of a graph \mathcal{G} is positive semidefinite⁷. The largest entry of the matrix appears on the diagonal and if a diagonal entry is equal to zero, all the entries of the corresponding row and column are also equal to zero.*

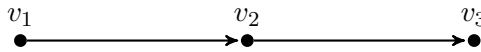
Hier ga ik nog enkele relevante eigenschappen van positieve semidefinitie matrices toevoegen, dit bewijs toch net iets te kort door de bocht me dunkt.

Proof. Since $A = B$, the compact form of Theorem 2.2.15 becomes:

$$Z^{(k+1)} = \frac{BZ^{(k)}A^T + B^T Z^{(k)}A}{\|BZ^{(k)}A^T + B^T Z^{(k)}A\|_F}, \quad Z^{(0)} = \mathbf{1},$$

It is clear that all matrices $Z^{(k)}$ are positive semidefinite because the scaled sum of two positive semidefinite matrices is also positive semidefinite. Since the positive semidefinite matrices form a closed set (in the usual topology), the limit S will also be positive semidefinite. The rest of the theorem are well known properties of positive semidefinite matrices. \square

Example 2.2.21. The self-similarity matrix of the graph:

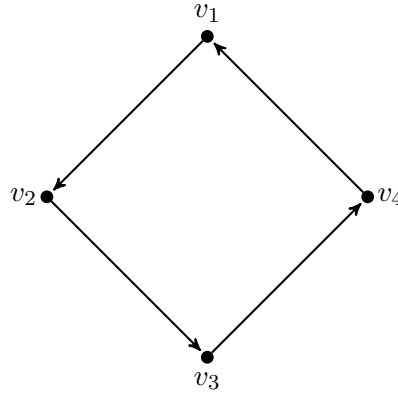


is equal to:

$$\begin{pmatrix} 0.5774 & 0 & 0 \\ 0 & 0.5774 & 0 \\ 0 & 0 & 0.5774 \end{pmatrix}$$

Example 2.2.22. The self-similarity matrix of the graph:

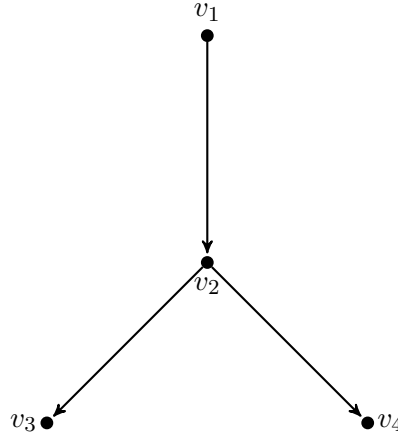
⁷A $n \times n$ -matrix A is called positive-semidefinite if $\mathbf{x}^T A \mathbf{x} \geq 0$ for all \mathbf{x} in \mathbb{R}^n .



is equal to:

$$\begin{pmatrix} 0.250 & 0.250 & 0.250 & 0.250 \\ 0.250 & 0.250 & 0.250 & 0.250 \\ 0.250 & 0.250 & 0.250 & 0.250 \\ 0.250 & 0.250 & 0.250 & 0.250 \end{pmatrix}$$

Example 2.2.23. The self-similarity matrix of the graph:



is equal to:

$$\begin{pmatrix} 0.4082 & 0 & 0 & 0 \\ 0 & 0.4082 & 0 & 0 \\ 0 & 0 & 0.4082 & 0.4082 \\ 0 & 0 & 0.4082 & 0.4082 \end{pmatrix}$$

2.3 Node-edge similarity

The paper of Blondel et al. [BLONDEL] caused a flow of successive papers which build upon the concept of similarity between two graphs. For instance, the paper ‘Graph similarity scoring and matching’ of Laura Zager and Goerge Verghese [ZAGER] expands the notion of node similarity presented in the previous section to similarity between the edges of two graphs. The paper was presented in 2006. Intuitively an edge of a graph \mathcal{G} is similar to an edge of graph \mathcal{H} if their *source* and *terminal nodes* are similar. As a consequence, the notion of similarity between edges introduces a coupling between edge and node similarity scores.

The algorithm presented in this paper is therefore an extension of the algorithm presented in the previous section.

2.3.1 Coupled node-edge similarity scores

We now present the extended algorithm allowing us to calculate not only a node similarity scores, but also edge similarity scores. The algorithm will use a new sort of matrices that represent a graph. Recall Definition 1.5.6 of source and terminal nodes.

Definition 2.3.1. Let be $\mathcal{G} = (V, \rightarrow)$ be a graph with adjacency matrix A , numbered vertices $v_1, v_2, \dots, v_n \in V$ and numbered edges $e_1, e_2, \dots, e_m \in \rightarrow$. We define the **source-edge matrix** A_S as a $n \times m$ matrix with entries:

$$(A_S)_{ij} = \begin{cases} 1 & \text{if } s_{\mathcal{G}}(e_j) = v_i \\ 0 & \text{otherwise} \end{cases},$$

the notation A_S is derived from the adjacency matrix A , when the graph would have another adjacency matrix, for instance B , we would write B_S .

Definition 2.3.2. Let be $\mathcal{G} = (V, \rightarrow)$ be a graph with adjacency matrix A , numbered vertices $v_1, v_2, \dots, v_n \in V$ and numbered edges $e_1, e_2, \dots, e_m \in \rightarrow$. We define the **terminus-edge matrix** A_T as a $n \times m$ matrix with entries:

$$(A_T)_{ij} = \begin{cases} 1 & \text{if } t_{\mathcal{G}}(e_j) = v_i \\ 0 & \text{otherwise} \end{cases},$$

the notation A_T is derived from the adjacency matrix A , when the graph would have another adjacency matrix, for instance B , we would write B_T .

Property 2.3.3. Let $\mathcal{G} = (V, \rightarrow)$ be a graph, then $A_S A_S^T$ is a diagonal matrix where the i th diagonal entry is equal the outdegree of vertex v_i .

Proof. By direct computation, we get:

$$(A_S A_S^T)_{ij} = \sum_{k=1}^m (A_S)_{ik} (A_S)_{kj}^T = \sum_{k=1}^m (A_S)_{ik} (A_S)_{jk}$$

Assume $i \neq j$. Then for each k , $(A_S)_{ik} (A_S)_{jk} = 0$ since vertex v_i and vertex v_j can't be both the source node of edge k .

When $i = j$, then for each k , $(A_S)_{ik} (A_S)_{jk} = ((A_S)_{ik})^2$ equals 0 or 1 depending on whether v_i is a starting point or not, so 1 is added to $(A_S A_S^T)_{ii}$ each time an edge 'departs' from v_i , this is exactly the outdegree of vertex v_i . \square

In an analogous way, we prove:

Property 2.3.4. Let $\mathcal{G} = (V, \rightarrow)$ be a graph, then $A_T A_T^T$ is a diagonal matrix where the i th diagonal entry is equal the indegree of vertex v_i .

Property 2.3.5. Let $\mathcal{G} = (V, \rightarrow)$ be a graph, then the adjacency matrix A is equal to $A_S A_T^T$.

