國 立 交 通 大 學

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碩 士 論 文

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A simple method on estimating spectral radius for some directed graphs

研究生　：陳科翰

指導教授　：翁志文 教授

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摘　要

　　矩陣的譜半徑為其特徵值絕對值的最大值，而一有向圖的譜半徑則定義為其鄰接矩陣之譜半徑。本論文給出一個尋找方陣譜半徑上界的方法，將此方法應用於有向圖的鄰接矩陣，我們可以簡易估算出此圖的譜半徑。

關鍵詞：譜半徑、鄰接矩陣

A simple method on estimating spectral radius for some directed graphs

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Department of Applied Mathematics

National Chiao Tung University

Abstract

The spectral radius of a square matrix is the largest magnitude of its eigenvalues. And the spectral radius of a directed graph is defined as the spectral radius of the corresponding adjacency matrix. In this paper, we give an approach to obtain an upper bound for the spectral radius of a square matrix. By applying this method on the adjacency matrix of a directed graph, we can estimate the spectral radius of this directed graph simply.

Keywords: spectral radius, adjacency matrix

Contents

1 Introduction

Let $\mathbb{R}$ and $\mathbb{C}$ denote the field of real numbers and complex numbers, respectively. Let C be an $n \times n$ real square matrix. If there is a nonzero column vector $u \in \mathbb{R}^n$ such that $Cu = \lambda u$ for some scalar $\lambda \in \mathbb{C}$, then the scalar λ is called the eigenvalue of C with corresponding eigenvector u. And the spectral radius of a matrix C is the largest magnitude (or complex modulus) of its eigenvalues, denoted by $\rho(C)$. We are interested in the spectral radius of the following matrix associated with a simple directed graph.

Definition 1.1. Given an directed graph G, the *adjacency matrix* of G is the square matrix $A = (a_{ij})$ indexed by vertices of G, and

$$a_{ij} = \begin{cases} 1, \text{if } i \text{ is adjacent to } j, \\ 0, \text{otherwise.} \end{cases}$$

Given a directed graph G, the spectral radius of G is the spectral radius of the adjacency matrix of G, denoted by $\rho(G)$. Note that the spectral radius $\rho(G)$ is independent of the ordering of the vertex set of G.

The spectral radius is an important indicator to specify the relation of connected vertices in a graph, so it is meaningful to find a simple method to estimate the spectral radius. A simple and excellent executable method to estimate the spectral radius has some features, first, the bios is minimized, and second, there must be a way to prove it sensible. Enumerate these factors and prove it correctly would make this method reliable.

In [1], Cheng and Weng give many bounds of the spectral radius of a nonnegative square matrix. And based on their theory and Perron-Frobenius theorem, we give another approach to obtain an upper bound of the spectral radius and apply it on the adjacency matrix of a directed graph.

2 Preliminaries

The following is Perron–Frobenius theorem, which provides a feature of nonnegative eigenvector to nonnegative matrices.

Theorem 2.1. *[3] If C is a nonnegative square matrix, then the spectral radius $\rho(C)$ is an eigenvalue of C with a corresponding nonnegative right eigenvector and a corresponding nonnegative left eigenvector.*

We introduce a notation of submatrix, which is taken from some columns and some rows of a matrix.

Definition 2.2. For a matrix $C = (c_{ij})$ and subsets α, β of row indices and column indices of C, respectively, we use $C[\alpha|\beta]$ to denote the submatrix of C with size $|\alpha| \times |\beta|$ that has entries c_{ij} for $i \in \alpha$ and $j \in \beta$.

Our theory is based on the following theorem, which is from [1], and we introduce two square matrices P and Q in the following theorem first. The matrix P is a permutation matrix which is multiplied to the left side, and the matrix Q is the sum of an elementary matrix and a certain binary matrix. In which P generalize row permutation on cases of C matrix, and Q is the transform from C' to C', which is the first $n-1$ columns and sum of certain columns. We aim to find C' such that C' majors C, i.e. $C \leq C'$.

