Estrada index and subgraph centrality of hypergraphs via tensors

Hong Zhou, Lizhu Sun, Changjiang Bu

College of Mathematical Sciences, Harbin Engineering University, Harbin 150001, PR China

Abstract

Uniform hypergraphs have a natural one-to-one correspondence to tensors. In this paper, we investigate the Estrada index and subgraph centrality of an m-uniform hypergraph $\mathcal{H}$ via the adjacency tensor. We establish some bounds for the Estrada index and give expressions of the subgraph centrality in terms of graph parameters of the multi-digraphs associated with $\mathcal{H}$. When $\mathcal{H}$ is 2-uniform, the above Estrada index and subgraph centrality are the Estrada index and subgraph centrality of a graph.

Keywords: hypergraph, Estrada index, subgraph centrality, adjacency tensor, eigenvalue

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1. Introduction

For a simple undirected graph H, its *Estrada index*

$$EE(H) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all the eigenvalues of the adjacency matrix of H [1]. The study of Estrada index has attracted extensive attention[2, 3, 4, 5, 6]. The Estrada index of graphs has wide applications in biology [1], chemistry [7] and complex networks [8, 9]. The Estrada index of graphs is closely related to the subgraph centrality of a vertex in graphs and the trace of the adjacency matrix of graphs [2, 8].

Email address: sunlizhu678876@126.com (Lizhu Sun)

Let A be the adjacency matrix of the graph H and $\mu_d(j) = (A^d)_{jj}$. Then $\mu_d(j)$ is the number of closed walks of length d starting and ending at the vertex j in H [10].

$$C(j) = \sum_{d=0}^{\infty} \frac{\mu_d(j)}{d!} \tag{1.1}$$

is called the *subgraph centrality* of a vertex j in H [8]. The subgraph centrality is a topological parameter to measure the importance of nodes in networks, which is widely used in the real-world network analysis [8, 11].

The *dth order spectral moment* of H is the sum of d powers of all the eigenvalues of A, denoted by $S_d(H)$. Since the trace $tr(A^d) = \sum_{j=1}^{n} \mu_d(j) = S_d(H)$ [10],

$$\sum_{j=1}^{n} C(j) = \sum_{d=0}^{\infty} \sum_{j=1}^{n} \frac{\mu_d(j)}{d!} = \sum_{d=0}^{\infty} \frac{tr(A^d)}{d!} = \sum_{d=0}^{\infty} \sum_{i=1}^{n} \frac{\lambda_i^d}{d!} = \sum_{i=1}^{n} e^{\lambda_i} = EE(H). \tag{1.2}$$

Since uniform hypergraphs have a natural one-to-one correspondence to tensors, in this paper, we investigate the Estrada index and subgraph centrality of hypergraphs via tensors. Next, we introduce some notations and concepts for tensors and hypergraphs. Let $[n] = \{1, 2, \ldots, n\}$, $[n]^m = \{i_1 i_2 \cdots i_m | \ i_k \in [n], \ k = 1, \ldots, m\}$ and $\mathbb{C}$ be complex field. An order m dimension n complex tensor

$$\mathcal{T} = (t_\alpha), \text{ for } \alpha \in [n]^m, t_\alpha \in \mathbb{C},$$

is a multidimensional array with n^m entries. When $m = 2$, $\mathcal{T}$ is an $n \times n$ matrix [12, 13].

A hypergraph $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ is called *m-uniform* if $|e| = m \geq 2$ for all $e \in E(\mathcal{H})$. For $e = \{i_1, i_2, \ldots, i_m\} \in E(\mathcal{H})$, e is also written $i_1 i_2 \cdots i_m$ in this paper. For an m-uniform hypergraph $\mathcal{H}$, its *adjacency tensor* is the order m dimension n tensor $\mathcal{A}_{\mathcal{H}} = (h_\alpha)$, where

$$h_\alpha = \begin{cases} \frac{1}{(m-1)!}, & \text{if } \alpha \in E(\mathcal{H}), \\ 0, & \text{otherwise}. \end{cases}$$

Clearly, $\mathcal{A}_{\mathcal{H}}$ is the adjacency matrix of $\mathcal{H}$ when $\mathcal{H}$ is 2-uniform. The eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are also called the eigenvalues of $\mathcal{H}$ [14].

In 2005, the concept of eigenvalues of tensors was proposed by Qi [12] and Lim

[13], independently. The eigenvalues of tensors and related problems are important research topics of spectral hypergraph theories [15, 16, 17, 18], especially the trace of tensors [18, 19, 20, 21, 22].

Morozov and Shakirov gave an expression of the dth order trace $Tr_d(\mathcal{T})$ of a tensor $\mathcal{T}$ [19]. Hu et al. proved that $Tr_d(\mathcal{T})$ is equal to the sum of d powers of all eigenvalues of $\mathcal{T}$ [20]. For a uniform hypergraph $\mathcal{H}$, the sum of d powers of all eigenvalues of $\mathcal{A}_{\mathcal{H}}$ is called the *dth order spectral moment* of $\mathcal{H}$, denoted by $S_d(\mathcal{H})$. Then $Tr_d(\mathcal{A}_{\mathcal{H}}) = S_d(\mathcal{H})$. Shao et al. established some formulas for the dth order trace of tensors in terms of some graph parameters [21]. Clark and Cooper expressed the spectral moments of hypergraphs by the numbers of Veblen multi-hypergraphs and used this result to give the "Harary-Sachs" coefficient theorem for hypergraphs [18]. Chen et al. gave a formula for the spectral moment of a hypertree in terms of the numbers of some subhypertrees [22].

In this paper, we define the Estrada index and subgraph centrality of a uniform hypergraph $\mathcal{H}$ via the adjacency tensor. The bounds for the Estrada index are established. We give two expressions of the subgraph centrality by the number of Eulerian closed walks of the multi-digraphs associated with $\mathcal{H}$ and the number of arborescences of the multi-digraphs associated with $\mathcal{H}$, respectively. Similar to the Estrada index of a graph as in Equation (1.2), the Estrada index of a uniform hypergraph $\mathcal{H}$ is equal to the sum of the subgraph centrality measures of all vertices in $\mathcal{H}$.