Proof. By direct computation, we get:

$$(A_S A_T^T)_{ij} = \sum_{k=1}^m (A_S)_{ik} (A_T)_{kj}^T = \sum_{k=1}^m (A_S)_{ik} (A_T)_{jk}$$

The terms $(A_S)_{ik} (A_T)_{jk}$ equal 1 if edge k goes from v_i to v_j and since the sum is taken over all edges we conclude:

$$(A_S A_T^T)_{ij} = A_{ij}.$$

□

Let $\mathcal{G}(V, \rightarrow)$, $\mathcal{H}(U, \rightarrow')$ be two (directed) graphs, \mathcal{G} has $n_{\mathcal{G}}$ vertices and $m_{\mathcal{G}}$ edges and \mathcal{H} has $n_{\mathcal{H}}$ vertices and $m_{\mathcal{H}}$. Remember the following updating equation from (2.5), which returns the (node) similarity score between vertices u_i from \mathcal{H} and v_j from \mathcal{G} :

$$x_{ij}^{(k+1)} = \sum_{r: (u_r, u_i) \in \rightarrow', w: (v_w, v_j) \in \rightarrow} x_{rw}^{(k)} + \sum_{r: (u_i, u_r) \in \rightarrow', w: (v_j, v_w) \in \rightarrow} x_{rw}^{(k)},$$

if we number the edges of \mathcal{G} and \mathcal{H} as $e_1, e_2, \dots, e_{m_{\mathcal{G}}} \in \rightarrow$ and $e'_1, e'_2, \dots, e'_{m_{\mathcal{H}}} \in \rightarrow'$, this can be rewritten as:

$$x_{ij}^{(k+1)} = \sum_{t_{\mathcal{H}}(e'_p)=u_i, t_{\mathcal{G}}(e_q)=v_j} x_{s_{\mathcal{H}}(e'_p) s_{\mathcal{G}}(e_q)}^{(k)} + \sum_{s_{\mathcal{H}}(e'_p)=u_i, s_{\mathcal{G}}(e_q)=v_j} x_{t_{\mathcal{H}}(e'_p) t_{\mathcal{G}}(e_q)}^{(k)}.$$

We now extend this mutually reinforcing relation with the notion of edge similarity. x_{ij} denotes again the node similarity score between vertex u_i from \mathcal{H} and vertex v_j from \mathcal{G} and y_{pq} denotes the edge similarity score between edge p from \mathcal{H} and edge q in \mathcal{G} , the update equations for edge and node similarity scores take now the following form:

$$y_{pq}^{(k+1)} = x_{s_{\mathcal{H}}(e'_p) s_{\mathcal{G}}(e_q)}^{(k)} + x_{t_{\mathcal{H}}(e'_p) t_{\mathcal{G}}(e_q)}^{(k)} \quad (2.11)$$

$$x_{ij}^{(k+1)} = \sum_{t_{\mathcal{H}}(e'_r)=u_i, t_{\mathcal{G}}(e_w)=v_j} y_{rw}^{(k)} + \sum_{s_{\mathcal{H}}(e'_t)=u_i, s_{\mathcal{G}}(e_w)=v_j} y_{rw}^{(k)} \quad (2.12)$$

With the same reasoning as presented in the previous section, these scores can be assembled into matrices $Y^{(k)}$ and $X^{(k)}$ by using the source-edge matrices A_S and the terminus-edge matrices A_T . Let A be the adjacency matrix of \mathcal{G} and B be the adjacency matrix of \mathcal{H} , let $X^{(k)}$ be the $n_{\mathcal{H}} \times n_{\mathcal{G}}$ -matrix with entries x_{ij} , the node similarity scores at iteration step k and let $Y^{(k)}$ be the $m_{\mathcal{H}} \times m_{\mathcal{G}}$ -matrix with entries y_{pq} , the edge similarity scores at step k . The equations (2.11) and (2.12) can be rewritten as:

$$Y'^{(k+1)} = B_S^T X^{(k)} A_S + B_T^T X^{(k)} A_T \quad (2.13)$$

$$X'^{(k+1)} = B_S Y^{(k)} A_S^T + B_T Y^{(k)} A_T^T \quad (2.14)$$

for $k = 0, 1, \dots$

Of course we want to customize this equations in a way that we can apply Theorem 2.2.10 to prove convergence. This will be completely analogous to Theorem 2.2.15, but we can achieve a slightly better result: not only the even and odd iterates will converge, the iteration converges as a whole. Lastly, remember that one of the conditions of Theorem 2.2.10 is to normalize the results at each iteration step. Therefore, the following theorem comes as no surprise:

Theorem 2.3.6. *Let \mathcal{G} and \mathcal{H} be two graphs with adjacency matrices A and B , \mathcal{G} has $n_{\mathcal{G}}$ vertices and $m_{\mathcal{G}}$ edges and \mathcal{H} has $n_{\mathcal{H}}$ vertices and $m_{\mathcal{H}}$ edges, define:*

$$Y^{(k+1)} = \frac{B_S^T X^{(k)} A_S + B_T^T X^{(k)} A_T}{\|B_S^T X^{(k)} A_S + B_T^T X^{(k)} A_T\|_F} \quad (2.15)$$

$$X^{(k+1)} = \frac{B_S Y^{(k)} A_S^T + B_T Y^{(k)} A_T^T}{\|B_S Y^{(k)} A_S^T + B_T Y^{(k)} A_T^T\|_F} \quad (2.16)$$

for $k = 0, 1, \dots$

Then the matrix subsequences $X^{(2k)}, Y^{(2k)}$ and $X^{(k+1)}, Y^{(k+1)}$ converge to $X_{\text{even}}, Y_{\text{even}}$ and $X_{\text{odd}}, Y_{\text{odd}}$. If we take⁸:

$$\begin{aligned} X^{(0)} &= J \in \mathbb{R}^{n_{\mathcal{H}} \times n_{\mathcal{G}}} \\ Y^{(0)} &= J \in \mathbb{R}^{m_{\mathcal{H}} \times m_{\mathcal{G}}} \end{aligned}$$

as initial matrices, then $X_{\text{even}}(\mathbf{1}) = X_{\text{odd}}(\mathbf{1})$, $Y_{\text{even}}(\mathbf{1}) = Y_{\text{odd}}(\mathbf{1})$ are the unique matrices of largest 1-norm among all possible limits with positive initial matrices and the matrix sequence $X^{(k)}, Y^{(k)}$ converges has a whole.

Proof. By Theorem 2.2.14 we can rewrite (2.13) as follows:

$$\begin{aligned} Y'^{(k+1)} &= B_S^T X'^{(k)} A_S + B_T^T X'^{(k)} A_T \\ \Leftrightarrow \text{vec}(Y'^{(k+1)}) &= \text{vec}(B_S^T X'^{(k)} A_S + B_T^T X'^{(k)} A_T) \\ \Leftrightarrow \text{vec}(Y'^{(k+1)}) &= \text{vec}(B_S^T X'^{(k)} A_S) + \text{vec}(B_T^T X'^{(k)} A_T) \\ \Leftrightarrow \text{vec}(Y'^{(k+1)}) &= (A_S^T \otimes B_S^T) \text{vec}(X'^{(k)}) + (A_T^T \otimes B_T^T) \text{vec}(X'^{(k)}) \\ \Leftrightarrow \text{vec}(Y'^{(k+1)}) &= (A_S^T \otimes B_S^T + A_T^T \otimes B_T^T) \text{vec}(X'^{(k)}) \end{aligned}$$

Completely analogous we can also rewrite (2.14):

$$\text{vec}(X'^{(k+1)}) = (A_S \otimes B_S + A_T \otimes B_T) \text{vec}(Y^k),$$

define $\mathbf{y}^{(k)} = \text{vec}(Y'^{(k+1)})$ and $\mathbf{x}^{(k)} = \text{vec}(X'^{(k+1)})$, we get:

$$\begin{aligned} \mathbf{y}^{(k+1)} &= (A_S^T \otimes B_S^T + A_T^T \otimes B_T^T) \mathbf{x}^{(k)} \\ \mathbf{x}^{(k+1)} &= (A_S \otimes B_S + A_T \otimes B_T) \mathbf{y}^{(k)} \end{aligned}$$

If we define $G = A_S^T \otimes B_S^T + A_T^T \otimes B_T^T$, then with Lemma 2.2.13 and the well known properties of transpose matrices:

$$\begin{aligned} G^T &= (A_S^T \otimes B_S^T + A_T^T \otimes B_T^T)^T \\ &= ((A_S \otimes B_S)^T + (A_T \otimes B_T)^T)^T \\ &= ((A_S \otimes B_S)^T)^T + ((A_T \otimes B_T)^T)^T \\ &= A_S \otimes B_S + A_T \otimes B_T \end{aligned}$$