Theorem 2.3. *Let $C = (c_{ij})$, $C' = (c'_{ij})$, P and Q be $n \times n$ matrices. Assume that*

(i) $PCQ \leq PC'Q$;

(ii) there exist a nonnegative column vector $u = (u_1, u_2, \ldots, u_n)^T$ and a scalar $\lambda' \in \mathbb{R}$ such that λ' is an eigenvalue of C' with associated eigenvector Qu;

(iii) there exist a nonnegative row vector $v^T = (v_1, v_2, \ldots, v_n)$ and a scalar $\lambda \in \mathbb{R}$ such that λ is an eigenvalue of C with associated left eigenvector $v^T P$; and

(iv) $v^T P Q u > 0$.

Then $\lambda \leq \lambda'$. Moreover, $\lambda = \lambda'$ if and only if

$$(PC'Q)_{ij} = (PCQ)_{ij} \qquad \text{for } 1 \leq i, j \leq n \text{ with } v_i \neq 0 \text{ and } u_j \neq 0. \quad (1)$$

Proof. Multiplying the nonnegative vector u in assumption (ii), where Qu is eigenvector of C', to the right of both terms of (i),

$$PCQu \leq PC'Qu = \lambda' PQu. \quad (2)$$

Multiplying the nonnegative left eigenvector v^T of C for λ in assumption (iii) to the left of all terms in (2), where $v^T P$ is left eigenvector of C for λ, thus we have

$$\lambda v^T P Q u = v^T P C Q u \leq v^T P C' Q u = \lambda' v^T P Q u. \quad (3)$$

Now delete the positive term $v^T P Q u$ by assumption (iv) to obtain $\lambda \leq \lambda'$ and finish the proof of the first part. Assume that $\lambda = \lambda'$, so the inequality in (3) is an equality. Especially $(PCQu)_i = (PC'Qu)_i$ for any i with $v_i \neq 0$. Hence, $(PCQ)_{ij} = (PC'Q)_{ij}$ for any i with $v_i \neq 0$ and any j with $u_j \neq 0$. Conversely, (1) implies

$$v^T P C Q u = \sum_{i,j} v_i (PCQ)_{ij} u_j = \sum_{i,j} v_i (PC'Q)_{ij} u_j = v^T P C' Q u,$$

so $\lambda = \lambda'$ by (3). $\qquad \square$

3 Our Method

We use $[n-1]$ as notation of the set of elements from one to $n-1$, which is $\{1, 2, ..., n-1\}$. Throughout fix $k \in [n-1]$, let E_{kn} denote the $n \times n$ binary matrix with a unique 1 appearing in the position k, n of E_{kn}. Now we apply the previous Theorem 2.3 with $P = I$ and

$$Q = I + E_{kn} = \begin{pmatrix} 1 & & & & & 0 \\ & 1 & & & & \\ & & \ddots & & 1 & \\ & & & & 1 & \\ 0 & & & & & 1 \end{pmatrix}, \tag{4}$$

so the matrix $PC'Q$ in assumption (i) of Theorem 2.3 is

$$PC'Q = \begin{pmatrix} c'_{11} & c'_{12} & \cdots & c'_{1k} + c'_{1n} \\ c'_{21} & c'_{22} & \cdots & c'_{2k} + c'_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c'_{n1} & c'_{n2} & \cdots & c'_{nk} + c'_{nn} \end{pmatrix}, \tag{5}$$

where c'_{ij} denote the (i, j)-entry of C.

Definition 3.1. A column vector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ is called K-*rooted* if $v'_j \geq 0$ for $1 \leq j \leq n$ and $v'_k \geq v'_n$.

The following Lemma is immediate from the above definition.

Lemma 3.2. *If $u = (u_1, u_2, \ldots, u_n)^T$ and $v' = (v'_1, v'_2, \ldots, v'_n) := Qu = (u_1, \ldots, u_{k-1}, u_k + u_n, u_{k+1}, \ldots, u_n)^T$, then*

(i) v' is k-rooted if and only if u is nonnegative;

(ii) $u_k > 0$ if and only if $v'_k > v'_n$.

