On Clique Incidence Matrices and Derivatives of Clique Polynomials

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Abstract

The ordinary generating function of the number of complete subgraphs (cliques) of \( G \), denoted by \( C(G, x) \), is called the clique polynomial of the graph \( G \). In this paper, we first introduce some clique incidence matrices associated by a simple graph \( G \) as a generalization of the classical vertex-edge incidence matrix of \( G \). Then, using these clique incidence matrices, we obtain two clique-counting identities that can be used for deriving two combinatorial formulas for the first and the second derivatives of clique polynomials. Finally, we conclude the paper with several open questions and conjectures about possible extensions of our main results for higher derivatives of clique polynomials.

1 Introduction

The reconstruction problems in discrete setting can be considered as a theoretical foundation for many inverse problems in the area of computer science and information technology. In graph-theoretical setting, the well-know Kelly-Ulam [1] reconstruction conjecture simply states that any graph with
at least three vertices can be reconstructed from its vertex-deck. We recall that a vertex deck of a given graph $G$ is the collection of (not necessarily distinct) vertex-deleted subgraphs; that is $\{G - v\}_{v \in V(G)}$. We will denote this collection by $\text{deck}_v(G)$. It seems that finding the general solution for this longstanding open problem is a quite challenging problem.

In another direction, one can try to reconstruct the key invariants of a given graph rather than reconstructing the graph itself. It seems that the collection of complete subgraphs (that we call them cliques), plays an essential role in reconstructing key invariants of graphs. In this respect, one of our main goal in this paper is to obtain some interesting clique-counting identities. A common approach to tackle these kind of problems is to use the two ideas of incidence matrices and the double-counting method. In the classical literature of graph theory, the classical vertex-edge incidence matrix has been already introduced. A generalization of this idea has been also introduced in the context of graph homology [7] under the name of boundary maps of simplicial complexes as higher-dimensional generalizations of graphs. Indeed, one can construct edge-triangle incidence matrix and their higher-order cliques generalizations simply by defining a $(0,1)$-matrix where non-zero entries shows that a lower-dimensional clique (here we call it the subclique) contained in is a subgraph of a higher-dimensional one (here we call it the superclique).

In this paper, based on the motivation originating form the reconstruction problem, we construct other kinds of incidence matrices which we call them the clique incidence matrices. Using this idea, we obtain two important
clique-counting identities that relates the number of $k$-cliques ($k = 1, 2$) in
the graph $G$ itself to the number of $k$-cliques in the clique-deck of $G$. Then, we
establish two combinatorial formulas for the first and the second derivatives
of clique polynomials. A formula very similar to that of our first derivative
has been already mentioned in the literature [3], but our formula for the sec-
ond derivative of clique polynomials, to the best of our knowledge, is a new
combinatorial formula. Indeed, there is no formula in the literature for the
second or higher derivatives of many graph polynomials. For this reason, we
also include a discussion about possible future directions in this fascinating
area of clique-counting graph polynomials.

2 The Generalized Incidence Matrices

All graphs here are finite, simple and undirected. For the terminologies not
defined here, one can consult the reference [2].

For a given graph $G = (V, E)$ and a vertex $v \in V(G)$, it’s vertex-deleted
subgraph denoted by $G - v$ is defined as an induced subgraph obtained from
$G$ by deleting the vertex $v$. The collection of all vertex-deleted subgraphs of
$G$ is called a vertex-deck of $G$ and denoted by $\text{deck}_v(G)$. One can similarly
define the edge-deleted subgraph of $G$ which we denote it by $G - e$. The collection of all edge-deleted subgraphs of $G$ is called an edge-deck of $G$ and is
denoted by $\text{deck}_e(G)$. The open neighborhood of the vertex $v$ in $G$ is the set
of vertices adjacent to $v$ and is denoted by $N_G(v)$. A $k$-clique of a graph $G$
is denoted by $Q_k$ is defined as a complete subgraph $G$ on $k$ vertices. The set
$\Delta_k(G)$ denotes the set of all $k$-cliques of $G$. We will also denote the number
of $k$-cliques of $G$ by $c_k(G)$. In general, for any clique $Q_k \in \Delta_k(G)$, we define the *clique-deck* of $G$ as the collection of all *clique-deleted* subgraphs of $G$.

