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Efficient computation of Ihara coefficients using the Bell polynomial recursion

Samuel Rota Bulò [a,*], Edwin R. Hancock [b], Furqan Aziz [b], Marcello Pelillo [a]

[a] Dipartimento di Scienze Ambientali, Informatica e Statistica, Università Ca' Foscari Venezia, via Torino 155, 30172 Mestre, Venezia, Italy
[b] Department of Computer Science, The University of York, York YO10 5DD, UK

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ABSTRACT

The Ihara zeta function has proved to be a powerful tool in the analysis of graph structures. It is determined by the prime cycles of a finite graph $G = (V, E)$ and can be characterized in terms of a quasi characteristic polynomial of the adjacency matrix T of the oriented line graph associated to G. The coefficients of this polynomial, referred to as Ihara coefficients, have been used to characterize graphs in a permutation-invariant manner, and allow for an efficient evaluation of the Ihara zeta function. In this paper we present a novel method for computing the Ihara coefficients. We first establish a characterization of the Ihara coefficients in terms of complete Bell polynomials and, by exploiting a recursive relation for the latter, we show how the Ihara coefficients can be efficiently computed in $O(|E|^2)$, provided that the eigenvalues of T are known.

1. Introduction

The Ihara zeta function is defined on a finite graph, and is closely akin to the Selberg zeta function [12]. Originally introduced by Ihara [5,6], it has attracted sustained interest in the graph theory literature. For instance, Hashimoto [4] has deduced explicit factorizations for the Ihara zeta function on bi-regular bipartite graphs. Bass [1] has generalized Hashimoto's factorization to all finite graphs. Recently, Stark and Terras [13–15] have published a series of articles on the topic. Commencing from an up-to-date survey of the Ihara zeta function and its properties, they generalize the Ihara zeta function

* Corresponding author.
E-mail addresses: srotabul@dsi.unive.it (S. Rota Bulò), erh@cs.york.ac.uk (E.R. Hancock), furqan@cs.york.ac.uk (F. Aziz) pelillo@dsi.unive.it (M. Pelillo).

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to develop edge and path based variants. Recently, Storm has further developed and refined the Ihara zeta function for hypergraphs [16].

The Ihara zeta function is determined by the prime cycles of a graph G, and can be used to link the number of closed paths to the spectrum of the adjacency matrix. It can be expressed in terms of a quasi characteristic polynomial of the adjacency matrix T of the oriented line graph $\vec{L}(G)$ associated to G. The coefficients of this polynomial, referred to as Ihara coefficients, are related to the frequencies of prime cycles of different lengths in the graph. They can be computed from symmetric polynomials of the eigenvalues of T.

The Ihara zeta function has recently attracted attention in the pattern analysis and machine learning literature. For instance, Zhao and Tang [18] have used Savchenko's formulation of the zeta function [11], expressed in terms of cycles, to generate merge weights for clustering over a graph-based representation of pairwise similarity data. Their formulation is based on a representation of oriented line graphs, which is an intermediate step in the development of the Ihara zeta function. Watanabe and Fukumizu [17] have presented an approach to the analysis of Loopy Belief Propagation (LBP) by establishing a formula that connects the Hessian of the Bethe free energy with the edge Ihara zeta function. Peng, Wilson and Hancock have investigated the use of the Ihara zeta function for clustering weighted and unweighted graphs [10] and have then extended this work to hypergraphs [9]. In more recent work [8], Peng, Aleksic, Wilson and Hancock demonstrate a relationship between the Ihara zeta function and discrete-time quantum walks on graphs.

Unfortunately, despite its attractions as a compact representation of graph structure, applications of the Ihara zeta function have been limited due to the computational overheads required to calculate it. For the graph $G = (V, E)$, with node-set V and edge-set E, the adjacency matrix T of the oriented line graph $\vec{L}(G)$ of G is of size $|E|^2$. For graphs of large edge density, this makes computing the spectrum of T and hence the Ihara zeta function or its polynomial coefficients burdensome.

The aim in this paper is to address this issue by developing an efficient recursive scheme for evaluating the Ihara coefficients. Our approach is as follows. We commence by expressing the Ihara zeta function as the exponential of a series in traces of powers of the adjacency matrix T of $\vec{L}(G)$. We show how this exponential can be expressed as a power series whose coefficients are Bell polynomials. By exploiting a recursive formula for the Bell polynomials [2,3], which is proven here for completeness, we show how to recursively compute the Ihara coefficients in $O(|E|^2)$, provided that the eigenvalues of T are known.