2. Preliminaries

Let $\mathbb{C}^n$ be the set of n-dimension complex vectors and $\mathbb{C}^{[m,n]}$ be the set of complex tensors with order m dimension n. For a tensor $\mathcal{T} = (t_{i\alpha}) \in \mathbb{C}^{[m,n]}$ and $x = (x_1, \ldots, x_n)^{\mathrm{T}} \in \mathbb{C}^n$, $\mathcal{T}x^{m-1}$ is a vector in $\mathbb{C}^n$ whose i-th component is

$$(\mathcal{T}x^{m-1})_i = \sum_{\alpha \in [n]^{m-1}} t_{i\alpha} x^{\alpha},$$

where $x^{\alpha} = x_{i_1} x_{i_2} \cdots x_{i_{m-1}}$ for $\alpha = i_1 i_2 \cdots i_{m-1}$. A number $\lambda \in \mathbb{C}$ is called an *eigenvalue* of $\mathcal{T}$ if there exists a nonzero vector $x \in \mathbb{C}^n$ such that

$$\mathcal{T}x^{m-1} = \lambda x^{[m-1]},$$

where $x^{[m-1]} = \left(x_1^{m-1}, \ldots, x_n^{m-1}\right)^{\mathrm{T}}$. The number of eigenvalues of $\mathcal{T}$ is $k = n(m-1)^{n-1}$ [12, 13]. Let $\rho = \max\{|\lambda_1|, |\lambda_2|, \ldots, |\lambda_k|\}$ be the spectral radius of $\mathcal{T}$, where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all the eigenvalues of $\mathcal{T}$.

The *dth order trace* $Tr_d(\mathcal{T})$ of a tensor $\mathcal{T} = (t_\alpha) \in \mathbb{C}^{[m,n]}$ is expressed as follows [19]:

$$\begin{aligned} & Tr_d(\mathcal{T}) \\ & = (m-1)^{n-1} \sum_{d_1+\cdots+d_n=d} \prod_{i=1}^{n} \frac{1}{(d_i(m-1))!} \Big(\sum_{\alpha_i \in [n]^{m-1}} t_{i\alpha_i} \frac{\partial}{\partial a_{i\alpha_i}} \Big)^{d_i} tr(A^{d(m-1)}), \end{aligned} \quad (2.1)$$

where $A = (a_{ij})$ is an $n \times n$ auxiliary matrix, $d_1, \ldots, d_n$ are nonnegative integers and $\frac{\partial}{\partial a_{i\alpha_i}} := \frac{\partial}{\partial a_{ii_2}} \cdots \frac{\partial}{\partial a_{ii_m}}$ for $\alpha_i = i_2 \cdots i_m$.

In [14], the dth order traces of the adjacency tensor of an m-uniform hypergraph were given for $d = 0, 1, 2, \ldots, m$.

Lemma 2.1. *[14] Let $\mathcal{H}$ be an m-uniform hypergraph with n vertices and q edges. Then*

(1) $Tr_0(\mathcal{A}_\mathcal{H}) = n(m-1)^{n-1}$;
(2) $Tr_d(\mathcal{A}_\mathcal{H}) = 0$ for $d = 1, 2, \ldots, m-1$;
(3) $Tr_m(\mathcal{A}_\mathcal{H}) = qm^{m-1}(m-1)^{n-m}$.

Since uniform hypergraphs have a natural one-to-one correspondence to tensors, we define the Estrada index and subgraph centrality of a uniform hypergraph via the adjacency tensor.

Definition 2.2. *For an m-uniform hypergraph $\mathcal{H}$ with n vertices,*

$$\sum_{i=1}^{k} e^{\lambda_i}$$

is called the Estrada index of $\mathcal{H}$, denoted by $EE(\mathcal{H})$, where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all the eigenvalues of $\mathcal{A}_\mathcal{H}$.

Clearly, when $\mathcal{H}$ is 2-uniform, the above index is the Estrada index of a graph [1].

Let $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ be an m-uniform hypergraph with n vertices. For $j \in V(\mathcal{H})$, let $\mu_d(j)$ be the term corresponding to the vertex j in $Tr_d(\mathcal{A}_\mathcal{H})$ which is expressed by Equation (2.1), that is

$$\mu_d(j) = (m-1)^{n-1} \sum_{d_1+\cdots+d_n=d} \prod_{i=1}^{n} \frac{1}{(d_i(m-1))!} \Big(\sum_{\alpha_i \in [n]^{m-1}} h_{i\alpha_i} \frac{\partial}{\partial a_{i\alpha_i}}\Big)^{d_i} (A^{d(m-1)})_{jj}. \quad (2.2)$$

Thus,

$$\sum_{j=1}^{n} \mu_d(j) = Tr_d(\mathcal{A}_{\mathcal{H}}). \quad (2.3)$$

Definition 2.3. *For an m-uniform hypergraph $\mathcal{H}$ with n vertices,*

$$\sum_{d=0}^{\infty} \frac{\mu_d(j)}{d!} \quad (2.4)$$

is called the subgraph centrality of a vertex j in $\mathcal{H}$, denoted by $C(j)$, where $\mu_d(j)$ is given by Equation (2.2).

By Equation (2.2), we know $C(j)$ is a real number. When $\mathcal{H}$ is 2-uniform, since $\mu_d(j) = (\mathcal{A}_{\mathcal{H}}^d)_{jj}$ [19], $C(j)$ is the subgraph centrality of a graph as in Equation (1.1).

