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k-Combinations of an unlabelled graph

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ABSTRACT. In this paper we extend the notion of the binomial coefficient $\binom{n}{k}$ into a new notion $\binom{[G]}{k}$, where $[G]$ is an unlabelled graph with n vertices and $0 \leqslant k \leqslant n$. We call $\binom{[G]}{k}$ as the graph binomial coefficient and a version of the graph binomial expansion is also studied. As an application of this notion, we enumerate the number of ways to color vertices of a path and beads of a necklace.

1. INTRODUCTION AND PRELIMINARIES

Let n be a positive integer and $0 \leqslant k \leqslant n$. The *binomial coefficient* $\binom{n}{k}$ is the number of k-*combinations* of a set with n elements. This is equal to $\frac{n!}{k!(n-k)!}$ and satisfies the recursive relation $\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}$. The summation $\sum_{k=0}^{n} \binom{n}{k}$ is then equal to the number of ways to choose a subset of a fixed set with n elements which is obviously equal to 2^n. The mentioned fixed set with n elements can be vertices of a given *labelled graph*. But if we omit the labels then the number of k-combinations is not necessarily equal to $\binom{n}{k}$. For a simple example, if we have an unlabelled path with 3 vertices, then the number of 2-combinations is not 3. In fact the two ends of the path play the same role.

Let G be a graph with n vertices labelled by $1, 2, \ldots, n$. If we ignore the labels we have an *unlabelled graph*, denoted by $[G]$, with n vertices. We can formally say that $[G]$ is the class of all graphs G' which are isomorphic to G. Whence, as a good question we can enumerate the number of k-combinations of an unlabelled graph $[G]$. We denote this number by $\binom{[G]}{k}$ and we aim to find some formulas for this. We can also evaluate $\sum_{k=0}^{n} \binom{[G]}{k}$ for a given graph G. The number can be interpreted as the number of ways to color the vertices of $[G]$ with two different colors. We apply this for some special cases such as paths, directed cycles and indirected cycles.

In the following, we use *Burnside's Lemma*, [4], [2] and [6], which asserts that if a group $\mathcal{G}$ acts on a set X, then the number of orbits of $\mathcal{G}$ is equal to $\frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} |X_g|$, where X_g is the set of all $x \in X$ with $(g, x) = x$. To see a simple proof of Burnside's Lemma the reader is referred to [1]. A discussion about *Pólya Enumeration Theorem*, [7], which uses Burnside's Lemma, can be found in [8].

Recall that the *complement* of a graph G is a graph $\overline{G}$ on the same vertices such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. An *automorphism* of a graph $G = (V, E)$ is a permutation σ of the vertex set V, such that the pair of vertices (u, v) form an edge if and only if the pair $(\sigma(u), \sigma(v))$ also form an edge. The set of all automorphisms of a graph G, with the operation of composition of permutations, is a permutation group which is denoted by $\mathrm{Aut}(G)$. See [3] for the terminology and main

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results of permutation group theory. A graph and its complement have the same automorphism group. Frucht [5] proved that every group is the automorphism group of a graph. Moreover, if the group is finite, the graph can be taken to be finite.

Furthermore, recall that a graph G is called *vertex transitive* if for each two vertices u and v of G there is an automorphism $\sigma \in \mathrm{Aut}(G)$ such that $\sigma(u) = v$.

2. An explicit formula

In the following, for a labelled graph G we denote the class of all graphs G' which are isomorphic to G by $[G]$. This is called the *unlabelled graph induced by* G.

Definition 2.1. Let $[G]$ be an unlabelled graph with n vertices, where n is a positive integer. For $0 \leqslant k \leqslant n$, a *k-combination* of $[G]$ is a way of selecting members from $[G]$, such that the order of members in the selection does not matter. The number of k-combinations of $[G]$ is denoted by $\binom{[G]}{k}$ (read as $[G]$ *choose* k) and is called the *graph binomial coefficient*.