So we get:

$$\mathbf{y}^{(k+1)} = G \mathbf{x}^{(k)} \quad (2.17)$$

$$\mathbf{x}^{(k+1)} = G^T \mathbf{y}^{(k)}, \quad (2.18)$$

⁸J is a matrix of all ones

G is a $m_{\mathcal{G}}m_{\mathcal{H}} \times n_{\mathcal{G}}n_{\mathcal{H}}$ -matrix, the previous expressions can be concatenated to a single matrix update equation (we define matrix M and $\mathbf{z}^{(k+1)}$):

$$\mathbf{z}^{(k+1)} = \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^{(k+1)} = \begin{pmatrix} \mathbf{0}_{m_{\mathcal{G}}m_{\mathcal{H}}} & G^T \\ G & \mathbf{0}_{n_{\mathcal{G}}n_{\mathcal{H}}} \end{pmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^{(k)} = M\mathbf{z}^{(k)},$$

M is clearly nonnegative because G and G^T consists of sums of Kronecker products of A_S, B_S, A_T and/or B_T , all matrices with entries equal to zero or one, M is as a $(n_{\mathcal{G}}n_{\mathcal{H}} + m_{\mathcal{G}}m_{\mathcal{H}}) \times (n_{\mathcal{G}}n_{\mathcal{H}} + m_{\mathcal{G}}m_{\mathcal{H}})$ -matrix clearly symmetric, so the result follows immediately from Theorem 2.2.10. The appearance of the Perron norm can be explained in the same way as in Theorem 2.2.15, note that we write $Y^{(k)}$ and $X^{(k)}$ for the normalized results at iteration step k . We still have to prove that odd and even iterates are the same and that M has only positive eigenvalues, meaning that the sequence converges to $\frac{\Pi\mathbf{z}^{(0)}}{\|\Pi\mathbf{z}^{(0)}\|_2}$, this can be done easily by expanding the matrix equation:

$$\mathbf{x}^{(k)} = \begin{cases} (G^T G)^{\frac{k}{2}} \mathbf{x}^{(0)} & k \text{ even} \\ (G^T G)^{\frac{k-1}{2}} G^T \mathbf{y}^{(0)} & k \text{ odd} \end{cases} \quad \text{and} \quad \mathbf{y}^{(k)} = \begin{cases} (GG^T)^{\frac{k}{2}} \mathbf{y}^{(0)} & k \text{ even} \\ (GG^T)^{\frac{k-1}{2}} G \mathbf{x}^{(0)} & k \text{ odd} \end{cases}$$

The matrix G is the sum of two matrices $(A_S^T \otimes B_S^T)$ and $(A_T^T \otimes B_T^T)$. Now, A_S^T is a $m_{\mathcal{G}} \times n_{\mathcal{G}}$ -matrix and has in each row a single ‘1’-entry, simply because an edge has at most one source node. The same holds for B_S^T . Therefore, taking the Kronecker product of those two matrices results in the matrix $A_S^T \otimes B_S^T$ which also has just a single ‘1’ entry in each row. With the same reasoning, we conclude that also $A_T^T \otimes B_T^T$ has also just a single ‘1’-entry in each row. Taking the sum of $(A_S^T \otimes B_S^T)$ and $(A_T^T \otimes B_T^T)$ results thus in the matrix G with exactly two 1 entries in each row. If we know choose the initial conditions as $\mathbf{x}^{(0)} = \mathbf{1} \in \mathbb{R}^{n_{\mathcal{H}}n_{\mathcal{G}}}$ and $\mathbf{y}^{(0)} = \mathbf{1} \in \mathbb{R}^{m_{\mathcal{H}}m_{\mathcal{G}}}$. Then we conclude:

$$G\mathbf{x}^{(0)} = 2\mathbf{y}^{(0)},$$

we get:

$$\begin{aligned} \mathbf{x}^{(k)} &= \begin{cases} (G^T G)^{\frac{k-2}{2}} G^T G \mathbf{x}^{(0)} = \frac{1}{2} (G^T G)^{\frac{k-2}{2}} G^T \mathbf{y}^{(0)} & k \text{ even} \\ (G^T G)^{\frac{k-1}{2}} G^T \mathbf{y}^{(0)} & k \text{ odd} \end{cases} \\ \mathbf{y}^{(k)} &= \begin{cases} (GG^T)^{\frac{k}{2}} \mathbf{y}^{(0)} & k \text{ even} \\ (GG^T)^{\frac{k-1}{2}} G \mathbf{x}^{(0)} = (GG^T)^{\frac{k-1}{2}} \frac{1}{2} \mathbf{y}^{(0)} & k \text{ odd} \end{cases} \end{aligned}$$

First, observe that the matrices GG^T and $G^T G$ are besides being symmetric (for example, $(GG^T)^T = GG^T$) and nonnegative, are also positive semi-definite and thus have only nonnegative eigenvalues. Note that the factor $\frac{1}{2}$ that appears in the odd iterates will be eliminated by the normalization in each step. So in the limit as $k \rightarrow \infty$, the even and odd iterates are the same. □

We define now $X_{\text{even}}(\mathbf{1})$ as the node similarity matrix and $Y_{\text{even}}(\mathbf{1})$ as the edge similarity matrix.

Data: A_S : the $n_{\mathcal{G}} \times m_{\mathcal{G}}$ source-edge matrix of a graph \mathcal{G} A_T : the $n_{\mathcal{G}} \times m_{\mathcal{G}}$ terminal-edge matrix of a graph \mathcal{G} B_S : the $n_{\mathcal{H}} \times m_{\mathcal{H}}$ source-edge matrix of a graph \mathcal{H} B_T : the $n_{\mathcal{H}} \times m_{\mathcal{H}}$ terminal-edge matrix of a graph \mathcal{H}

TOL: tolerance for the estimation error.

Result: X : the node similarity matrix between \mathcal{G} and \mathcal{H} Y : the edge similarity matrix between \mathcal{G} and \mathcal{H} **begin** node_edge_similarity_matrix(A_S, A_T, B_S, B_T, TOL) $k = 1$; $X^{(0)} = \mathbf{1}$ ($n_{\mathcal{H}} \times n_{\mathcal{G}}$ -matrix with all entries equal to 1); $Y^{(0)} = \mathbf{1}$ ($m_{\mathcal{H}} \times m_{\mathcal{G}}$ -matrix with all entries equal to 1); $\mu_X = n_{\mathcal{H}} \times n_{\mathcal{G}}$ -matrix with all entries equal to TOL; $\mu_Y = m_{\mathcal{H}} \times m_{\mathcal{G}}$ -matrix with all entries equal to TOL;**repeat**

$$Y^{(k)} = \frac{B_S^T X^{(k-1)} A_S + B_T^T X^{(k-1)} A_T}{\|B_S^T X^{(k-1)} A_S + B_T^T X^{(k-1)} A_T\|_F};$$

$$X^{(k)} = \frac{B_S Y^{(k)} A_S^T + B_T Y^{(k)} A_T^T}{\|B_S Y^{(k)} A_S^T + B_T Y^{(k)} A_T^T\|_F};$$

 $k = k + 1$;**until** $|X^{(k)} - X^{(k-1)}| < \mu_X$ and $|Y^{(k)} - Y^{(k-1)}| < \mu_Y$;**return** $X^{(k)}, Y^{(k)}$;**end**

Algorithm 6: Algorithm for calculating the node and edge similarity matrix X and Y between \mathcal{G} and \mathcal{H} .

2.3.2 The algorithm

The algorithm to calculate the node and edge similarity scores is presented in pseudo-code in Algorithm 6. Remember that the absolute value that is mentioned is the same as in Notation 1.1.8. Besides the different calculations, the main difference with the algorithm of the previous section (Algorithm 5) is that the whole sequence converges, not only the even (or odd) iterates, making this algorithm twice as fast. Also notice that we implement a *sequential* update: when $Y^{(k)}$ is calculated, the result is immediately used in $X^{(k)}$. This is not according to Theorem 2.3.6, which suggest *simultaneous* updating equations: in that case $X^{(k)}$ uses $Y^{(k-1)}$ in its calculations. It is not difficult to see, by an analogous argument of Theorem 2.3.6, that both approaches yield the same set of similarity scores. Numerical analysts, however, will always prefer the sequential update procedure because it performs slightly better (see section 3.2 in [ADHEMAR]).