Since the dth order trace of the adjacency tensor $Tr_d(\mathcal{A}_{\mathcal{H}}) = \sum_{i=1}^{k} \lambda_i^d$ [20] and Equation (2.3),

$$\sum_{j=1}^{n} C(j) = \sum_{d=0}^{\infty} \sum_{j=1}^{n} \frac{\mu_d(j)}{d!} = \sum_{d=0}^{\infty} \frac{Tr_d(\mathcal{A}_{\mathcal{H}})}{d!} = \sum_{i=1}^{k} \sum_{d=0}^{\infty} \frac{\lambda_i^d}{d!} = \sum_{i=1}^{k} e^{\lambda_i} = EE(\mathcal{H}),$$

where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$.

3. Bounds for the Estrada index of hypergraphs

The spectrum of an m-uniform hypergraph is said to be *m-symmetric* if this spectrum is invariant under a rotation of an angle $2\pi/m$ in the complex plane [21]. In this section, for a 3-uniform hypergraph $\mathcal{H}$ whose spectrum is 3-symmetric, we give an upper bound for the Estrada index in terms of energy of $\mathcal{H}$. And for m-uniform hypergraphs, we establish some bounds for the Estrada index.

The spectra of m-uniform power hypergraphs and hypertrees have attracted extensive attention [23, 24]. Their spectra are all m-symmetric [14, 21, 24, 25].

Lemma 3.1. *[21] Let $\mathcal{H}$ be an m-uniform hypergraph whose spectrum is m-symmetric. If $m \nmid d$, then $Tr_d(\mathcal{A}_{\mathcal{H}}) = 0$.*

Let $\mathcal{H}$ be an m-uniform hypergraph with n vertices and $\lambda_1, \lambda_2, \ldots, \lambda_k$ be all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$. In this paper, $\sum_{j=1}^{k} |\lambda_j|$ is called the *energy* of $\mathcal{H}$, denoted by $\mathcal{E}(\mathcal{H})$. When $m = 2$, bounds for the Estrada index of a graph $\mathcal{H}$ were given by energy of $\mathcal{H}$ [2, 26, 27].

For a 3-uniform hypergraph $\mathcal{H}$ whose spectrum is 3-symmetric, we establish an upper bound by energy of $\mathcal{H}$ for the Estrada index.

Theorem 3.2. *Let $\mathcal{H}$ be a 3-uniform hypergraph with n vertices and q edges ($q \geq 1$). If the spectrum of $\mathcal{H}$ is 3-symmetric, then*

$$EE(\mathcal{H}) \leq \frac{2(\cosh \rho - 1)}{3\rho} \mathcal{E}(\mathcal{H}) + k,$$

where ρ is the spectral radius of $\mathcal{A}_{\mathcal{H}}$ and $k = 2^{n-1}n$.

Proof. It follows from Lemma 3.1 that

$$EE(\mathcal{H}) = \sum_{d=0}^{\infty} \frac{Tr_d(\mathcal{A}_{\mathcal{H}})}{d!} = \sum_{l=0}^{\infty} \frac{Tr_{3l}(\mathcal{A}_{\mathcal{H}})}{(3l)!} = \sum_{l=0}^{\infty} \sum_{j=1}^{k} \frac{\lambda_j^{3l}}{(3l)!} \leq \sum_{j=1}^{k} \sum_{l=0}^{\infty} \frac{|\lambda_j|^{3l}}{(3l)!}, \quad (3.1)$$

where $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$.

Let $S(x) = \sum_{l=0}^{\infty} \frac{x^{3l}}{(3l)!}$, where x is a real variable. We have $\frac{d^3 S}{dx^3} = \sum_{l=1}^{\infty} \frac{x^{3l-3}}{(3l-3)!} = \sum_{l=0}^{\infty} \frac{x^{3l}}{(3l)!}$.

Hence, we get the differential equation $\frac{d^3 S}{dx^3} - S = 0$ satisfying the conditions $S(0) = 1$, $\frac{dS}{dx} \mid_{x=0} = 0$ and $\frac{d^2 S}{dx^2} \mid_{x=0} = 0$. Then $S(x) = \frac{2}{3} e^{-\frac{x}{2}} \cos(\frac{\sqrt{3}}{2} x) + \frac{1}{3} e^x$.

We have

$$\begin{aligned} S(|\lambda_j|) &= \frac{2}{3} e^{-\frac{|\lambda_j|}{2}} \cos(\frac{\sqrt{3}}{2} |\lambda_j|) + \frac{1}{3} e^{|\lambda_j|} \\ &\leq \frac{2}{3} \frac{e^{-|\lambda_j|} + (\cos(\frac{\sqrt{3}}{2}|\lambda_j|))^2}{2} + \frac{1}{3} e^{|\lambda_j|} \\ &\leq \frac{1}{3}(e^{-|\lambda_j|} + e^{|\lambda_j|}) + \frac{1}{3} = \frac{2}{3} \cosh |\lambda_j| + \frac{1}{3}. \end{aligned}$$

Let $f(x) = \frac{\cosh x - 1}{x}$, $x \in (0, \rho]$. We have $\frac{df(x)}{dx} = \frac{x \sinh x - \cosh x + 1}{x^2}$. Let $g(x) = x \sinh x - \cosh x + 1$, $x \in [0, \rho]$. We have $\frac{dg(x)}{dx} = x \cosh x \geq 0$ and $\frac{dg(x)}{dx} = 0$ if and only if $x = 0$. Thus, $g(x)$ is strictly monotone increasing function. For $0 < x \leq \rho$, we have $g(x) > g(0) = 0$. Hence, $\frac{df(x)}{dx} > 0$, $x \in (0, \rho]$. Then $f(x)$ is strictly monotone increasing function. So $\frac{\cosh x - 1}{x} \leq \frac{\cosh \rho - 1}{\rho}$, $x \in (0, \rho]$, that is

$\cosh x \leq \frac{\cosh\rho-1}{\rho}x+1$, $x\in(0,\rho]$. When $x=0$, the above inequality obviously holds. Thus, $\cosh x \leq \frac{\cosh\rho-1}{\rho}x+1$, $x\in[0,\rho]$.