Example 2.1. Let n be a positive integer. For the complete graph K_n and the star graph $K_{1,n-1}$ we have $\binom{[K_n]}{k} = 1$ and $\binom{[K_{1,n-1}]}{k} = 2$ for each $1 \leqslant k \leqslant n$.

Though for a vertex transitive graph $[G]$ the graph binomial coefficient $\binom{[G]}{1}$ is 1, but $\binom{[G]}{2}$ can be a number other than 1.

Example 2.2. Let Q_3 be the 3-dimensional cube with vertices labelled as

$$a = 000, b = 001, c = 010, d = 011, e = 100, f = 101, g = 110, h = 111,$$

where two vertices are adjacent if and only if they differ in just one position. If we ignore the labels then there are three 2-combinations of $[Q_3]$ which are ab, ad and ah. Note that any other 2-combination is isomorphic to these.

We have the following two obvious results.

Proposition 2.1. *Let G be a labelled graph with n vertices and let $0 \leqslant k \leqslant n$. Then*

$$\binom{[G]}{k} = \binom{[G]}{n-k} = \binom{[\overline{G}]}{k},$$

where $\overline{G}$ is the complement of G.

Proposition 2.2. *Let G and G' be two labelled graphs with n vertices and let $0 \leqslant k \leqslant n$. If $\mathrm{Aut}(G) \simeq \mathrm{Aut}(G')$ then*

$$\binom{[G]}{k} = \binom{[G']}{k}.$$

Theorem 2.1. *Let $G = (V, E)$ be a labelled graph with n vertices and let $1 \leqslant k \leqslant n$. Then*

$$\binom{[G]}{k} = \frac{1}{|\mathrm{Aut}(G)|} \sum_{\sigma \in \mathrm{Aut}(G)} |V_\sigma^k|,$$

where $V_\sigma^k = \{\{v_1, \ldots, v_k\} \subseteq V : \sigma(\{v_1, \ldots, v_k\}) = \{v_1, \ldots, v_k\}\}$.

Proof. Let X be the set of k-subsets of V. Then $\mathrm{Aut}(G)$ acts on X by the rule $(\sigma, A) = \sigma(A)$ for each $A \in X$. Now, by the Burnside's Lemma, the number of orbits of X under $\mathrm{Aut}(G)$, which is equal to $\binom{[G]}{k}$, is $\frac{1}{|\mathrm{Aut}(G)|} \sum_{\sigma \in \mathrm{Aut}(G)} |V_\sigma^k|$, where V_σ^k is the set of all members of X which are fixed under σ. □

Corollary 2.1. *Let P_n be the labelled path with n vertices and let $1 \leqslant k \leqslant n$. Then*

$$\binom{[P_n]}{k} = \begin{cases} \frac{1}{2}\binom{n}{k} & \text{if } n \text{ is even and } k \text{ is odd} \\ \frac{1}{2}\left(\binom{n}{k} + \binom{\lfloor \frac{n}{2} \rfloor}{\lfloor \frac{k}{2} \rfloor}\right) & \text{otherwise} \end{cases}$$

Proof. There are two automorphisms for P_n: the identity automorphism ι and the automorphism α defined by $\alpha(i) = n+1-i$ for $1 \leqslant i \leqslant n$. For ι we obviously have $|V_\iota^k| = \binom{n}{k}$ and for α we see that a subset $\{v_1, \ldots, v_k\}$ of V is in V_α^k if and only if $i \in \{v_1, \ldots, v_k\}$ implies $n+1-i \in \{v_1, \ldots, v_k\}$. If n is even and k is odd, the latter is impossible and for the other cases we should choose $\lfloor \frac{k}{2} \rfloor$ of the members of $\{v_1, \ldots, v_k\}$ from $\{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ and the reminder should be chosen by symmetry. Now we can apply Theorem 2.1 to see the result. □