A generalization of the concept of the *degree* of a vertex $v \in V(G)$ is called the *clique-value* which can be defined, as follows.

**Definition 2.1.** Let $G = (V, E)$ be a graph and let $Q_k$ be a $k$-clique of $G$. Then, we define the clique-value denoted by $\text{val}_G(Q_k)$, as follows

$$\text{val}_G(Q_k) = \bigcap_{v \in V(Q_k)} N_G(v). \quad (1)$$

As a generalization of standard vertex-edge incidence matrix, we define our first clique incidence matrix that we call it the *subclique-superclique incidence matrix* $I_{c,k}(G)$, as follows. From now on, we will assume $\Delta_k(G) = \{Q_{k,1}, Q_{k,2}, \ldots, Q_{k,r}\}$ in which $r = c_k(G)$.

**Definition 2.2.** For a given graph $G = (V, E)$, we define the subclique-superclique incidence matrix of order $k$ denoted by $I_{c,k}(G)$, as follows

$$(I_{c,k}(G))_{Q_k,i, Q_{k+1,j}} = \begin{cases} 1 & \text{if } Q_{k,i} \text{ is a subgraph of } Q_{k+1,j}, \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

It is clear that the subclique-superclique matrix of order 1 is exactly the classic vertex-edge incidence matrix $I(G)$ of a graph $G$.

**Lemma 2.1.** Let $G = (V, E)$ be a graph. Then, we have

$$\sum_{Q_k \in \Delta_k(G)} \text{val}_G(Q_k) = (k + 1)c_{k+1}(G). \quad (3)$$
Proof. We first note that the number of \( k \)-cliques of any \((k+1)\)-clique \( Q_{k+1,j} \) is equal to \( k + 1 \). We also note that the number of times that any given \( k \)-clique \( Q_k \) appears as a subset of another \((k + 1)\)-clique is equal to \( \text{val}_G(Q_k) \). Now, considering the definition of subclique-superclique incidence matrix \( I_{c,k}(G) \) and the double-counting technique, we get the desired result.

\[
\]

We also need to recall the definition and basic properties of clique polynomials \[6\].

The clique polynomial of a given graph \( G = (V, E) \) is defined as the ordinary generating function of the number \( k \)-cliques of \( G \). More precisely, we have

\[
C(G, x) = 1 + \sum_{k=1}^{\omega(G)} c_k(G)x^k, \tag{4}
\]

where \( \omega(G) \) is the size of the largest clique in \( G \).

One can easily prove that the polynomial \( C(G, x) \) satisfies the following vertex-recurrence relation.

\[
C(G, x) = C(G - v, x) + xC(G[N_G(v)], x), \quad (v \in V(G)). \tag{5}
\]

Similarly, we can prove the following edge-recurrence relation for clique polynomials.

\[
C(G, x) = C(G - e, x) + x^2C(G[N_G(e)], x), \quad (e = \{u, v\} \in E(G)), \tag{6}
\]

where by \( N_G(e) \), we mean the subgraph of \( G \) induced by the common neighbors of the end vertices of \( e \). In other words, we have \( N_G(e) = N_G(u) \cap N_G(v) \)
3 Main Results

In this section, we first obtain two interesting clique-counting identities related to the vertex-deck and the edge-deck of $G$.

We start with the following identity closely related to the vertex-deck of $G$.

**Lemma 3.1.** Let $G = (V, E)$ be a graph on $n$ vertices. Then, we have

\[(n - k)c_k(G) = \sum_{v \in V(G)} c_k(G - v) \quad (k \geq 1).\]  

(7)

**Proof.** Put $r = c_k(G)$. Let $\Delta_k(G) = \{Q_{k,1}, Q_{k,2}, \ldots, Q_{k,r}\}$ be the set of all $k$-cliques of $G$. Now, we consider our second clique incidence matrix $I_{H,k}(G)$ which is defined, as follows

\[
(I_{k,r}(G))_{Q_{k,i}, H - v_j} = \begin{cases} 
1 & \text{if } Q_{k,i} \text{ is a subgraph of } H - v_j , \\
0 & \text{otherwise}. 
\end{cases}
\]  

(8)

Now, it is obvious that the sum of rows is equal to $(n - k)c_k(G)$ and the sum of columns equals to $\sum_{v \in V(G)} c_k(G - v)$ . Hence, the proof is complete based on the double-counting method.

\[\square\]

In a similar way, one can prove the following clique-counting identity in close connection with edge-deck of a graph.