2. Ihara zeta function

Before introducing the Ihara zeta function we provide some basic definitions and notations. Let $G = (V, E)$ be a finite, connected graph, where V is the set of vertices and $E \subseteq V \times V$ is the set of oriented edges. Throughout we assume that each vertex has degree larger than 1, *i.e.* $|\{(u, v) \in E : v \in V\}| > 1$ for all $u \in V$. A *cycle* of G of length m is a closed path of m vertices, *i.e.* a $(m + 1)$-tuple $(v_0, \dots, v_m) \in V^{m+1}$ such that $v_0 = v_m$, and $(v_i, v_{i+1}) \in E$ for all $0 \leqslant i < m$. The *length* of a cycle C is denoted by $l(C)$. Two cycles $C_1 = (w_0, \dots w_m)$ and $C_2 = (v_0, \dots, v_m)$ are equivalent if there exists $0 \leqslant k < m$ such that $w_i = v_{i+k}$ for all $0 \leqslant i < m$ with subscripts modulo m. This equivalence relation identifies an equivalence class $[C]$ for all cycles C of G. Let C^r be the cycle obtained by moving r times through the cycle C. A cycle $(v_0, \dots, v_m)$ is called *backtrackless* if $v_{i-1} \neq v_{i+1}$ for all $0 < i < m$. A cycle $C = (v_0, \dots, v_m)$ is called *prime* if C and C^2 are backtrackless and $C \neq B^r$ for any other cycle B and $r > 1$. The *oriented line graph* of a graph $G = (V, E)$, denoted by $\vec{L}(G)$, is a graph (V_L, E_L) with vertex set $V_L = E$ and edge set

$$E_L = \{((u, v), (v, w)) \in E \times E : u \neq w\} .$$

The *Ihara zeta function* associated with graph G is a function of the complex variable $u \in \mathbb{C}$ defined as

$$\zeta_G(u) = \prod_{[C]} \left(1 - u^{l(C)}\right)^{-1}, \tag{1}$$

where $[C]$ runs over the set of all equivalence classes of prime cycles of G.

As shown in (1), the Ihara zeta function is generally an infinite product. However, $\zeta_G(u)^{-1}$ can be written in the form of a determinant [7], and can therefore be expressed as a polynomial:

$$\zeta_G^{-1}(u) = \det(I - uT) = \sum_{n=0}^{|E|} c_n u^n, \tag{2}$$

where $|E|$ denotes the cardinality of E, *i.e.* the number of (directed) edges of G, I is the $|E| \times |E|$ identity matrix, and T is the adjacency matrix of the oriented line graph $\vec{L}(G)$ of G.

Note that the coefficients c_n of the Ihara zeta function, referred to as *Ihara coefficients*, can be derived from (2) in terms of derivatives of $\zeta_G^{-1}(u)$ evaluated at $u = 0$ as follows:

$$c_n = \frac{1}{n!} \frac{d^n}{du^n} \zeta_G^{-1}(0). \tag{3}$$

Additionally, the Ihara zeta function can be written in terms of a power series of the variable u [7]:

$$\zeta_G(u) = \exp\left(\sum_{n=1}^{\infty} \frac{\mathrm{Tr}\,(T^n)}{n} u^n\right), \tag{4}$$

where $\mathrm{Tr}\,(\cdot)$ is the matrix trace operator.

3. Ihara coefficients and Bell polynomials

In this section, we provide a characterization of the Ihara coefficients in terms of the complete Bell polynomials.