So,

$$\begin{aligned} S(|\lambda_j|) &\leq \frac{2}{3}\cosh|\lambda_j| + \frac{1}{3} \\ &\leq \frac{2}{3}(\frac{\cosh\rho-1}{\rho}|\lambda_j|+1)+\frac{1}{3} = \frac{2(\cosh\rho-1)}{3\rho}|\lambda_j|+1. \end{aligned} \tag{3.2}$$

By Equation (3.1) and (3.2), we have

$$\begin{aligned} EE(\mathcal{H}) &\leq \sum_{j=1}^{k} S(|\lambda_j|) \\ &\leq \frac{2(\cosh\rho-1)}{3\rho}\sum_{j=1}^{k}|\lambda_j| + k = \frac{2(\cosh\rho-1)}{3\rho}\mathcal{E}(\mathcal{H})+k. \end{aligned}$$

□

The following is a lower bound for the Estrada index of m-uniform hypergraphs.

Theorem 3.3. *Let $\mathcal{H}$ be an m-uniform hypergraph with n vertices and q edges. Then*

$$EE(\mathcal{H}) \geq \frac{qm^{m-2}(m-1)^{n-m-1}}{(m-2)!} + n(m-1)^{n-1}, \tag{3.3}$$

equality holds if and only if $\mathcal{H}$ is an empty hypergraph.

Proof. From Lemma 2.1, we have

$$\begin{aligned} EE(\mathcal{H}) &= \sum_{d=0}^{\infty}\frac{Tr_d(\mathcal{A}_\mathcal{H})}{d!} = n(m-1)^{n-1} + \sum_{d=m}^{\infty}\frac{Tr_d(\mathcal{A}_\mathcal{H})}{d!} \\ &\geq n(m-1)^{n-1} + \frac{Tr_m(\mathcal{A}_\mathcal{H})}{m!} = n(m-1)^{n-1} + \frac{qm^{m-2}(m-1)^{n-m-1}}{(m-2)!}. \end{aligned}$$

When $\mathcal{H}$ is an empty hypergraph, all eigenvalues of $\mathcal{A}_\mathcal{H}$ are 0. It is easy to see $EE(\mathcal{H}) = \sum_{i=1}^{k} e^0 = k = n(m-1)^{n-1}$. Then the equality of Inequality (3.3) holds.

On the other hand, if the equality of Inequality (3.3) holds, it follows from the proof of the above inequality that $Tr_d(\mathcal{A}_{\mathcal{H}}) = 0$ for all $d \geq m+1$, that is

$$\sum_{j=1}^{k} \lambda_j^d = 0, \text{ for all } d \geq m+1, \tag{3.4}$$

where $\lambda_1, \lambda_2, \dots, \lambda_k$ are all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$. Without loss of generality, suppose that $\lambda_1, \lambda_2, \dots, \lambda_s$ are all the distinct eigenvalues among $\lambda_1, \lambda_2, \dots, \lambda_k$, and $l_i \geq 1$ is the multiplicity of λ_i, $i = 1, 2, \dots, s$.

If $s = 1$, then all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are the same. Since $Tr_1(\mathcal{A}_{\mathcal{H}}) = 0$, all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are 0.

If $s \geq 2$, let $M = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ \lambda_1 & \lambda_2 & \cdots & \lambda_s \\ \cdots & \cdots & \cdots & \cdots \\ \lambda_1^{s-1} & \lambda_2^{s-1} & \cdots & \lambda_s^{s-1} \end{pmatrix}$. By Equation (3.4), we have $M(l_1\lambda_1^{m+1}, l_2\lambda_2^{m+1}, \dots, l_s\lambda_s^{m+1})^{\mathrm{T}} = 0$. Since $\det(M) \neq 0$, $(l_1\lambda_1^{m+1}, l_2\lambda_2^{m+1}, \dots, l_s\lambda_s^{m+1})^{\mathrm{T}} = 0$, that is $\lambda_j = 0$, $j = 1, 2, \dots, s$. It contradicts $s \geq 2$.

So all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are 0. Then the spectral radius of $\mathcal{A}_{\mathcal{H}}$ is 0. The spectral radius is greater than or equal to the average degree of $\mathcal{H}$ [14]. Hence, the average degree is equal to 0, that is $\mathcal{H}$ is an empty hypergraph.

Thus, equality holds in Inequality (3.3) if and only if $\mathcal{H}$ is an empty hypergraph. $\square$

Next we establish an upper bound for the Estrada index of m-uniform hypergraphs with $m \geq 3$.

Theorem 3.4. *Let $\mathcal{H}$ be an m-uniform hypergraph with n vertices, q edges and $m \geq 3$. Then*

$$EE(\mathcal{H}) \leq k - 1 + e^r + \frac{qm^{m-2}(m-1)^{n-m-1}}{(m-2)!} - \sum_{d=1}^{m} \frac{r^d}{d!}, \tag{3.5}$$

where $r = \sqrt{2\sum_{j=1}^{k}(Re(\lambda_j))^2}$, $\lambda_1, \lambda_2, \dots, \lambda_k$ are all the eigenvalues of $\mathcal{A}_{\mathcal{H}}$, $k = n(m-1)^{n-1}$. Equality holds if and only if $\mathcal{H}$ is an empty hypergraph.