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Below is our first result, in which the first condition implies the first $n-1$ columns of C major to the columns of C', and the (k,n)-sum column of C is also major to C'. The second and the third condition suggest that C and C' have nonnegative eigenvectors which are K-rooted. And the forth condition is simpler but with the same meaning with Theorem 2.3

Theorem 3.3. *Let $C = (c_{ij})$, $C' = (c'_{ij})$ be $n \times n$ matrices. Assume that*

(i) $C[[n]][[n-1]] \leq C'[[n]][[n-1]]$ and $c_{ik} + c_{in} \leq c'_{ik} + c'_{in}$ for all $1 \leq i \leq n$;

(ii) there exists a K-rooted vector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ and a scalar $\lambda' \in \mathbb{R}$ such that λ' is an eigenvalue of C' with associated eigenvector v';

(iii) there exists a nonnegative vector $v^T = (v_1, v_2, \ldots, v_n)$ and a scalar $\lambda \in \mathbb{R}$ such that λ is an eigenvalue of C with associated left eigenvector v^T;

(iv) $v^T v' > 0$.

Then $\lambda \leq \lambda'$. Moreover, $\lambda = \lambda'$ if and only if

(a) $c_{ik} + c_{in} = c'_{ik} + c'_{in} \qquad$ for $1 \leq i \leq n$ with $v_i \neq 0$ and $v'_n \neq 0$;

(b) $c'_{ij} = c_{ij} \qquad$ for $1 \leq i \leq n$, $1 \leq j \leq n-1$, $j \neq k$ with $v_i \neq 0$;

(c) $c'_{ik} = c_{ik} \qquad$ for $1 \leq i \leq n$ and $v'_k > v'_n$

Proof. The proof is based on Theorem 2.3 with $P = I$ and $Q = I + E_{kn}$ in (4). The assumption (i) $PCQ \leq PC'Q$ of Theorem 2.3 holds by the condition (i) of this theorem. Let $u = Q^{-1} v'$. Then u is nonnegative and $C'Qu = \lambda'Qu$ by the condition (ii) and (i) in Lemma 3.2. Hence the

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assumption (ii) of Theorem 2.3 holds. The assumptions (iii) and (iv) of Theorem 2.3 clearly hold by conditions (iii), (iv) of this theorem since $P = I$ and $v' = Qu$. Hence $\lambda \leq \lambda'$ by the necessary condition of Theorem 2.3. Moreover, $\lambda = \lambda'$ if and only if (1) holds, and this is equivalent to conditions (a), (b) and (c) of this theorem. $\qquad\square$

We are interested in the matrices C' that have K-rooted eigenvectors. Motivated by the condition (i) of Theorem 2.3, we provide the following two definitions. This is the definition of (k, n)-sum.

Definition 3.4. For an $n \times n$ matrix $C' = (c'_{ij})$, the (k, n)-sum vector of C' is the vector of the sum of the k-th and n-th columns of C', where $k \leq n - 1$.

Note that the last column of $C'Q$ is the (k, n)-sum vector of C'. Below is the definition of K-rooted matrix.

Definition 3.5. A matrix $C' = (c'_{ij})$ is called K-*rooted* if its first $n - 1$ columns and its (k, n)-sum vector are all K-rooted.

Remark 3.6.

$$Q^{-1} = I - E_{kn} = \begin{pmatrix} 1 & & & & & 0 \\ & 1 & & & & \\ & & \ddots & & -1 & \\ & & & 1 & & \\ 0 & & & & & 1 \end{pmatrix}.$$

The following lemma shows that a K-rooted matrix has a K-rooted eigenvector.