We distinguish between partial and complete Bell polynomials. The *partial Bell polynomials* are a triangular array of polynomials given for $1 \leqslant k \leqslant n$ by

$$B_{n,k}(x_1, \ldots, x_{n-k+1}) = \sum \frac{n!}{\prod_{\ell=1}^{n-k+1} j_\ell!} \prod_{\ell=1}^{n-k+1} \left(\frac{x_\ell}{\ell!}\right)^{j_\ell},$$

where the sum extends over all sequences $j_1, j_2, \ldots, j_{n-k+1}$ of non-negative integers such that

$$\sum_{\ell=1}^{n-k+1} j_\ell = k \quad \text{and} \quad \sum_{\ell=1}^{n-k+1} j_\ell\, \ell = n.$$

The sum of the partial Bell polynomials $B_{n,k}(x_1, \ldots, x_{n-k+1})$ over all values of k gives the *complete Bell polynomials* $B_n(x_1, \ldots, x_n)$, *i.e.*

$$B_n(x_1, \ldots, x_n) = \sum_{k=1}^{n} B_{n,k}(x_1, \ldots, x_{n-k+1}).$$

The complete Bell polynomials $B_n(x_1, \ldots, x_n)$ have the following generating function:

$$\exp\left(\sum_{n=1}^{\infty} \frac{x_n}{n!} u^n\right) = \sum_{n=0}^{\infty} \frac{1}{n!} B_n(x_1, \ldots, x_n) u^n \tag{5}$$

and, additionally, it can be shown that they satisfy the following identity:

$$B_n(x_1, \ldots, x_n) = \det \begin{bmatrix} x_1 & \binom{n-1}{1}x_2 & \binom{n-1}{2}x_3 & \binom{n-1}{3}x_4 & \ldots & x_n \\ -1 & x_1 & \binom{n-2}{1}x_2 & \binom{n-2}{2}x_3 & \ldots & x_{n-1} \\ 0 & -1 & x_1 & \binom{n-3}{1}x_2 & \ldots & x_{n-2} \\ 0 & 0 & -1 & x_1 & \ldots & x_{n-3} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & -1 & x_1 \end{bmatrix}. \tag{6}$$

The following lemma provides a characterization of the Ihara coefficients in terms of the complete Bell polynomials.

Lemma 1. *Let G be a graph, T be the adjacency matrix of $\vec{L}(G)$ and let c_n denote the nth Ihara coefficient related to G. The following identity holds:*

$$c_n = \frac{B_n(\alpha_1, \ldots, \alpha_n)}{n!},$$

where $\alpha_\ell = -(\ell-1)!Tr\left(T^\ell\right)$.

Proof. By (4) and (5) we have

$$\zeta_G^{-1}(u) = \exp\left(-\sum_{n=1}^{\infty} \frac{\mathrm{Tr}\,(T^n)}{n} u^n\right) = \exp\left(\sum_{n=1}^{\infty} \frac{\alpha_n}{n!} u^n\right) = \sum_{n=0} \frac{1}{n!} B_n(\alpha_1, \ldots, \alpha_n) u^n.$$

Finally, the result derives from (3), by noting that $\frac{d^n}{du^n}\zeta_G^{-1}(0) = B_n(\alpha_1, \ldots, \alpha_n)$. $\square$

This result justifies a possible method for computing the Ihara coefficients, which makes use of (6). Indeed, one could compute a Ihara coefficient by calculating the determinant of a matrix, which has in general complexity $O(|E|^3)$.

4. A recursive formula for the complete Bell polynomials

We introduce here a recursive formula that can be used for the computation of the Bell polynomials. This result will then play a fundamental role in Section 5, where we propose our efficient method for computing the Ihara coefficients.

Although the recursive relation for the Bell polynomials is already known (see, *e.g.* [2,3]), we provide here a self-contained proof for completeness. To this end, we prove the following lemma first, which can be considered as a special instance of the general Leibniz rule for the *n*th derivative of the product of functions.

Lemma 2. *Let* $g(u) = \exp(f(u))$. *Then for all* $n \geqslant 1$,

$$g^{(n)}(u) = \sum_{\ell=0}^{n-1} \binom{n-1}{\ell} f^{(n-\ell)}(u) g^{(\ell)}(u),$$

where $f^{(n)}(u)$ and $g^{(n)}(u)$ denote the nth-order derivatives of f and g, respectively.