**Lemma 3.2.** Let $G = (V, E)$ be a graph on $n$ vertices and $m$ edges. Then, we have
\[(m - \binom{k}{2})c_k(G) = \sum_{e \in E(G)} c_k(G - e), \quad (k \geq 2). \quad (9)\]

The following graph-theoretical interpretation of the first derivative of clique polynomials is similar to that of [3]. Here, we also include the proof which is based on Lemma [3.1].

**Theorem 3.3.** Let \( G = (V, E) \) be a graph. Then, we have

\[
\frac{d}{dx}C(G, x) = \sum_{v \in V(G)} C(G[N(v)], x). \quad (10)
\]

**Proof.** By multiplying both sides of formula (5) by \( x^i \) and then summing over all \( i \ (i \geq 0) \), we get

\[
\sum_{i \geq 0} (n - i)c_i(G)x^i = \sum_{i \geq 0} \sum_{v \in V(G)} c_i(G - v)x^i,
\]

or equivalently, by interchanging the summation order, we have

\[
(n \sum_{i \geq 0} c_i(G)x^i - x \sum_{i \geq 1} ic_i(G)x^{i-1} = \sum_{v \in V(G)} \left( \sum_{i \geq 0} c_i(G - v)x^i \right). \quad (11)
\]

On the other hand, by the definition of a clique polynomial of a graph, it’s first derivative is equal to

\[
\frac{d}{dx}C(G, x) = \sum_{i \geq 1} ic_i(G)x^{i-1}. \quad (12)
\]

Hence, considering relation (12) and the definition of a clique polynomial, we can rewrite equation (11) as follows

\[
n.C(G, x) - x \frac{d}{dx}C(G, x) = \sum_{v \in V(G)} C(G - v, x),
\]
or equivalently,

\[ \frac{d}{dx} C(G, x) = \sum_{v \in V(G)} \frac{C(G, x) - C(G - v, x)}{x}. \]  \tag{13} 

Thus, considering relations (13) and (5) we finally get the desired result.

Next, we give the graph-theoretical interpretation of the second derivative of the clique polynomials which is a new combinatorial formula to the best of our knowledge.

**Theorem 3.4.** For any simple graph \( G = (V, E) \), we have

\[ \frac{1}{2!} \frac{d^2}{dx^2} C(G, x) = \sum_{e \in E(G)} C(G[N(e)], x). \]  \tag{14} 

**Proof.** We first multiplying both sides of formula (6) by \( x^i \) and then summing over all \( i \) \((i \geq 0)\), we get

\[ \sum_{i \geq 0} \left( m - \binom{i}{2} \right) c_i(G)x^i = \sum_{i \geq 0} \sum_{e \in E(G)} c_i(G - e)x^i, \]

or equivalently, by interchanging the summation order, we obtain

\[ m \sum_{i \geq 0} c_i(G)x^i - x^2 \sum_{i \geq 2} \binom{i}{2} c_i(G)x^{i-2} = \sum_{e \in E(G)} \left( \sum_{i \geq 0} c_i(G - e)x^i \right). \]  \tag{15} 

Next, by the definition of a clique polynomial of a graph, it’s second derivative is equal to

\[ \frac{1}{2!} \frac{d^2}{dx^2} C(G, x) = \sum_{i \geq 2} \binom{i}{2} c_i(G)x^{i-2}. \]  \tag{16}
Therefore, considering relation (16) and the definition of a clique polynomial, we can rewrite equation (15) as follows

\[ m.C(G, x) - x^2 \left( \frac{1}{2!} \frac{d^2}{dx^2} C(G, x) \right) = \sum_{e \in E(G)} C(G - e, x). \]

or equivalently,

\[ \frac{1}{2!} \frac{d^2}{dx^2} C(G, x) = \sum_{e \in E(G)} \frac{C(G, x) - C(G - e, x)}{x^2}. \]  

(17)

Finally, the relations (17) and (6) imply the desired result. □

4 Triangle-deck Identity and Third Derivative

In this section, we are going to develop a graph-theoretical interpretation of the third derivative of a clique polynomial.