Corollary 2.2. *Let $\overrightarrow{C_n}$ be the labelled cycle with n vertices which is clockwise directed and let $1 \leqslant k \leqslant n$. Then*

$$\binom{[\overrightarrow{C_n}]}{k} = \frac{1}{n} \sum_{d \mid \gcd(n,k)} \varphi(d) \binom{\frac{n}{d}}{\frac{k}{d}}.$$

Proof. We know that $\mathrm{Aut}(\overrightarrow{C_n})$ is the cyclic group generated by the permutation $\alpha = (12\ldots n)$. Thus $\mathrm{Aut}(\overrightarrow{C_n}) = \{\alpha, \alpha^2, \ldots, \alpha^n\}$. This group has $\varphi(d)$ elements of order d for each divisor d of n. An element of order d has $\frac{n}{d}$ cycles of length d. For a subset $\{v_1, \ldots, v_k\}$ of V and $\sigma \in \mathrm{Aut}(\overrightarrow{C_n})$, we have $\sigma(\{v_1, \ldots, v_k\}) = \{v_1, \ldots, v_k\}$ if and only if these k elements consist of full cycles of σ. Whence if d does not divide k then V_σ^k is empty and if $d|n$ then choosing a subset $\{v_1, \ldots, v_k\}$ with the property $\sigma(\{v_1, \ldots, v_k\}) = \{v_1, \ldots, v_k\}$ is equivalent to choosing $\frac{k}{d}$ cycles of the $\frac{n}{d}$ cycles of σ. □

Corollary 2.3. *Let C_n be the labelled cycle with n vertices and let $1 \leqslant k \leqslant n$. Then*

$$\binom{[C_n]}{k} = \begin{cases} \frac{1}{2n} \sum_{d \mid \gcd(n,k)} \varphi(d) \binom{\frac{n}{d}}{\frac{k}{d}} + \frac{1}{2}\binom{\lfloor \frac{n}{2} \rfloor - 1}{\lfloor \frac{k}{2} \rfloor} & \text{if } n \text{ is even and } k \text{ is odd} \\ \frac{1}{2n} \sum_{d \mid \gcd(n,k)} \varphi(d) \binom{\frac{n}{d}}{\frac{k}{d}} + \frac{1}{2}\binom{\lfloor \frac{n}{2} \rfloor}{\lfloor \frac{k}{2} \rfloor} & \text{otherwise} \end{cases}$$

Proof. $\mathrm{Aut}(G)$ is the dihedral group consisting of a cyclic subgroup of order n and n reflections. If n is odd then a reflection consists of a cycle with order one and $\frac{n-1}{2}$ cycles of order two. And if n is even then we have $\frac{n}{2}$ reflections with $\frac{n}{2}$ cycles of order two and $\frac{n}{2}$ reflections with two cycles of order one and $\frac{n-2}{2}$ cycles of order two. Now we can do as in the previous corollary. □

3. Two recursive formulas

A famous recursive relation for the binomial coefficient is $\binom{n}{k} = \binom{n-1}{k-1} + \binom{n-1}{k}$. This simply says that a k-combination of the set $[n] = \{1, 2, \ldots, n\}$ can be chosen in two ways: $\{n\}$ union by a $(k-1)$-combination of the set $[n-1]$ or a k-combination of the set $[n-1]$. Using this idea, we aim to give a recursive formula for the graph binomial coefficient. Prior to this, we need some preliminaries.

Definition 3.2. Let $G = (V, E)$ be a labelled graph with n vertices, where n is a positive integer, and let H be a vertex induced subgraph of G. For $0 \leqslant k \leqslant n$, a *$k$-combination of H in $[G]$* is a way of selecting members from H, such that the order of members in the selection does not matter. The number of k-combinations of H in $[G]$ is denoted by $\binom{[H\subseteq G]}{k}$ and is called the *graph binomial coefficient of H with respect to $[G]$*.