A Matlab implementation can be found in Listing A.3 in Appendix A. Because giving source-edge matrices and terminal-edge matrices as input is quite unnatural, in Listing A.4 and Listing A.5 some Matlab code is also presented to transform an adjacency matrix into a source-edge matrix and a terminal-edge matrix. The resulting matrices represent an edge numbering left-to-right, based on the entries of the adjacency matrix. The algorithm to

calculate the source-edge matrix based on the adjacency matrix is also written in pseudo-code in Algorithm 7, the calculation of the terminal-edge matrix is completely analogous. A Matlab implementation of Algorithm 6 that takes two adjacency matrices as input can be found in Listing A.6.

Data:

A : the $n \times n$ adjacency matrix of a graph \mathcal{G}

Result:

A_S : the source-edge matrix of graph \mathcal{G}

begin source_edge_matrix(A)

$m = \text{sum of all entries of } A$;

$A_S = \text{initialize a } n \times m\text{-matrix with all entries equal to } 0$;

 current_edge = 1;

for $i : 1 \text{ to } n$ **do**

for $j : 1 \text{ to } n$ **do**

if $(A)_{ij} > 0$ **then**

for $e : 1 \text{ to } (A)_{ij}$ **do**

$(A_S)_{i, \text{current_edge}} = 1$;

 current_edge = current_edge + 1 ;

end

end

end

end

end

return A_S ;

Algorithm 7: Algorithm for calculating the source-edge matrix A_S based on the adjacency matrix A of a graph \mathcal{G} .

2.3.3 Difference with node similarity

It is clear that the node-edge similarity algorithm is different from Algorithm 5 from the previous section. We will make this a little more explicit and show how different the resulting node similarity matrix is exactly. We first need another property of the Kronecker property.

Property 2.3.7. (mixed-product proeperty of Kronecker products) Let $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{r \times s}$, $C \in \mathbb{R}^{n \times p}$ and $D \in \mathbb{R}^{s \times t}$ then:

$$(A \otimes B)(C \otimes D) = AC \otimes BD \quad (\in \mathbb{R}^{mr \times pt})$$

Proof.

$$\begin{aligned} (A \otimes B)(C \otimes D) &= \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix} \begin{pmatrix} c_{11}D & \dots & c_{1p}D \\ \vdots & \ddots & \vdots \\ a_{n1}D & \dots & a_{np}D \end{pmatrix} \\ &= \begin{pmatrix} \sum_{k=1}^n a_{1k}c_{k1}BD & \dots & \sum_{k=1}^n a_{1k}c_{kp}BD \\ \vdots & \ddots & \vdots \\ \sum_{k=1}^n a_{mk}c_{k1}BD & \dots & \sum_{k=1}^n a_{mk}c_{kp}BD \end{pmatrix} \\ &= AC \otimes BD. \end{aligned}$$

□

Now take equations (2.17) and (2.18) and consider only the even iterates. We consider only the even iterates because Algorithm 5 does, remember that in Algorithm 6 the even and odd iterates yield the same set of similarity scores, we get:

$$\begin{aligned}
\mathbf{x}^{(k)} &= (G^T G) \mathbf{x}^{(k-2)} \\
&= ((A_S \otimes B_S + A_T \otimes B_T)(A_S^T \otimes B_S^T + A_T^T \otimes B_T^T)) \mathbf{x}^{(k-2)} \\
&= ((A_S \otimes B_S)(A_S^T \otimes B_S^T) + (A_S \otimes B_S)(A_T^T \otimes B_T^T) \\
&\quad + (A_T \otimes B_T)(A_S^T \otimes B_S^T) + (A_T \otimes B_T)(A_T^T \otimes B_T^T)) \mathbf{x}^{(k-2)} \\
&= (A_S A_S^T \otimes B_S B_S^T + A_S A_T^T \otimes B_S B_T^T \\
&\quad + A_T A_S^T \otimes B_T B_S^T + A_T A_T^T \otimes B_T B_T^T) \mathbf{x}^{(k-2)} \\
&= (A_S A_S^T \otimes B_S B_S^T + A \otimes B + A^T \otimes B^T + A_T A_T^T \otimes B_T B_T^T) \mathbf{x}^{(k-2)} \\
&= (A \otimes B + A^T \otimes B^T + A_S A_S^T \otimes B_S B_S^T + A_T A_T^T \otimes B_T B_T^T) \mathbf{x}^{(k-2)}
\end{aligned}$$

Where A, B are the adjacency matrices of \mathcal{G}, \mathcal{H} (Property 2.3.5), $A_S A_S^T, B_S B_S^T$ are the diagonal matrices with the outdegrees of the vertices on the diagonal (Property 2.3.3) and $A_T A_T^T, B_T B_T^T$ are the diagonal matrices with the indegree of the vertices on the diagonal (Property 2.3.4). The iteration suggested in Theorem 2.2.15 in the previous section has the following form (see equation (2.10)):

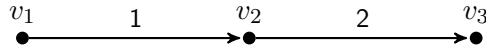
$$\mathbf{x}^{(k)} = A \otimes B + A^T \otimes B^T \mathbf{x}^{(k-2)},$$

thus Algorithm 6 differs from Algorithm 5 in three important ways:

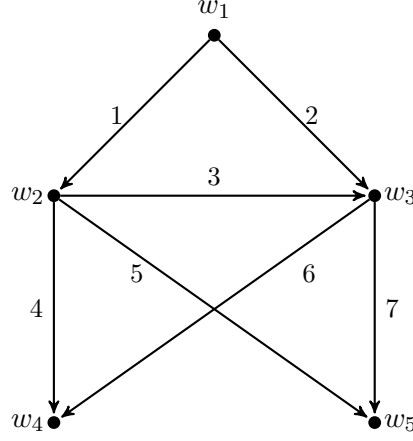
- In Algorithm 6 the inclusion of additional diagonal terms serve to amplify the scores of nodes that are highly connected in the node similarity matrix,
- Algorithm 6 returns a node similarity matrix and an edge similarity matrix, Algorithm 5 returns only a node similarity matrix,
- The whole sequence in Algorithm 6 converges, not only the even and odd iterates.

2.3.4 Example

Example 2.3.8. We retake Example 2.2.2 and number the edges as follows, let $\mathcal{G} = (V, \rightarrow)$ be :



Let $\mathcal{H} = (W, \rightarrow)$ be the following graph:



Then the node similarity matrix is:

$$X = \begin{pmatrix} 0.2338 & 0.0718 & 0 \\ 0.2472 & 0.3230 & 0.0128 \\ 0.1841 & 0.7553 & 0.3185 \\ 0 & 0.0935 & 0.2338 \\ 0 & 0.0441 & 0.0576 \end{pmatrix},$$

and the edge similarity matrix equals:

$$Y = \begin{pmatrix} 0.2166 & 0.0329 \\ 0.3847 & 0.1518 \\ 0.3899 & 0.2495 \\ 0.1325 & 0.2166 \\ 0.1133 & 0.1480 \\ 0.3653 & 0.4176 \\ 0.1080 & 0.3847 \end{pmatrix}$$

If you look at the structure of \mathcal{H} and compare it with the structure of \mathcal{G} , then intuitively it is not surprising that edge 3 of \mathcal{H} is most similar to edge 1 of \mathcal{G} and edge 6 of \mathcal{H} is most similar to edge 2 of \mathcal{G} because they are both very central edges with source nodes and terminal nodes that are very similar.

2.4 Colored graphs

In this last section, we extend the notion of similarity to colored graphs. The paper [VANDOREN] is written by two Belgian professors Paul Van Dooren and Catherine Fraikin from the Catholic University of Louvain in 2009.

Graph coloring is already introduced in paragraph 1.5.1 and we will construct a method that returns similarity matrices for two graphs where the coloring is on the nodes or on the edges of both graphs.