Proof. Let $\lambda_j = \alpha_j + \mathbf{i}\beta_j$, $\alpha_j, \beta_j \in \mathbb{R}$, $j = 1, 2, \dots, k$, $\mathbf{i}^2 = -1$. From $Tr_2(\mathcal{A}_{\mathcal{H}}) =$

$\sum_{j=1}^{k}\lambda_j^2$ and Lemma 2.1 (2), we have

$$Tr_2(\mathcal{A}_{\mathcal{H}})=\sum_{j=1}^{k}(\alpha_j^2-\beta_j^2)+\mathbf{i}\sum_{j=1}^{k}2\alpha_j\beta_j=0.$$

Then

$$\sum_{j=1}^{k}(\alpha_j^2-\beta_j^2)=0.$$

So

$$\sum_{j=1}^{k}|\lambda_j|^2=\sum_{j=1}^{k}(\alpha_j^2+\beta_j^2)=2\sum_{j=1}^{k}\alpha_j^2. \tag{3.6}$$

Note that $EE(\mathcal{H})$, $Tr_d(\mathcal{A}_{\mathcal{H}})$ are nonnegative real numbers, $d=0,1,2,\ldots$, and $\sum_{d=0}^{\infty}\frac{|\lambda_j|^d}{d!}$ is convergent. We have

$$\begin{aligned}EE(\mathcal{H})&=\sum_{d=0}^{m}\frac{Tr_d(\mathcal{A}_{\mathcal{H}})}{d!}+\sum_{d=m+1}^{\infty}\frac{\sum_{j=1}^{k}\lambda_j^d}{d!}\\&\le\sum_{d=0}^{m}\frac{Tr_d(\mathcal{A}_{\mathcal{H}})}{d!}+\sum_{d=m+1}^{\infty}\frac{1}{d!}\sum_{j=1}^{k}|\lambda_j|^d.\end{aligned}$$

For $|\lambda_j|, j\in[k]$ and integer $d\ge 2$, by Cauchy-Schwarz Inequality, we have

$$\begin{aligned}(\sum_{j=1}^{k}|\lambda_j|^d)^2&=(\sum_{j=1}^{k}(|\lambda_j|^{d-1}|\lambda_j|))^2\\&\le\sum_{j=1}^{k}|\lambda_j|^{2(d-1)}\sum_{j=1}^{k}|\lambda_j|^2=\sum_{j=1}^{k}(|\lambda_j|^2)^{(d-1)}\sum_{j=1}^{k}|\lambda_j|^2\\&\le(\sum_{j=1}^{k}|\lambda_j|^2)^{d-1}\sum_{j=1}^{k}|\lambda_j|^2=(\sum_{j=1}^{k}|\lambda_j|^2)^d,\end{aligned}$$

that is $\sum_{j=1}^{k}|\lambda_j|^d \le (\sum_{j=1}^{k}|\lambda_j|^2)^{\frac{d}{2}}$. So,

$$EE(\mathcal{H}) \le \sum_{d=0}^{m}\frac{Tr_d(\mathcal{A_H})}{d!} + \sum_{d=m+1}^{\infty}\frac{1}{d!}(\sum_{j=1}^{k}|\lambda_j|^2)^{\frac{d}{2}}.$$

It follows from Equation (3.6) that

$$\begin{aligned}EE(\mathcal{H}) &\le \sum_{d=0}^{m}\frac{Tr_d(\mathcal{A_H})}{d!} + \sum_{d=m+1}^{\infty}\frac{1}{d!}(2\sum_{j=1}^{k}\alpha_j^2)^{\frac{d}{2}}\\ &= \sum_{d=0}^{m}\frac{Tr_d(\mathcal{A_H})}{d!} + e^{\sqrt{2\sum\limits_{j=1}^{k}\alpha_j^2}} - \sum_{d=0}^{m}\frac{(2\sum\limits_{j=1}^{k}\alpha_j^2)^{\frac{d}{2}}}{d!}.\end{aligned}$$

By Lemma 2.1, we have

$$EE(\mathcal{H}) \le k-1+e^{\sqrt{2\sum\limits_{j=1}^{k}\alpha_j^2}} + \frac{Tr_m(\mathcal{A_H})}{m!} - \sum_{d=1}^{m}\frac{(2\sum\limits_{j=1}^{k}\alpha_j^2)^{\frac{d}{2}}}{d!},$$

where $Tr_m(\mathcal{A_H}) = qm^{m-1}(m-1)^{n-m}$. Thus, we obtain Inequality (3.5).

If $\mathcal{H}$ is an empty hypergraph, all eigenvalues of $\mathcal{A_H}$ are 0. It is easy to see $EE(\mathcal{H}) = \sum_{i=1}^{k} e^0 = k$. Then the equality in Inequality (3.5) holds.

On the other hand, suppose the equality in Inequality (3.5) holds. From the proof of the above inequality, we have $\sum_{d=m+1}^{\infty}\frac{1}{d!}(\sum_{j=1}^{k}|\lambda_j|^d - \sum_{j=1}^{k}\lambda_j^d) = 0$ and note that $\sum_{j=1}^{k}\lambda_j^d$ is a nonnegative real number, $d = m+1, m+2, \ldots$. Then

$$\sum_{j=1}^{k}\lambda_j^d = \sum_{j=1}^{k}|\lambda_j|^d, d = m+1, m+2, \ldots.$$

Let $\lambda_j = |\lambda_j|e^{\mathbf{i}\theta_j}, j = 1,2,\ldots,k$. We have

$$\sum_{j=1}^{k}|\lambda_j|^d(1-\cos(\theta_j d)) = 0, d = m+1, m+2, \ldots.$$

Then $|\lambda_j|^d(1-\cos(\theta_j d)) = 0$, $d = m+1, m+2, \ldots,$ and $j = 1,2,\ldots,k$. Thus, we have $\lambda_j = 0$ or $\cos(\theta_j d) = 1$, $d = m+1, m+2, \ldots,$ for each $j \in [k]$. If there exists