The following key lemma from [4,5] is essential in our future arguments. We recall that by \( G - M \), where \( M \) is the set of edges of \( G \), we mean a graph obtained from \( G \) by deleting only edges of \( M \) from \( G \).

Lemma 4.1. Let \( G = (V, E) \) be a simple graph and the set of edges \( M \) induces a clique in \( G \), then we have

\[ C(G, x) = C(G - M, x) + \sum_{r=2}^{\lfloor |M| / 2 \rfloor} (-1)^r (r-1) x^r \sum_{S \subseteq M \ | S | = \frac{|M|}{2}} C(G[N_G(S)], x). \]  

(18)

We are mainly interested the particular case where \( M \) induces a triangle \( \delta \).
Theorem 4.2. For any simple graph \( G = (V, E) \) and a triangle \( \delta = \{e_1, e_2, e_3\} \in \Delta_3(G) \), we have

\[
C(G, x) = C(G - \delta, x) + I_2(G, x)x^2 - 2I_3(G, x)x^3,
\]

in which

\[
I_2(G, x) = \sum_{i=1}^{3} C(G[N_G(e_i)]), \quad I_3(G, x) = C(G[N_G(\delta)], x).
\]

One of the interesting question that naturally arise is that of triangle-recurrence for clique polynomials. In other words, we are searching for the class of graphs for which the following triangle-recurrence relation holds.

\[
C(G, x) = C(G - \delta, x) + x^3C(G[N_G(\delta)], x).
\]

Note that the above condition is equivalent to the following clique-counting identity

\[
\sum_{i=1}^{3} C(G[N_G(e_i)]) = 3xC(G[N_G(\delta)], x)
\]

In the case of having symmetric property for the edge-neighborhoods; that is \( G[N_G(e_i)] \ (i = 1, 2, 3) \) are the same, the above condition reduced to the following simple one.

\[
C(G[N_G(e)]) = xC(G[N_G(\delta)], x).
\]

Next, we prove the following theorem.

Theorem 4.3. Let \( G = (V, E) \) be a connected \( K_5 \)-free graph. Then, we have
\[
\frac{1}{3!} \frac{d^3}{dx^3} C(G, x) = \sum_{\delta \in \Delta_3(G)} C(G[N_G(\delta)], x). \tag{24}
\]

**Proof.** We first define
\[
Diff(G, x) = C(G, x) - C(G - \delta, x). \tag{25}
\]
Now, considering the identity (19), we equivalently have
\[
C(G[N_G(\delta)], x) = \frac{I_2(G, x)x^2 - Diff(G, x)}{2x^3}. \tag{26}
\]
Our ultimate goal is to prove that
\[
\sum_{\delta \in \Delta_3(G)} C(G[N_G(\delta)], x) = \frac{1}{3!} \frac{d^3}{dx^3} C(G, x). \tag{27}
\]
Next, we note that since \( G \) is a connected \( K_5 \)-free graph, then we conclude that
\[
C(G, x) = 1 + c_1(G)x + c_2(G)x^2 + c_3(G)x^3 + c_4(G)x^4. \tag{28}
\]
Based on the proof of (1), one can also show that
\[
C(G - \delta, x) = 1 + c_1(G - \delta)x + c_2(G - \delta)x^2 + c_3(G - \delta)x^3 + c_4(G - \delta)x^4, \tag{29}
\]
in which
\[
c_1(G - \delta) = c_1(G),
c_2(G - \delta) = c_2(G) - 3,
c_3(G - \delta) = c_3(G) - \sum_{i=1}^{3} val_G(e_i) + 2,
c_4(G - \delta) = c_4(G) - \sum_{i=1}^{3} c_2(G[N_G(e_i)]) + 2val_G(\Delta). \tag{30}
\]
By considering above formulas, we obtain

\[
\text{Diff}(G, x) = 3x^2 + (c_3(G) - \sum_{i=1}^{3} \text{val}_G(e_i) - 2)x^3
\]

\[
+ \left( \sum_{i=1}^{3} c_2(G[N_G(e_i)]) - 2\text{val}_G(\Delta) \right)x^4,
\]