2.4.1 Colored nodes

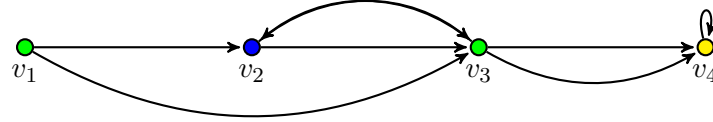
We first extend the node similarity introduced in section 2.2 to node colored graphs. Take two node colored graphs $\mathcal{G} = (V, \rightarrow, C, a)$ and $\mathcal{H} = (U, \rightarrow', C, a')$ with $|C|$ (remember that a ,

a' are surjective) different colors and assume that the nodes in both graphs are renumbered such that those of color 1 come first, then those of color 2,... The adjacency matrices A (of graph \mathcal{G}) and B (of graph \mathcal{H}) can then be partitioned as follows:

$$A = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1|C|} \\ A_{21} & A_{22} & \dots & A_{2|C|} \\ \vdots & \vdots & \ddots & \vdots \\ A_{|C|1} & A_{|C|2} & \dots & A_{|C||C|} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1|C|} \\ B_{21} & B_{22} & \dots & B_{2|C|} \\ \vdots & \vdots & \ddots & \vdots \\ B_{|C|1} & B_{|C|2} & \dots & B_{|C||C|} \end{pmatrix}$$

Remember that $c_{\mathcal{G}}(i)$ denotes the number of vertices of color i in graph \mathcal{G} , then each block $A_{ij} \in \mathbb{R}^{c_{\mathcal{G}}(i) \times c_{\mathcal{G}}(j)}$ and $B_{ij} \in \mathbb{R}^{c_{\mathcal{H}}(i) \times c_{\mathcal{H}}(j)}$ describes the adjacency relations between the nodes of color i to the vertices of color j in both A and B . In fact, by just renumbering the vertices such that the nodes with the same color succeed each other, you immediately get such partitioning. If you see this renumbering as a permutation on the nodes, then performing on the original adjacency matrix a left and right multiplication with the corresponding permutation matrix (see Definition 1.1.1) leads to this adjusted adjacency matrix. To make the idea more comprehensible, we give an example.

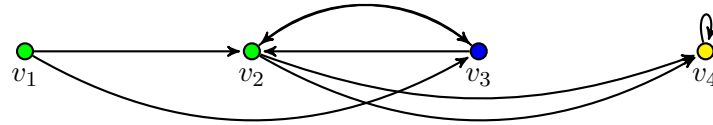
Example 2.4.1. Let \mathcal{G} be following graph:



The adjacency matrix equals:

$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

If we order the colors as: {green, blue, yellow} (so color 1 = green, color 2 = blue, color 3 = yellow), we can renumber the vertices and get the following graph:



The adjacency matrix equals:

$$A' = PAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 2 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

which can be partitioned in blocks as follows (we have 3 colors: 1 = green, 2 = blue, 3 = yellow):

$$A' = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 1 \\ 1 \end{pmatrix} & \begin{pmatrix} 0 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{pmatrix}.$$

Now, we will only compare the nodes of the same color in both graphs, so that we define similarity matrices $S_{ii} \in \mathbb{R}^{c_{\mathcal{G}}(i) \times c_{\mathcal{H}}(i)}$, with $i = 1, \dots, |C|$, which we can put in a block-diagonal similarity matrix:

$$S = \begin{pmatrix} S_{11} & 0 & \dots & 0 \\ 0 & S_{12} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & S_{|C||C|} \end{pmatrix}$$

Theorem 2.4.2. *Let $\mathcal{G} = (V, \rightarrow, C, a)$ and $\mathcal{H} = (V, \rightarrow, C, a')$ be two node colored graphs and define:*

$$\begin{aligned} Z_1^{(k+1)} &= \sum_{i \in \{1, \dots, |C|\}} B_{1i} S_{ii}^{(k)} A_{1i}^T + B_{i1}^T S_{ii}^{(k)} A_{i1} \\ Z_2^{(k+1)} &= \sum_{i \in \{1, \dots, |C|\}} B_{2i} S_{ii}^{(k)} A_{2i}^T + B_{i2}^T S_{ii}^{(k)} A_{i2} \\ &\vdots \\ Z_{|C|}^{(k+1)} &= \sum_{i \in \{1, \dots, |C|\}} B_{|C|i} S_{ii}^{(k)} A_{|C|i}^T + B_{i|C|}^T S_{ii}^{(k)} A_{i|C|} \\ (S_{11}, S_{22}, \dots, S_{|C||C|})^{(k+1)} &= \frac{(Z_1^{(k+1)}, Z_2^{(k+1)}, \dots, Z_{|C|}^{(k+1)})}{\|(Z_1^{(k+1)}, Z_2^{(k+1)}, \dots, Z_{|C|}^{(k+1)})\|_F} \end{aligned}$$

for $k = 0, 1, \dots$

Then the the matrix subsequences $Z_j^{(2k)}$ for every $j \in \{1, \dots, |C|\}$ and $(S_{11}, S_{22}, \dots, S_{|C||C|})^{(2k)}$ converge to Z_j^{even} and $(S_{11}, S_{22}, \dots, S_{|C||C|})^{even}$. Also the odd subsequences converge. If we take:

$$S_{jj}^{(0)} = \mathbf{1} \in \mathbb{R}^{c_{\mathcal{H}}(j) \times c_{\mathcal{G}}(j)}$$

as initial matrices, then the resulting $S_{jj}^{even}(\mathbf{1})$ are the unique matrices of largest 1-norm among all possible limits with positive start vector.

Proof. By induction on $|C|$. Remember from Definition 1.5.16 that the function c is surjective, meaning that C only consists of colors that are actually used.

For $|C| = 1$, we have a graph with all vertices having the same color, which can be seen as an uncoloured graph. This just the normal case as proved in Theorem 2.2.15.

Although redundant, it is instructive to prove the case $|C| = 2$ separately, because the generalization in the induction step is then immediately clear, so consider the partitioned adjacency matrices:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

the equations of the theorem are in this case:

$$\begin{aligned} Z_1^{(k+1)} &= B_{11}S_{11}^{(k)}A_{11}^T + B_{11}^TS_{11}^{(k)}A_{11} + B_{12}S_{22}^{(k)}A_{12}^T + B_{21}^TS_{22}^{(k)}A_{21} \\ Z_2^{(k+1)} &= B_{21}S_{11}^{(k)}A_{21}^T + B_{12}^TS_{11}^{(k)}A_{12} + B_{22}S_{22}^{(k)}A_{22}^T + B_{22}^TS_{22}^{(k)}A_{22} \\ (S_{11}, S_{22})^{(k+1)} &= \frac{(Z_1^{(k+1)}, Z_2^{(k+1)})}{\|(Z_1^{(k+1)}, Z_2^{(k+1)})\|_F} \end{aligned}$$

Let $Z_1'^{(k+1)}$ be the not normalized version $Z^{(k+1)}$, then we can write (see Theorem 2.2.14):

$$\begin{aligned} Z_1'^{(k+1)} &= B_{11}Z_1'^{(k)}A_{11}^T + B_{11}^TZ_1'^{(k)}A_{11} + B_{12}Z_2'^{(k)}A_{12}^T + B_{21}^TZ_2'^{(k)}A_{21} \\ \Leftrightarrow \text{vec}(Z_1'^{(k+1)}) &= \text{vec}(B_{11}Z_1'^{(k)}A_{11}^T + B_{11}^TZ_1'^{(k)}A_{11} + B_{12}Z_2'^{(k)}A_{12}^T + B_{21}^TZ_2'^{(k)}A_{21}) \\ \Leftrightarrow \text{vec}(Z_1'^{(k+1)}) &= (A_{11} \otimes B_{11}) \text{vec } Z_1'^{(k)} + (A_{11}^T \otimes B_{11}^T) \text{vec}(Z_1'^{(k)}) \\ &\quad + (A_{12} \otimes B_{12}) \text{vec}(Z_2'^{(k)}) + (A_{21}^T \otimes B_{21}^T) \text{vec}(Z_2'^{(k)}) \\ \Leftrightarrow \text{vec}(Z_1'^{(k+1)}) &= (A_{11} \otimes B_{11} + A_{11}^T \otimes B_{11}^T) \text{vec}(Z_1'^{(k)}) \\ &\quad + (A_{12} \otimes B_{12} + A_{21}^T \otimes B_{21}^T) \text{vec}(Z_2'^{(k)}) \end{aligned}$$