$j \in [k]$ such that $\cos(\theta_j d) = 1$, $d = m+1, m+2, \ldots$. Then we have $\theta_j d = 2l_d\pi$, where l_d is an integer and $d = m+1, m+2, \ldots$. So,

$$\theta_j = \frac{l_{m+1}}{m+1}2\pi = \frac{l_{m+2}}{m+2}2\pi = \cdots.$$

Let $\frac{l_{m+1}}{m+1} = \frac{l_{m+2}}{m+2} = \cdots = t$. Then

$$l_{m+2} = t(m+2) = t(m+1) + t = l_{m+1} + t.$$

Since l_{m+1}, l_{m+2} are integers, t is an integer. So, θ_j is equal to an integer multiple of 2π. Hence, λ_j is a nonnegative real number. Since $Tr_1(\mathcal{A}_{\mathcal{H}}) = 0$, all eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are 0. In the proof of Theorem 3.3, we proved that $\mathcal{H}$ is an empty hypergraph when all eigenvalues of $\mathcal{A}_{\mathcal{H}}$ are 0. Thus, we get $\mathcal{H}$ is an empty hypergraph. Therefore, the equality holds in Inequality (3.5) if and only if $\mathcal{H}$ is an empty hypergraph. $\square$

4. Expressions for the subgraph centrality of hypergraphs

In this section, for a uniform hypergraph $\mathcal{H}$, we give two expressions of the subgraph centrality by the number of Eulerian closed walks of the multi-digraphs associated with $\mathcal{H}$ and the number of arborescences of the multi-digraphs associated with $\mathcal{H}$, respectively. The explicit expression of $\mu_d(j)$ of $\mathcal{H}$ is given for $d = 0, 1, 2, \ldots, m$.

For an integer $d > 0$, let $\alpha = i_1 \cdots i_d \in [n]^d$. If α satisfies $i_1 \leq \cdots \leq i_d$, then α is called *ascending order*. Let

$$\mathcal{F}_d = \{(i_1\alpha_1, \ldots, i_d\alpha_d) |\ 1 \leq i_1 \leq \cdots \leq i_d \leq n,\ \alpha_k \in [n]^{m-1},\ k = 1, \ldots, d\}.$$

Let $F = (i_1\alpha_1, \ldots, i_d\alpha_d) \in \mathcal{F}_d$, where $i_k\alpha_k = i_k j_1^{(k)} \cdots j_{m-1}^{(k)}$, $k = 1, 2, \ldots, d$. Let the set of arcs from i_k to $j_1^{(k)}, j_2^{(k)}, \ldots, j_{m-1}^{(k)}$ be

$$E(i_k\alpha_k) = \{(i_k, j_1^{(k)}), (i_k, j_2^{(k)}), \ldots, (i_k, j_{m-1}^{(k)})\}.$$

Let the arc multi-set

$$\widetilde{E}(F) = \bigcup_{k=1}^{d} E(i_k\alpha_k).$$

Let multi-digraph $D(F) = (V(\widetilde{E}(F)), \widetilde{E}(F))$. An *Eulerian tour* of the multi-digraph $D(F)$ is a closed walk that traverses each arc of $D(F)$ exactly once [28]. Let $\epsilon(F, j)$ be the set of all Eulerian tours starting and ending at the vertex j in

$D(F)$. For any arc (i, j) from i to j in $D(F)$, let $\omega(i, j)$ be multiplicity of arc (i, j). Let $\widehat{D}(F)$ be the digraph formed by removing duplicate arcs of $D(F)$. In this paper, an *Eulerian closed walk* of the multi-digraph $D(F)$ is a closed walk that uses each arc (i, j) of $\widehat{D}(F)$ exactly $\omega(i, j)$ times. Let $\mathbf{W}(F, j)$ be the set of all Eulerian closed walks of $D(F)$ starting and ending at the vertex j. The multi-digraph $D(F)$ is called *Eulerian* if $D(F)$ has Eulerian closed walks.

For $F = (i_1\alpha_1, \dots, i_d\alpha_d) \in \mathcal{F}_d$, let the differential operator $\partial(F) := \prod_{k=1}^{d} \frac{\partial}{\partial a_{i_k\alpha_k}}$.

Lemma 4.1. *Let $F \in \mathcal{F}_d$. Then*

$$\partial(F)(A^{d(m-1)})_{jj} = b(F)|\,\boldsymbol{W}(F, j)|,$$

where A is an auxiliary matrix of order n, and $b(F)$ is the product of the factorials of the multiplicities of all the arcs in $D(F)$.

Proof. For the matrix $A = (a_{ij})$, we have

$$\partial(F)(A^{d(m-1)})_{jj} = \sum_{l_2,\dots,l_{d(m-1)}=1}^{n} \partial(F)(a_{jl_2}a_{l_2l_3}\cdots a_{l_{d(m-1)}j}).$$

Since $a_{jl_2}a_{l_2l_3}\cdots a_{l_{d(m-1)}j}$ is a polynomial of degree $d(m-1)$, $\partial(F)(a_{jl_2}a_{l_2l_3}\cdots a_{l_{d(m-1)}j}) \neq 0$ if and only if $\partial(F)(a_{jl_2}a_{l_2l_3}\cdots a_{l_{d(m-1)}j}) = b(F)$. And in this case, the arc multi-set $\{(j, l_2), (l_2, l_3), \dots, (l_{d(m-1)}, j)\} = \widetilde{E}(F)$, that is there exists an Eulerian closed walk of $D(F)$ starting and ending at the vertex j. Hence,

$$\partial(F)(A^{d(m-1)})_{jj} = \sum_{l_2,\dots,l_{d(m-1)}=1}^{n} \partial(F)(a_{jl_2}a_{l_2l_3}\cdots a_{l_{d(m-1)}j}) = b(F)|\mathbf{W}(F, j)|.$$

$\square$

Let $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ be an m-uniform hypergraph with n vertices, where $V(\mathcal{H}) = \{1, \dots, n\}$. Let $\mathcal{F}_d(\mathcal{H}) = \{(i_1\alpha_1, \dots, i_d\alpha_d) \in \mathcal{F}_d | i_k\alpha_k \in E(\mathcal{H}), \alpha_k$ is ascending order, $k = 1, \dots, d\}$.