Example 3.3. Let $G=(V,E)$ be the graph with

$$V=\{1,2,3,4,5,6\},\quad E=\{12,23,31,34,45,56,64\}.$$

If H is the triangle $\{1,2,3\}$ then $\binom{[H]}{1}$ is 1, but $\binom{[H\subseteq G]}{1}$ is 2, since we have two different 1-combinations 1 and 3 of H.

Theorem 3.2. *Let $G=(V,E)$ be a labelled graph with n vertices, $1\leqslant k\leqslant n$ and let H be a vertex induced subgraph of G. Then*

$$\binom{[H\subseteq G]}{k}=\frac{1}{|\mathrm{Aut}(G)|}\sum_{\sigma\in\mathrm{Aut}(G)}|H_\sigma^k|,$$

where $H_\sigma^k=\{\{v_1,\ldots,v_k\}\subseteq H:\sigma(\{v_1,\ldots,v_k\})=\{v_1,\ldots,v_k\}\}$.

Proof. Let X be the set of k-subsets of H. Then $\mathrm{Aut}(G)$ acts on X by the rule $(\sigma,A)=\sigma(A)$ for each $A\in X$. Now, by the Burnside's Lemma, the number of orbits of X under $\mathrm{Aut}(G)$, which is equal to $\binom{[H\subseteq G]}{k}$, is $\frac{1}{|\mathrm{Aut}(G)|}\sum_{\sigma\in\mathrm{Aut}(G)}|H_\sigma^k|$, where H_σ^k is the set of all members of X which are fixed under σ. □

Definition 3.3. Let $G=(V,E)$ be a graph, v be a vertex of G and let $\sigma\in\mathrm{Aut}(G)$. We denote the set of all $u\in V$ such that u and v are in the same cycle of σ, in the cyclic representation of σ, by $\mathrm{Cycle}(v,\sigma)$. The set $\cup_{\sigma\in\mathrm{Aut}(G)}\mathrm{Cycle}(v,\sigma)$, denoted by $\mathrm{Tran}_G(v)$, is called *the v-transitive subset of G*. The v-transitive subset $\mathrm{Tran}_G(v)$ of G is called *strongly transitive* if for each $u_1,u_2\in\mathrm{Tran}_G(v)$ and $u\in G$, there is a $\sigma\in\mathrm{Aut}(G)$ such that $\sigma(u_1)=u_2$ and $\sigma(u)=u$. For a vertex induced subgraph H of G we say that H is *v-transitive* if there is a $\sigma\in\mathrm{Aut}(G)$ with $H=V(v,\sigma)$. The set of v-transitive vertex induced subgraphs of G is denoted by $\mathcal{T}_G(v)$.

Example 3.4. Let $G=(V,E)$ be the graph with

$$V=\{1,2,3,4,5\},\quad E=\{12,13,23,24,35,45\}.$$

Then $\mathrm{Tran}_G(1)=\{1\},\mathrm{Tran}_G(2)=\{2,3\}$ and $\mathrm{Tran}_G(4)=\{4,5\}$. Here, $\mathrm{Tran}_G(1)$ is strongly transitive but $\mathrm{Tran}_G(2)$ and $\mathrm{Tran}_G(4)$ are not. To see this note that for $2,3\in\mathrm{Tran}_G(2)$ and $4\in G$ there is no $\sigma\in\mathrm{Aut}(G)$ with $\sigma(2)=3$ and $\sigma(4)=4$.

The following result is something similar to the recursive relation $\binom{n}{k}=\binom{n-1}{k-1}+\binom{n-1}{k}$.

Theorem 3.3. *Let $G=(V,E)$ be a graph with n vertices, v be a fixed vertex of G and let $1\leqslant k\leqslant n$. Then*

$$\binom{[G]}{k}=\sum_{H\in\mathcal{T}_G(v)}(\binom{[H^c\subseteq G]}{k-|H|}+\binom{[H^c\subseteq G]}{k}),$$

where H^c is the vertex induced subgraph of G whose vertex set is the complement of the vertex set of H.