In a similar way, we can write $Z_2'^{(k+1)}$, which is the not normalized version of $Z_2^{(k+1)}$, as:

$$\text{vec}(Z_2'^{(k+1)}) = (A_{21} \otimes B_{21} + A_{12}^T \otimes B_{12}^T) \text{vec } Z_1'^{(k)} + (A_{22} \otimes B_{22} + A_{22}^T \otimes B_{22}^T) \text{vec } Z_2'^{(k)}$$

If we define M, \mathbf{z}^{k+1} as follows, the previous expressions concatenate to a single matrix update equation:

$$\begin{aligned} \mathbf{z}^{k+1} &= \begin{pmatrix} \text{vec}(Z_1') \\ \text{vec}(Z_2') \end{pmatrix}^{(k+1)} \\ &= \begin{pmatrix} A_{11} \otimes B_{11} + A_{11}^T \otimes B_{11}^T & A_{12} \otimes B_{12} + A_{21}^T \otimes B_{21}^T \\ A_{21} \otimes B_{21} + A_{12}^T \otimes B_{12}^T & A_{22} \otimes B_{22} + A_{22}^T \otimes B_{22}^T \end{pmatrix} \begin{pmatrix} \text{vec}(Z_1') \\ \text{vec}(Z_2') \end{pmatrix}^{(k)} \\ &= M\mathbf{z}^{(k)} \end{aligned}$$

Notice that the diagonal blocks in M are related to links between the nodes with the same color, while the off diagonal blocks refer to links between nodes of another color. As always, we want to use Theorem 2.2.10 to get the result. M is clearly nonnegative, because every block A_{ij} and B_{ij} is nonnegative (it's derived from the nonnegative adjacency matrices A and B). Proving that M is symmetric a bit trickier, but notice that $A_{11} \otimes B_{11} + (A_{11} \otimes B_{11})^T$ is a symmetric $c_{\mathcal{G}}(1)c_{\mathcal{H}}(1) \times c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$ matrix (because it's the sum of a matrix with his transpose), and $A_{22} \otimes B_{22} + (A_{22} \otimes B_{22})^T$ is a symmetric $c_{\mathcal{G}}(2)c_{\mathcal{H}}(2) \times c_{\mathcal{G}}(2)c_{\mathcal{H}}(2)$. If we define $G = A_{21} \otimes B_{21} + A_{12}^T \otimes B_{12}^T$, G is a $c_{\mathcal{G}}(2)c_{\mathcal{H}}(2) \times c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$ -matrix. Now, notice the following relation between the off diagonal blocks:

$$\begin{aligned} G^T &= (A_{21} \otimes B_{21} + A_{12}^T \otimes B_{12}^T)^T \\ &= (A_{21} \otimes B_{21})^T + ((A_{12}^T \otimes B_{12}^T)^T)^T \\ &= A_{12} \otimes B_{12} + A_{21}^T \otimes B_{21}^T \end{aligned}$$

G^T is a $c_{\mathcal{G}}(1)c_{\mathcal{H}}(1) \times c_{\mathcal{G}}(2)c_{\mathcal{H}}(2)$ -matrix. So we can rewrite M as:

$$M = \begin{pmatrix} A_{11} \otimes B_{11} + A_{11}^T \otimes B_{11}^T & G^T \\ G & A_{22} \otimes B_{22} + A_{22}^T \otimes B_{22}^T \end{pmatrix}$$

M is a $(c_{\mathcal{G}}(1)c_{\mathcal{H}}(1) + c_{\mathcal{G}}(2)c_{\mathcal{H}}(2)) \times (c_{\mathcal{G}}(1)c_{\mathcal{H}}(1) + c_{\mathcal{G}}(2)c_{\mathcal{H}}(2))$ -matrix, we want to prove that $(M)_{ij} = (M)_{ji}$ and to do so we distinguish all possible cases:

- If $i \leq c_{\mathcal{G}}(1)c_{\mathcal{H}}(1), j \leq c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$, then $(M)_{ij}$ and $(M)_{ji}$ will both be entries of $A_{11} \otimes B_{11} + A_{11}^T \otimes B_{11}^T$ and this submatrix was symmetric.
- If $i \leq c_{\mathcal{G}}(1)c_{\mathcal{H}}(1), j > c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$, then $(M)_{ij}$ will be an entry of G^T and $(M)_{ji}$ will be an entry of G , so they are equal.
- If $i > c_{\mathcal{G}}(1)c_{\mathcal{H}}(1), j > c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$, then $(M)_{ij}$ and $(M)_{ji}$ will both be entries of $A_{22} \otimes B_{22} + A_{22}^T \otimes B_{22}^T$ and this submatrix was symmetric.
- If $i > c_{\mathcal{G}}(1)c_{\mathcal{H}}(1), j \leq c_{\mathcal{G}}(1)c_{\mathcal{H}}(1)$, then $(M)_{ij}$ will be an entry of G and $(M)_{ji}$ will be an entry of G^T , so they are equal.

The result immediately follows from Theorem 2.2.10. We motivated the usage of the Frobenius norm already in the proof of Theorem 2.2.15. Notice that the normalization after each iteration step happens ‘together’ by dividing by $\|(Z_1^{(k+1)}, Z_2^{(k+1)})\|_F$, because this is in accordance to the conditions of Theorem 2.2.10. Normalizing $Z_1^{(k+1)}, Z_2^{(k+1)}$ separately after the expressions is calculated, gives an iterative process that is different from the one described in Theorem 2.2.10.

We now prove the induction step $|C| = n - 1 \Rightarrow |C| = n$. The only crucial thing to prove is that M is again symmetric, the rest of the steps consist of an easy expansion of the case $|C| = 2$. M is in this case equal to:

$$M = \begin{pmatrix} A_{11} \otimes B_{11} & & A_{1(n-1)} \otimes B_{1(n-1)} & A_{1n} \otimes B_{1n} \\ +A_{11}^T \otimes B_{11}^T & \cdots & +A_{(n-1)1}^T \otimes B_{(n-1)1}^T & +A_{n1}^T \otimes B_{n1}^T \\ \vdots & \ddots & \vdots & \vdots \\ A_{(n-1)1} \otimes B_{(n-1)1} & \cdots & A_{(n-1)(n-1)} \otimes B_{(n-1)(n-1)} & A_{(n-1)n} \otimes B_{(n-1)n} \\ +A_{1(n-1)}^T \otimes B_{1(n-1)}^T & \cdots & +A_{(n-1)(n-1)}^T \otimes B_{(n-1)(n-1)}^T & +A_{n(n-1)}^T \otimes B_{n(n-1)}^T \\ A_{n1} \otimes B_{n1} & \cdots & A_{n(n-1)} \otimes B_{n(n-1)} & A_{nn} \otimes B_{nn} \\ +A_{1n}^T \otimes B_{1n}^T & \cdots & +A_{(n-1)n}^T \otimes B_{(n-1)n}^T & +A_{nn}^T \otimes B_{nn}^T \end{pmatrix}$$

which can be seen as:

$$M = \begin{pmatrix} & & A_{1n} \otimes B_{1n} \\ & & +A_{n1}^T \otimes B_{n1}^T \\ & & \vdots \\ & M' & A_{(n-1)n} \otimes B_{(n-1)n} \\ & & +A_{n(n-1)}^T \otimes B_{n(n-1)}^T \\ A_{n1} \otimes B_{n1} & \cdots & A_{n(n-1)} \otimes B_{n(n-1)} \\ +A_{1n}^T \otimes B_{1n}^T & \cdots & +A_{(n-1)n}^T \otimes B_{(n-1)n}^T & A_{nn} \otimes B_{nn} \\ & & & +A_{nn}^T \otimes B_{nn}^T \end{pmatrix}$$

From the induction hypothesis we now that M' is symmetric. It's clear that the entries in the last column of M are the transpose of the entries in the last row. It follows that M is again symmetric.

□

Chapter 3

Similarity on hypergraphs

3.1 Introduction

In this section, we explore similarity on hypergraphs: an undiscovered field as no papers can be found in journals about this subject. In this section, we try to formulate an answer to the question whether we can generalize the results of the previous section to the domain of hypergraphs.