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Lemma 3.7. *Let* $C' = (c'_{ij})$ *be an* $n \times n$ *nonnegative matrix. Then the following (i)-(iii) hold.*

(i) C' *is a* K*-rooted matrix if and only if* $Q^{-1}C'Q$ *is nonnegative,*

(ii) Assume that C' *is* K*-rooted and let* u *be the nonnegative eigenvector of* $Q^{-1}C'Q$ *corresponding to* $\rho(C')$*. Then* C' *has a* K*-rooted eigenvector* $v' = Qu$ *for* $\rho(C')$*,*

(iii) $\rho(C') = \rho(Q^{-1}C'Q)$*.*

Proof. (i) The matrix $Q^{-1}C'Q$ is

$$
\begin{pmatrix}
c'_{11} & c'_{12} & \cdots & c'_{1\ n-1} & c'_{1k} + c'_{1n} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
c'_{(k-1)1} & c'_{(k-1)2} & \cdots & c'_{(k-1)(n-1)} & c'_{(k-1)k} + c'_{(k-1)n} \\
c'_{k1} - c'_{n1} & c'_{k2} - c'_{n2} & \cdots & c'_{k(n-1)} - c'_{n(k-1)} & c'_{kk} + c'_{kn} - c'_{nk} - x'_{nn} \\
c'_{(k+1)1} & c'_{(k+1)2} & \cdots & c'_{(k+1)(n-1)} & c'_{(k+1)k} + c'_{(k+1)n} \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
c'_{n1} & c'_{n2} & \cdots & c'_{n(n-1)} & c'_{nk} + c'_{nn}
\end{pmatrix},
$$

which is nonnegative if and only if C' is K-rooted by the definition of nonnegative matrix and K-rooted matrix.

(ii) By Lemma 3.2, $v' = Qu$ is K-rooted. Since $Q^{-1}C'Qu = \rho(C')u$ by the assumption, we have

$$
Q^{-1}C'Qu = Q^{-1}\rho(C')Qu = \rho(C')u,
$$

which implies

$$C'Qu = \rho(C')Qu.$$

(iii) Since C' and $Q^{-1}C'Q$ have the same set of eigenvalues, clearly

$$\rho(C') = \rho(Q^{-1}C'Q).$$

$\square$

Lemma 3.8. *If a square matrix C' has a K-rooted eigenvector corresponding to λ', then $C'+dI$ also has the same K-rooted eigenvector corresponding to $\lambda' + d$, where d is a constant and I is the identity matrix with the same size of C'.*

Theorem 3.9. *Let C be an $n \times n$ nonnegative matrix. For $1 \leq i \leq n$ and $1 \leq j \leq n-1$, choose c'_{ij} such that $c'_{ij} \geq c_{ij}$ and $c'_{kj} \geq c'_{nj} > 0$, and choose r'_i such that $r'_i \geq c_{ik} + c_{in}$, and $r'_k \geq r'_n$. Moreover choose $c'_{in} := r'_i - c'_{ik}$. Then $\rho(C) \leq \rho(C')$, when $C' = (c'_{ij})$.*

Proof. These assumptions are necessary that $PCQ \leq PC'Q$, where $P = I$, $Q = I + E_{kn}$ and C' is K-rooted. Based on Lemma 3.7,

$$Q^{-1}C'Q = \begin{pmatrix} c'_{11} & c'_{12} & \cdots & c'_{1(n-1)} & c'_{1k} + c'_{1n} \\ \vdots & & & & \\ c'_{(k-1)1} & c'_{(k-1)2} & \cdots & c'_{(k-1)(n-1)} & c'_{(k-1)k} + c'_{(k-1)n} \\ c'_{k1} - c'_{n1} & c'_{k2} - c'_{n2} & \cdots & c'_{k(n-1)} - c'_{n(k-1)} & c'_{kk} + c'_{kn} - c'_{nk} - c'_{nn} \\ c'_{(k+1)1} & c'_{(k+1)2} & \cdots & c'_{(k+1)(n-1)} & c'_{(k+1)k} + c'_{(k+1)n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ c'_{n1} & c'_{n2} & \cdots & c'_{n(n-1)} & c'_{nk} + c'_{nn} \end{pmatrix}.$$

Then $Q^{-1}C'Q$ is nonnegative when $c'_{kj} \geq c'_{nj} > 0$ for $1 \leq j \leq n-1$ and $c'_{ij} \geq c_{ij}$, where C is nonnegative, and the last column $c'_{in} + c'_{ik} = r'_i \geq c_{in} + c_{ik}$ by assumption $r'_i \geq c_{ik} + c_{in}$.