Proof. We proceed by induction. For $n = 1$ we can easily see that

$$g^{(1)}(u) = \frac{d}{du}\left[\exp(f(u))\right] = f^{(1)}\exp(f(u)) = f^{(1)}(u)g(u).$$

For the general case n we have

$$\begin{aligned} g^{(n)}(u) &= \frac{d}{du}g^{(n-1)}(u) \\ &= \left[\sum_{\ell=0}^{n-2}\binom{n-2}{\ell}f^{(n-\ell)}(u)g^{(\ell)}(u)\right] + \left[\sum_{\ell=0}^{n-2}\binom{n-2}{\ell}f^{(n-1-\ell)}(u)g^{(\ell+1)}(u)\right], \end{aligned}$$

where we used the inductive hypothesis for $g^{(n-1)}(u)$. By taking the term $\ell = 0$ out of the first summation and the term $\ell = n-2$ out of the second one, we obtain after simple algebra:

$$\begin{aligned} g^{(n)}(u) &= f^{(n)}(u)g(u) + f^{(1)}(u)g^{(n-1)}(u) + \sum_{\ell=0}^{n-3}\binom{n-2}{\ell+1}f^{(n-1-\ell)}(u)g^{(\ell+1)}(u) \\ &\quad + \binom{n-2}{\ell}f^{(n-1-\ell)}(u)g^{(\ell+1)}(u) \\ &= f^{(n)}(u)g(u) + f^{(1)}(u)g^{(n-1)}(u) + \sum_{\ell=0}^{n-3}\binom{n-1}{\ell+1}f^{(n-1-\ell)}(u)g^{(\ell+1)}(u) \\ &= \sum_{\ell=0}^{n-1}\binom{n-1}{\ell}f^{(n-\ell)}(u)g^{(\ell)}(u). \quad \square \end{aligned}$$

Theorem 1. *The complete Bell polynomials can be expressed using the following recursive formula:*

$$B_n(x_1, \ldots, x_n) = \begin{cases} \sum_{\ell=0}^{n-1}\binom{n-1}{\ell}x_{n-\ell}B_\ell(x_1, \ldots, x_\ell) & \text{if } n > 0 \\ 1 & \text{otherwise.} \end{cases}$$

Proof. Let $f(u) = \sum_{n=1}^{\infty}\frac{x_n}{n!}u^n$. Then it easy to see that $f^{(n)}(0) = x_n$. Similarly, let $g(u) = \sum_{n=0}^{\infty}\frac{1}{n!}B_n(x_1, \ldots, x_n)u^n$. Then $g^{(n)}(0) = B_n(x_1, \ldots, x_n)$. By (5) and by Lemma 2 the result derives. $\square$

5. Efficient computation of Ihara coefficients

The recursive formula for the computation of the Bell polynomials introduced in Theorem 1, combined with the fact that the Ihara coefficients can be expressed in terms of the Bell polynomials, leads to a novel, easy and efficient way of computing the Ihara coefficients.

Theorem 2. *Let G be a graph and T be the adjacency matrix of $\vec{L}(G)$. The Ihara coefficients related to G can be computed through the following recursive formula:*

$$c_n = \begin{cases} -\frac{1}{n}\sum_{\ell=0}^{n-1} Tr\left(T^{n-\ell}\right)c_\ell & \text{if } n > 1 \\ 1 & \text{otherwise.} \end{cases}$$

Proof. By Theorem 1 and Lemma 1 we have that

$$c_n = \frac{1}{n!}\sum_{\ell=0}^{n-1}\binom{n-1}{\ell}\alpha_{n-\ell}\ell! c_\ell = \sum_{\ell=0}^{n-1}\frac{\alpha_{n-\ell}}{n(n-1-\ell)!}c_\ell = -\frac{1}{n}\sum_{\ell=0}^{n-1}\mathrm{Tr}\left(T^{n-\ell}\right)c_\ell. \quad \square$$

Note that $\mathrm{Tr}\,(T^n)$ can be computed efficiently in terms of the eigenvalues $\lambda_1, \ldots, \lambda_{|E|}$ of matrix T, since $\mathrm{Tr}\,(T^n) = \sum_{i=1}^{|E|}\lambda_i^n$. Assuming the eigenvalues of T known, we can compute by means of Theorem 2 the Ihara coefficients incrementally starting from $n = 1$ by exploiting for each new coefficient the previously computed ones. By so doing, the complexity of the computation of all the Ihara coefficients is $O(|E|^2)$. It is worth noting that this complexity becomes $O(|E|^3)$ if the spectrum of T is not available, since a preliminary eigenvalue decomposition of T is required in order to compute the terms $\mathrm{Tr}\,(T^n)$.

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