One of the most obvious ways to apply the concept of similarity to hypergraphs is looking to the corresponding graph representations of a hypergraph and apply the algorithms of the previous section. This is explained in the first section of this chapter. Although it the most logic way to introduce similarity on hypergraphs, it's also the least significant solution because most graph representations throw away a lot of information that the structure of a hypergraph contains.

A slightly smarter, more meaningful way to introduce similarity on hypergraphs is to work with the hypergraph variant of an adjacency matrix. As with graphs, also hypergraphs can be represented by a kind of matrix representation. The only difference with graphs is that there is no consensus at all in the literature about which matrix representation is the standard for hypergraphs (see [BERGE]).

The most common representation is a (two-dimensional) normal matrix representation, where the rows represent the nodes and the columns the edges and the entries $(A)_{ij}$ are equal to 1 if vertex i is contained in edge j and 0 otherwise. Although it's an easy representation that is applicable to hypergraphs with edges containing different numbers of nodes, the biggest drawbacks are that all edges must be undirected (there is no way to express which is the start node, the second node,..., terminal node) and that this representation is completely different to the structure of an adjacency matrix we are so used with graphs. The main reason why it's so popular is probably that the hypergraph can be represented by just a normal matrix, no other datastructure must be studied.

Another way to represent a hypergraph is through a multi-dimensional adjacency matrix. Also referred to as an hypermatrix or an adjacency tensor. Take, for example, a 3-hypergraph (see Definition ??), then the adjacency tensor \mathcal{A} is $n \times n \times n$ -tensor, with n the number of vertices. The element $(\mathcal{A})_{ijk}$ is equal to the number of 3-edges between vertices v_i, v_j and v_k . Besides that it is the natural generalization of adjacency matrices we know from graphs, it's also a richer structure, this is explained in the final reflection in subsection 3.6.1.

For now, we consider only k -uniform hypergraphs with undirected edges. Meaning that

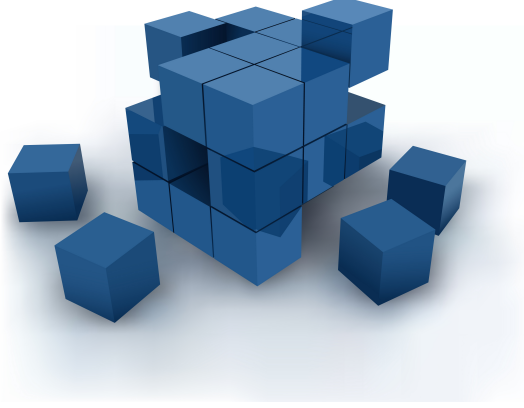


Figure 3.1.1: Just as a cube can be decomposed into a square and even to a straight line, a hypermatrix can be decomposed into a matrix and next into a vector. (Source: *istock-photo.com*)

symmetry elements given by permutations of the index set in the hypermatrix have the same value, so in our 3-uniform hypergraph this means that

$$(\mathcal{A})_{ijk} = (\mathcal{A})_{ikj} = (\mathcal{A})_{jik} = (\mathcal{A})_{jki} = (\mathcal{A})_{kij} = (\mathcal{A})_{kji}.$$

How do we generalize similarity by working with adjacency tensor representations of hypergraphs? Intuitively, it's not so hard to understand: all the algorithms described in section 2 consist of a matrix sequences of which the convergence is proved by Theorem 2.2.10. All these proofs have one thing in common: they use a vectorization of the matrix sequence, so the sequence can be rewritten in the form:

$$\mathbf{z}^{(k)} = M\mathbf{z}^{(k-1)}$$

when M meets certain conditions (being nonnegative and symmetric), our convergence theorem can be applied and we're done. Now, we can apply the same trick with hypermatrices, instead of a vectorization we can apply a *matricization* on an adjacency tensor turning the tensor into a 'normal', two-dimensional matrix. If this returns the matrix sequences of section 2, we know that the generalized methods will converge. A beautiful visualization of this idea can be found in Figure 3.1.1: think of a 3-uniform hypergraph with n nodes. The corresponding tensor will be of dimension $n \times n \times n$, which can be visually represented as a cube. Just as a cube can be decomposed into a square and next into a straight line, we can decompose the hypermatrix into a matrix and next into a vector.

There is only one difficult aspect when we bring similarity to hypergraphs and use their hypermatrix representation: the result will be a similarity hypermatrix. This means that by calculating the similarity hypergraph of two k -uniform hypergraphs, we don't get similarity scores to compare nodes (or edges) two-by-two but we get similarity scores to compare two groups of k nodes at the same time. We will propose some solutions to transform the resulting similarity hypermatrices in such way we can compare nodes two-by-two.

3.2 Similarity through corresponding graph representations

One way to look at similarity on hypergraphs is to represent a hypergraph as a graph and use the similarity algorithms from the previous section. Almost every generalization with hypergraphs starts by looking at corresponding graph representations ([BERGE]), and therefore it's interesting to do this for the notion of similarity too. We describe three representations of hypergraphs as a graph: the line-graphs, the 2-section graphs and the incidence graphs. For each representation we use the same examples to see the differences between the graph representations.

3.2.1 Line-graphs

In this subsection, we describe the representation of a hypergraph as a line-graph. We then show some relevant properties and examples and we conclude by looking at similarity between hypergraphs through this representation.

Definition 3.2.1. Let $\mathcal{H} = (V, E)$ be a hypergraph with $E \neq \emptyset$ and $E = \{e_1, \dots, e_m\}$. The **line-graph** of \mathcal{H} is the graph denoted by $\mathcal{G}_1 = (V', \rightarrow)$ with:

1. $V' = E$,
2. $e_i \rightarrow e_j$ if and only if $e_i \cap e_j \neq \emptyset$

It's immediately clear that line-graphs are simple graphs (see Definition 1.5.14). We will now prove that every simple, undirected graph is the line-graph of an hypergraph. More specifically, we will show that any connected graph is the line-graph of a linear hypergraph.

Definition 3.2.2. A **linear hypergraph** is a hypergraph where each pair of edges intersects in at most one vertex.

Theorem 3.2.3. Every connected, simple graph $\mathcal{G} = (V, \rightarrow)$ with vertices $v_1, \dots, v_n \in V$ and edges $e_1, \dots, e_m \in E$ is the line-graph of a linear hypergraph \mathcal{H} .

Proof. Construct the hypergraph $\mathcal{H} = (V', E')$ in the following way:

- Let $V' = \rightarrow$, this is possible since \mathcal{G} is simple so there is at most one edge that connects two vertices.
- The collection of edges E' is the family e'_i where e'_i is the set of all edges of \mathcal{G} that connect vertex v_i so:

$$\mathcal{H} = (V', E') = (\rightarrow, \{e'_1, \dots, e'_n\}),$$

with:

$$e'_i = \{e \in \rightarrow \mid v_i \text{ is a node connected by } e\}$$

If \mathcal{G} has only one edge ($m = 1$) e_1 then

$$V = v_1, v_2 \quad \text{and} \quad e'_1 = e'_2,$$

so $\mathcal{H} = (\{e_1\}, \{e'_1, e'_2\})$, this is the only case where \mathcal{H} will have a repeated edge. Notice that $\mathcal{H} = (\{e_1\}, \{e'_1, e'_2\})$ is a linear hypergraph as $e'_1 \cap e'_2 = \{e_1\}$. If $m > 1$, $i \neq j$ and $e'_i \cap e'_j \neq \emptyset$, then there is exactly one $e \in \rightarrow$ such that $e \in (e'_i \cap e'_j)$ with $e = \{v_i, v_j\}$ because \mathcal{G} is a simple graph. Notice that \mathcal{G} must be connected, otherwise \mathcal{G} could have isolated vertices which would never appear in the line-graph representation