Let $\mathcal{F}_d^{(j)}(\mathcal{H}) = \{F \in \mathcal{F}_d(\mathcal{H}) | D(F)$ is Eulerian and contains the vertex $j\}$.

Theorem 4.2. *Let $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ be an m-uniform hypergraph with n vertices. Then*

$$C(j) = \sum_{d=0}^{\infty} \frac{\mu_d(j)}{d!},$$

where
$$\mu_d(j) = (m-1)^{n-1} \sum_{F \in \mathcal{F}_d^{(j)}(\mathcal{H})} \frac{b(F)}{c(F)} |\,\boldsymbol{W}(F,j)|,$$
$j \in V(\mathcal{H})$, $b(F)$ is the product of the factorials of the multiplicities of all the arcs in $D(F)$, $c(F)$ is the product of the factorials of the outdegrees of all the vertices in $D(F)$ and $\boldsymbol{W}(F,j)$ is the set of all Eulerian closed walks of $D(F)$ starting and ending at the vertex j.

Proof. Let $V(\mathcal{H}) = \{1, \ldots, n\}$, the adjacency tensor $\mathcal{A}_{\mathcal{H}} = (h_\alpha)$, $F = (i_1\alpha_1, \ldots, i_d\alpha_d) \in \mathcal{F}_d$ and $\pi_F(\mathcal{A}_{\mathcal{H}}) = \prod_{k=1}^{d} h_{i_k\alpha_k}$. Using Formula (2.9) in [21]
$$\sum_{d_1+\cdots+d_n=d} \prod_{i=1}^{n} \frac{1}{(d_i(m-1))!} \Big(\sum_{\alpha_i \in [n]^{m-1}} h_{i\alpha_i} \frac{\partial}{\partial a_{i\alpha_i}} \Big)^{d_i} = \sum_{F \in \mathcal{F}_d} \frac{1}{c(F)} \pi_F(\mathcal{A}_{\mathcal{H}}) \partial(F),$$
we get
$$\mu_d(j) = (m-1)^{n-1} \sum_{F \in \mathcal{F}_d} \frac{1}{c(F)} \pi_F(\mathcal{A}_{\mathcal{H}}) \partial(F) (A^{d(m-1)})_{jj}.$$
By Lemma 4.1, we have
$$\mu_d(j) = (m-1)^{n-1} \sum_{F \in \mathcal{F}_d} \frac{b(F)}{c(F)} \pi_F(\mathcal{A}_{\mathcal{H}}) |\mathbf{W}(F,j)|. \tag{4.1}$$

According to the definition of adjacency tensors, we have
$$\pi_F(\mathcal{A}_{\mathcal{H}}) = \prod_{k=1}^{d} h_{i_k\alpha_k} = \begin{cases} \frac{1}{((m-1)!)^d}, & \text{if } \ i_k\alpha_k \in E(\mathcal{H}), k = 1, \ldots, d, \\ 0, & \text{otherwise.} \end{cases}$$
Then the F in Equation (4.1) such that $\pi_F(\mathcal{A}_{\mathcal{H}}) \neq 0$ if and only if $i_k\alpha_k \in E(\mathcal{H})$, $k = 1, \ldots, d$. For $F = (i_1\alpha_1, \ldots, i_d\alpha_d) \in \mathcal{F}_d(\mathcal{H})$, α_k is ascending order, $k = 1, \ldots, d$. Thus, each $F \in \mathcal{F}_d(\mathcal{H})$ corresponds to $((m-1)!)^d$ elements in $\mathcal{F}_d$.

Hence,

$$\begin{aligned}
\mu_d(j) &= (m-1)^{n-1} \sum_{F\in\mathcal{F}_d(\mathcal{H})} ((m-1)!)^d \frac{b(F)}{c(F)} \frac{1}{((m-1)!)^d} |\mathbf{W}(F,j)| \\
&= (m-1)^{n-1} \sum_{F\in\mathcal{F}_d(\mathcal{H})} \frac{b(F)}{c(F)} |\mathbf{W}(F,j)| \\
&= (m-1)^{n-1} \sum_{F\in\mathcal{F}_d^{(j)}(\mathcal{H})} \frac{b(F)}{c(F)} |\mathbf{W}(F,j)|. \qquad (4.2)
\end{aligned}$$

Substituting Equation (4.2) into Equation (2.4), we obtain the expression of $C(j)$ by the number of Eulerian closed walks of the multi-digraphs associated with $\mathcal{H}$. $\square$

For a uniform hypergraph $\mathcal{H}$, the following is the expression of $C(j)$ by the number of arborescences of the multi-digraphs associated with $\mathcal{H}$.

Theorem 4.3. *Let $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ be an m-uniform hypergraph with n vertices. Then*

$$C(j) = \sum_{d=0}^{\infty} \frac{\mu_d(j)}{d!},$$

where

$$\mu_d(j) = (m-1)^{n-1} \sum_{F\in\mathcal{F}_d^{(j)}(\mathcal{H})} \frac{t(F)}{\prod_{v\in V(\widetilde{E}(F))/\{j\}} d^+(v)},$$

$j \in V(\mathcal{H})$, $d^+(v)$ is the outdegree of a vertex v in $D(F)$ and $t(F)$ is the number of arborescences of $D(F)$.

Proof. Let $V(\mathcal{H}) = \{1,\dots,n\}$ and $F \in \mathcal{F}_d^{(j)}(\mathcal{H})$. Since $F \in \mathcal{F}_d^{(j)}(\mathcal{H})$, $D(F)$ is Eulerian and contains the vertex j. In order to get the Theorem 4.3, we first give the representation of $|\mathbf{W}(F,j)|$. Let $\epsilon(F,e_1)$ be the set of all Eulerian tours starting with a fixed arc e_1 in $D(F)$. Farrell and Levine [28] proved

$$|\epsilon(F,e_1)| = \frac{\sum_{e\in\widetilde{E}(F)} |\epsilon(F,e)|}{\sum_{v\in V(\widetilde{E}(F))} d^+(v)}. \qquad (4.3)$$

By Equation (4.3), we have $|\epsilon(F,e_1)| = |\epsilon(F,e_2)|$, for all $e_1, e_2 \in \widetilde{E}(F)$. Thus,

$$|\epsilon(F,j)| = d^+(j)|\epsilon(F,e_1)|.$$

Let $\mathfrak{E}(F)$ be the set of all Euler circuits in $D(F)$. There are $|\widetilde{E}(F)||\mathfrak{E}(F)|$ Euler tours in $\widetilde{E}(F)$ [18]. Then $\sum_{e\in\widetilde{E}(F)}|\epsilon(F,e)| = |\widetilde{E}(F)||\mathfrak{E}(F)|$.