For $1 \leq i \leq n$ and $1 \leq j \leq n-1$, choose c'_{ij} such that $c'_{ij} \geq c_{ij}$, which implies $C[[n]][[n-1]] \leq C'[[n]][[n-1]]$. And under the same condition for i and j, choose r'_i such that $r'_i \geq c_{ik} + c_{in}$, which implies $c_{ik} + c_{in} \leq c'_{ik} + c'_{in} = r'_i$; C' is K-rooted matrix, then by conditions (ii) and (iii) in Lemma 3.7, there exists a K-rooted vector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ and a scalar $\lambda' \in \mathbb{R}$ such that λ' is an eigenvalue of C' with associated eigenvector v'. Since C is nonnegative, by Theorem 2.1, we claim there exists $v^T = w^T P$, such that v^T is nonnegative left eigenvector of C, and a scalar $\lambda \in \mathbb{R}$ such that λ is an eigenvalue of C with associated left eigenvector v^T. Due to v' and v^T are nonnegative, $v^T v' > 0$, unless they are orthogonal, i.e, $v^T v' = 0$.

Here we can summarize the facts we know so far as the following:

(i) $C[[n]][[n-1]] \leq C'[[n]][[n-1]]$ and $c_{ik} + c_{in} \leq c'_{ik} + c'_{in}$ for all $1 \leq i \leq n$;

(ii) there exists a K-rooted vector $v' = (v'_1, v'_2, \ldots, v'_n)^T$ and a scalar $\lambda' \in \mathbb{R}$ such that λ' is an eigenvalue of C' with associated eigenvector v';

(iii) there exists a nonnegative vector $v^T = (v_1, v_2, \ldots, v_n)$ and a scalar $\lambda \in \mathbb{R}$ such that λ is an eigenvalue of C with associated left eigenvector v^T;

(iv) $v^T v' > 0$,

which come from Theorem 3.3.

By Lemma 3.8, for certain d, if $C' + dI$ is K-rooted, then it has a K-rooted eigenvector with its spectral radius $\lambda + d$. C' would share the same eigenvector with $C' + dI$ and has eigenvalue λ. So $C' + dI$ and $C + dI$ meet the conditions of Theorem 3.3, and we can show that $\rho(C'+dI) \geq \rho(C+dI)$ and then $\rho(C') \geq \rho(C)$ $\qquad\qquad\qquad\qquad\qquad\qquad\quad$ $\square$