□

3.3 Node similarity

3.4 Node-edge similarity

3.5 Similarity on colored hypergraphs

hypergraph.tex

3.6 Final reflection

3.6.1 Why hypermatrices are the best representation of a hypergraph

3.6.2 The curse of dimensionality

3.7 Applications

Appendix A

Listings

Listing A.1: The MatLab code for the Power Method described in algorithm 1

```
function [ y, lambda, it_num ] = power_method ( n, a, y, it_max, tol )

% Force Y to be a column vector.
y = y ( : );
lambda = 0;

% Force Y to be a vector of unit norm.

y = y / norm ( y );

it_num = 0;

y_old = y;

ay = a * y;
lambda = y' * ay;
y = ay / norm ( ay );
if ( lambda < 0.0 )
    y = - y;
end

val_dif = 0.0;

cos_yly2 = y' * y_old;
sin_yly2 = sqrt ( ( 1.0 - cos_yly2 ) * ( 1.0 + cos_yly2 ) );

for it_num = 1 : it_max

    lambda_old = lambda;
    y_old = y;

    ay = a * y;
    lambda = y' * ay;
    y = ay / norm ( ay );
    if ( lambda < 0.0 )
        y = - y;
    end
```

```

    val_dif = abs ( lambda - lambda_old );

    sin_yly2 = 0;
    cos_yly2 = y' * y_old;
    sin_yly2 = sqrt ( ( 1.0 - cos_yly2 ) * ( 1.0 + cos_yly2 ) );

    if ( val_dif <= tol )
        break
    end

end

y = ay / lambda;

return
end

```

Listing A.2: The MatLab code for algorithm 5.

```

function [Z] = similarity_matrix(A,B, TOL)
    Z_0 = ones(size(B,1),size(A,1));
    mu(1:size(B,1),1:size(A,1)) = TOL;
    Z = Z_0;
    Z_previouslyeven = Z_0;
    k=1;
    while true;
        Y = norm((B*Z*transpose(A)+transpose(B)*Z*A), 'fro');
        X = B*Z*transpose(A)+transpose(B)*Z*A;
        Z = X/Y;
        if mod(k,2) == 0
            difference = abs(Z-Z_previouslyeven);
            disp(difference);
            Z_previouslyeven = Z;
            if (difference < mu)
                break;
            end
        end
        k = k + 1;
    end
    return;
end

```

Listing A.3: The MatLab code for algorithm 6.

```

function [X, Y] = node_edge_similarity_matrices(AS, AT, BS, BT, TOL)
    X = ones(size(BS,1),size(AS,1));
    Y = ones(size(BS,2),size(AS,2));
    mu_X(1:size(BS,1),1:size(AS,1)) = TOL;
    mu_Y(1:size(BS,2),1:size(AS,2)) = TOL;
    X_previouslyeven = X;
    Y_previouslyeven = Y;
    k=1;
    while true;
        Y = (transpose(BS)*X*AS+transpose(BT)*X*AT)
            /norm(transpose(BS)*X*AS+transpose(BT)*X*AT, 'fro');
    end

```



```

X = (BS*Y*transpose(AS)+BT*Y*transpose(AT))
    /norm(BS*Y*transpose(AS)+BT*Y*transpose(AT), 'fro');

difference_X = abs(X-X_previous);
difference_Y = abs(Y-Y_previous);
X_previous = X;
Y_previous = Y;
    if difference_X < mu_X
        if difference_Y < mu_Y
            break;
        end
    end
end
return;
end

```

Listing A.4: The MatLab code to converse an adjacency matrix to a source-edge matrix (edges are numbered left-to-right based on the adjacency matrix).

```

function [AS] = source_edge_matrix(A)
    number_of_edges = sum(A(:));
    AS = zeros(size(A,1), number_of_edges); %initialize the souce-edge matrix A_S
    current_edge = 1;
    for i=1:size(A,1)
        for j=1:size(A,2)
            if A(i,j) > 0
                for e=1:A(i,j)
                    AS(i,current_edge) = 1;
                    current_edge = current_edge + 1;
                end
            end
        end
    end
end
end

```

Listing A.5: The MatLab code to converse an adjacency matrix to a terminal-edge matrix (edges are numbered left-to-right based on the adjacency matrix).

```

function [AS] = terminal_edge_matrix(A)
    number_of_edges = sum(A(:));
    AS = zeros(size(A,1), number_of_edges); %initialize the terminal-edge matrix A_T
    current_edge = 1;
    for i=1:size(A,1)
        for j=1:size(A,2)
            if A(i,j) > 0
                for e=1:A(i,j)
                    AS(j,current_edge) = 1;
                    current_edge = current_edge + 1;
                end
            end
        end
    end
end
end

```

Listing A.6: The MatLab code for algorithm 6 but with adjacency matrices as input (edges are numbered left-to-right based on the adjacency matrices).

```
function [X,Y] = node_edge_similarity_matrices_with_adjacency_matrix(A, B, TOL)
    AS = source_edge_matrix(A);
    AT = terminal_edge_matrix(A);
    BS = source_edge_matrix(B);
    BT = terminal_edge_matrix(B);
    [X,Y] = node_edge_similarity_matrix(AS, AT, BS, BT, TOL);
end
```

Appendix B

Results of the Eurovision Song Contest 2009-2014

Table B.1: Eurovision Song Contest 2009

	Albania	Armenia	Azerbaijan	Belarus	Belgium	Bosnia & Herzegovina	Bulgaria	Croatia	Cyprus	Czech Republic	Denmark	Estonia	F.Y.R. Macedonia	Finland	France	Germany	Greece	Hungary	Iceland	Ireland	Israel	Latvia	Lithuania	Malta	Moldova	Montenegro	Norway	Poland	Portugal	Romania	Russia	Serbia	Slovakia	Slovenia	Spain	Sweden	Switzerland	The Netherlands	Turkey	Ukraine	United Kingdom	Points	Place	Authority Score	Hub Score	
Norway	7	10	8	8	12	10	2	8	10	3	12	12	8	8	8	12	10	12	12	8	12	12	12	8	8	10	12	5	12	10	10	10	10	10	12	12	12	8	12	3	12	10	387	10	311382108	0.107545693
Iceland	6	8	5	2			5	2	5	2	10	8	2	10		7	4	7	12	10	12	10	8	8	12	3	5	12	1	8	10	3	6	5	10	5	7	2	8	218	20	175683413	0.113493313			
Azerbaijan	4	1	10	3	3	8	10	8	10	8	7	3	2	1			8	10				6	4	5	1	10	6	10	6	4	7	4	1	8	10	12	10	3	207	30	165946697	0.109357170				
Turkey	10	4	12	12	7	10	1	1	6	1	6	12	5	12	10	3	5	3	5			3		5	3	7	3	7	3	6				2	6	12	8	10	12	10	3	207	30	165946697	0.109357170	
United Kingdom	8	4	7	3	4	7	4	7	6	3			6		4	8	12	1	6	10	4	2	3	10	1	2	4	10	6	8	7	3	10			3	6	173	50	137107599	0.133630498					
Estonia			4	4				6	3	5		12		12	1	5	6	10	6	10	10	10	7		7		8		8	1	8	12			7		4	129	60	106793281	0.131401482					
Greece	12	10	5	5	5	12	7	12							6		4						7		2				8	4	6	4	1	2	2	1	5	120	70	096460793	0.148053884					
France	2	3	6	7	1	6					2		4	4	3	6		6	3	5	5	6		1	1					10	3	7	3	7	6	3	1	107	80	087462271	0.109033937					

Table B.4: Eurovision Song Contest 2012

[illegible]

Table B.6: Eurovision Song Contest 2014 (continued)

Portugal	Albania	
	Armenia	
	Austria	
	Azerbaijan	
	Belarus	
	Belgium	
	Denmark	
	Estonia	
	F.Y.R. Macedonia	
	Finland	
	France	
	Georgia	
	Germany	
	Greece	
	Hungary	
	Iceland	
	Ireland	
	Israel	
	Italy	
	Latvia	
	Lithuania	
	Malta	
	Moldova	
	Montenegro	
	Norway	
	Poland	
	Portugal	
	Romania	
	Russia	
	San Marino	
	Slovenia	
	Spain	
	Sweden	
	Switzerland	
	The Netherlands	
	Ukraine	
	United Kingdom	
	Points	
	Place	
	Authority Score	
	Hub Score	00.173610946

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