(31)

and

\[
N_2(G, x) = (1 + \text{val}_G(e_1)x + c_2(G[N_G(e_1)])x^2)
\]

\[
+ (1 + \text{val}_G(e_2)x + c_2(G[N_G(e_2)])x^2)
\]

\[
+ (1 + \text{val}_G(e_3)x + c_2(G[N_G(e_3)])x^2).
\]

Finally, from (2) and (3), we get

\[
C(G[N_G(\Delta)], x) = \frac{2x^3 + 2\text{val}_G(\Delta)x^4}{2x^3} = 1 + \text{val}_G(\Delta)x.
\]

(32)

Thus, considering (4) and clique handshaking lemma for \(\omega(G) = 4\), we get

\[
\sum_{\delta \in \Delta_3(G)} C(G[N_G(\Delta)], x) = |\Delta_3(G)| + 4c_4(G)x
\]

\[
= c_3(G) + 4c_4(G)
\]

\[
= \frac{1}{3!} \frac{d^3}{dx^3} C(G, x),
\]

(33)

which is the desired result.

\[\square\]

5 Open Questions and Conjectures

Here, we propose several interesting open questions and conjectures regarding subgraph-counting polynomials. The first open question is related to another
similar clique-counting polynomial \[3\], as follows.

**Open question 1.** Let \( c(G, x) \) be a clique-counting polynomial defined by

\[
c(G, x) = 1 + \sum_{k=1}^{n} c_k(G)x^{n-k}. \tag{34}
\]

Can we find the similar formulas for the first and second derivatives of \( c(G, x) \)?

**Conjecture 1.** Let \( G = (V, E) \) be a simple graph. Then, we have

\[
\frac{d}{dx} c(G, x) = \sum_{v \in V(G)} c(G - v, x). \tag{35}
\]

Moreover, we also have

\[
\frac{1}{2!} \frac{d^2}{dx^2} c(G, x) = \sum_{e \in E(G)} c(G - e, x). \tag{36}
\]

**Open question 2.**

Do we have a *triangle-version* of Lemma \[3.2\]? In other words, is the following identity true in general?

Let \( G = (V, E) \) be a graph on \( m \) edges and \( H \) be any graph with \( k \) vertices without isolated vertices such that \( |V(H)| \leq |V(G)| \), \( |E(H)| \leq |E(G)| \) and \( |\Delta_3(H)| < |\Delta_3(G)| \). Then, we have

\[
\left( t - \binom{k}{3} \right) c_k(G) = \sum_{\delta \in \Delta_3(G)} c_k(G - \delta) \quad (k \geq 3), \tag{37}
\]

where \( t \) denotes the number of triangles in \( G \).

It is not worthy that when you delete a vertex or an edge it has no effects in
other cliques.

**Definition 5.1.** For a given graph $G = (V, E)$, its triangle graph denoted by $T(G)$ is the graph whose vertex set is the set of triangles of $G$ and two vertices of $T(G)$ are connected if their corresponding triangles share an edge.

**Conjecture 2.**

For a given graph $G$ such that its triangle graph $T(G)$ is an empty graph, then the *triangle-version* of Lemma 3.2 holds for $G$.

As a possible extension of the derivatives of the clique polynomial, we believe that the following conjecture is also true.

**Conjecture 3.**

We have the following formula for the *third derivative* of the clique polynomial:

$$
\frac{1}{3!} \frac{d^3}{dx^3} C(G, x) = \sum_{\delta \in \Delta_3(G)} C(G - \delta, x),
$$

(38)

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