Thus,

$$|\mathbf{W}(F,j)| = \frac{|\epsilon(F,j)|}{b(F)} = \frac{d^+(j)\frac{|\widetilde{E}(F)||\mathfrak{E}(F)|}{\sum\limits_{v\in V(\widetilde{E}(F))} d^+(v)}}{b(F)} = \frac{d^+(j)|\mathfrak{E}(F)|}{b(F)},$$

where $b(F)$ is the product of the factorials of the multiplicities of all the arcs in $D(F)$.

Tutte et al.[29] and Aardenne-Ehrenfest et al.[30] proved the BEST Theorem

$$|\mathfrak{E}(F)| = t(F)\prod_{v\in V(\widetilde{E}(F))}(d^+(v)-1)!.$$

Then

$$|\mathbf{W}(F,j)| = \frac{d^+(j)t(F)\prod_{v\in V(\widetilde{E}(F))}(d^+(v)-1)!}{b(F)}. \tag{4.4}$$

By Theorem 4.2, Equation (4.4) and $c(F) = \prod_{v\in V(\widetilde{E}(F))} d^+(v)!$, we get

$$\begin{aligned}\mu_d(j) &= (m-1)^{n-1}\sum_{F\in\mathcal{F}_d^{(j)}(\mathcal{H})}\frac{b(F)d^+(j)t(F)\prod_{v\in V(\widetilde{E}(F))}(d^+(v)-1)!}{c(F)b(F)}\\ &= (m-1)^{n-1}\sum_{F\in\mathcal{F}_d^{(j)}(\mathcal{H})}\frac{t(F)}{\prod\limits_{v\in V(\widetilde{E}(F))/\{j\}} d^+(v)}. \qquad (4.5)\end{aligned}$$

Substituting Equation (4.5) into Equation (2.4), we obtain the expression of $C(j)$ by the number of arborescences of the multi-digraphs associated with $\mathcal{H}$. $\square$

Next, we give the following explicit formula of $\mu_d(j)$ ($d = 0,1,2,\ldots,m$) for m-uniform hypergraphs.

Theorem 4.4. *Let $\mathcal{H} = (V(\mathcal{H}), E(\mathcal{H}))$ be an m-uniform hypergraph with n vertices. Then*

$$\mu_d(j) = \begin{cases} m^{m-2}(m-1)^{n-m}d(j), & \text{if } d = m,\\ 0, & \text{if } d = 1,2,\ldots,m-1,\\ (m-1)^{n-1}, & \text{if } d = 0,\end{cases}$$

where $j \in V(\mathcal{H})$ and $d(j)$ is the degree of j in $\mathcal{H}$.

Proof. Let $V(\mathcal{H}) = \{1, \ldots, n\}$ and $E_j(\mathcal{H}) = \{e \in E(\mathcal{H}) | j \in e\}$. Since $\mathcal{F}_m^{(j)}(\mathcal{H}) = \{(i_1 i_2 \cdots i_m, i_2 i_1 i_3 i_4 \cdots i_m, \ldots, i_m i_1 i_2 \cdots i_{m-1}) | i_1 i_2 \cdots i_m \in E_j(\mathcal{H}), i_1 i_2 \cdots i_m$ is ascending order$\}$, we have $|\mathcal{F}_m^{(j)}(\mathcal{H})| = d(j)$.

For $F \in \mathcal{F}_m^{(j)}(\mathcal{H})$, $D(F)$ is a complete digraph with m vertices. We have $\prod_{v \in V(\widetilde{E}(F))/\{j\}} d^+(v) = (m-1)^{m-1}$. The number of arborescences of $D(F)$ is m^{m-2} (Cayley's formula [31]). By Theorem 4.3 and the above discussion, we get

$$\mu_m(j) = \frac{(m-1)^{n-1} d(j) m^{m-2}}{(m-1)^{m-1}} = m^{m-2}(m-1)^{n-m} d(j).$$

From Lemma 2.1 (2), we know $Tr_d(\mathcal{A}_{\mathcal{H}}) = 0$, $d = 1, 2, \ldots, m-1$, by Equation (2.3), we know $\sum_{j=1}^{n} \mu_d(j) = Tr_d(\mathcal{A}_{\mathcal{H}})$ and by Theorem 4.2, we get $\mu_d(j) \geq 0, d = 1, 2, \ldots, m-1$. Thus, we have

$$\mu_d(j) = 0, d = 1, 2, \ldots, m-1.$$

By Equation (2.2), we easily get $\mu_0(j) = (m-1)^{n-1}$. $\square$

For an m-uniform hypergraph $\mathcal{H}$ with n vertices and $m \geq 2$, the subgraph centrality $C(j) = \sum_{d=0}^{\infty} \frac{\mu_d(j)}{d!}$, by Theorem 4.4, we have $\sum_{d=0}^{m} \frac{\mu_d(j)}{d!} = (m-1)^{n-1} + \frac{m^{m-3}(m-1)^{n-m-1} d(j)}{(m-2)!}$, $j = 1, 2, \ldots, n$. The ranking from taking $\sum_{d=0}^{m} \frac{\mu_d(j)}{d!}$ as centrality is the same as degree centrality for the m-uniform hypergraph.

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