3.1 Example

For the following 4×4 matrix

$$C = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$
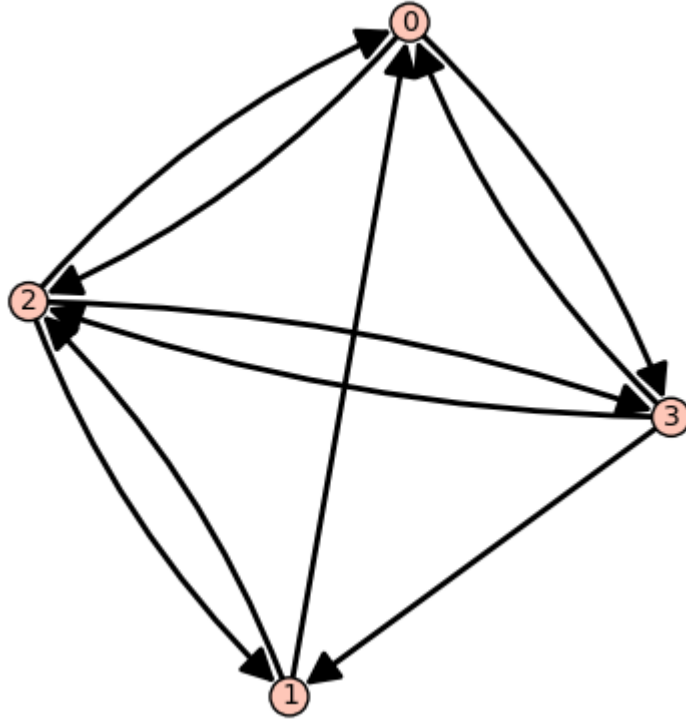
and corresponding directed graph, [4, sage]
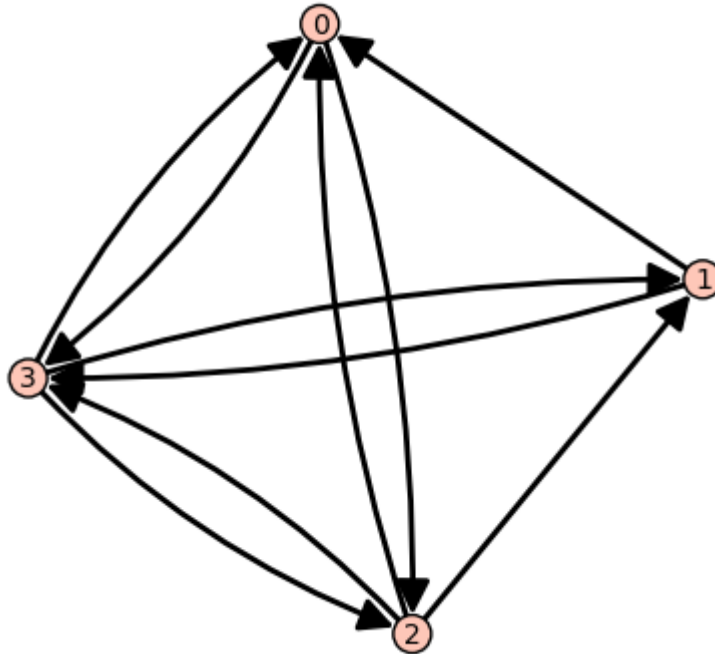
we choose the matrix
$$C' = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$
which satisfies the assumptions in Theorem 3.9. Hence $\rho(C) \leq \rho(C')$. Actually, both of the values of $\rho(C)$ and $\rho(C')$ are close to 2.511547, and we have $\rho(C') - \rho(C) > 0$ by calculating on computer. Moreover, the corresponding directed graph of matrix C' is, [4, sage]

3.2 Counterexample

For the following two 4×4 matrices

$$
C = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \quad
C' = \begin{pmatrix} 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{pmatrix},
$$

specify $n=4$, $k=3$ in $Q = I + E_{kn} = I + E_{34}$, then

$$
CQ = \begin{pmatrix} 0 & 0 & 1 & 2 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \quad
C'Q = \begin{pmatrix} 0 & 0 & 1 & 2 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{pmatrix},
$$

and we have $CQ \leq C'Q$, but $\rho(C) = 2.234 \nleq 2.148 = \rho(C')$. This is because $c'_{33} + c'_{34} \ngeq c'_{43} + c'_{44}$.

References

[1] Yen-Jen Cheng, *A matrix realization of spectral bounds of the spectral radius of a nonnegative matrix*, Ph.D. Thesis, NCTU, 2018.

[2] A. E. Brouwer, W. H. Haemers, *Spectra of graphs*, Springer, 2012

[3] R. A. Horn , C. R. Johnson, *Matrix analysis*, Cambrigde University Press, 1985.

[4] [Sage] SageMath, the Sage Mathematics Software System (Version 9.2), The Sage Developers, 2020, https://www.sagemath.org.