Proof. Let $\sigma\in\mathrm{Aut}(G)$ and $H=V(v,\sigma)$. Then

$$\begin{aligned}V_\sigma^k &= \{\{v_1,\ldots,v_k\}:H\subseteq\{v_1,\ldots,v_k\},\sigma(\{v_1,\ldots,v_k\})=\{v_1,\ldots,v_k\}\}\\ &\quad\cup\{\{v_1,\ldots,v_k\}:H\cap\{v_1,\ldots,v_k\}=\emptyset,\sigma(\{v_1,\ldots,v_k\})=\{v_1,\ldots,v_k\}\}\\ &= \{\{v_{|H|+1},\ldots,v_k\}:\{v_{|H|+1},\ldots,v_k\}\subseteq H^c,\sigma(\{v_{|H|+1},\ldots,v_k\})=\{v_{|H|+1},\ldots,v_k\}\}\\ &\quad\cup\{\{v_1,\ldots,v_k\}:\{v_1,\ldots,v_k\}\subseteq H^c,\sigma(\{v_1,\ldots,v_k\})=\{v_1,\ldots,v_k\}\}.\end{aligned}$$

The above equality is true since for a subset $\{v_1,\ldots,v_k\}$ of V with $\sigma(\{v_1,\ldots,v_k\}) = \{v_1,\ldots,v_k\}$, the set should contain a full cycle of σ or none of the members of a cycle.

Since the union is disjoint, we have

$$|V_\sigma^k| = |(H^c)_\sigma^{k-|H|}| + |(H^c)_\sigma^k|.$$

We now can apply Theorem 3.2. □

For the binomial coefficient $\binom{n}{k}$ we have also the recursive relation $\binom{n}{k} = \sum_{\ell=0}^{t}\binom{t}{\ell}\binom{n-t}{k-\ell}$, where t can be any fixed integer with $0 \leqslant t \leqslant n$. This simply says that choosing a k-combination from a group of t boys and $n-t$ girls is equivalent to choosing ℓ boys and $k-\ell$ girls, where ℓ can be 0 or 1 or ... or t.

Theorem 3.4. *Let $G = (V,E)$ be a graph with n vertices, v be a fixed vertex of G and let $1 \leqslant k \leqslant n$. If $\mathrm{Tran}_G(v)$ is strongly transitive then*

$$\binom{[G]}{k} = \sum_{\ell=0}^{|\mathrm{Tran}_G(v)|}\binom{[\mathrm{Tran}_G(v)\subseteq G]}{\ell}\binom{[(\mathrm{Tran}_G(v))^c\subseteq G]}{k-\ell}.$$

Proof. Let $\{v_1,\ldots,v_k\}$ be a subset of V. Moreover, suppose that $\{v_1,\ldots,v_k\}\cap\mathrm{Tran}_G(v) = \{v_1,\ldots,v_\ell\}$, where $0\leqslant \ell \leqslant |\mathrm{Tran}_G(v)|$. Then $\sigma(\{v_1,\ldots,v_k\}) = \{v_1,\ldots,v_k\}$ if and only if

$$\sigma(\{v_1,\ldots,v_\ell\}) = \{v_1,\ldots,v_\ell\},\quad \sigma(\{v_{\ell+1},\ldots,v_k\}) = \{v_{\ell+1},\ldots,v_k\}.$$

This shows that

$$|V_\sigma^k| = \sum_{\ell=0}^{|\mathrm{Tran}_G(v)|} |(\mathrm{Tran}_G(v))_\sigma^\ell| \times |((\mathrm{Tran}_G(v))^c)_\sigma^{k-\ell}|.$$

Theorem 2.1 and Theorem 3.2 now give the result. □

4. Graph binomial expansion

Recall that the binomial expansion says $\sum_{k=0}^{n}\binom{n}{k}a^kb^{n-k} = (a+b)^n$. In this section we want to find a graph version of the binomial expansion.

Definition 4.4. Let $G = (V,E)$ be a labelled graph with n vertices, where n is a positive integer, and let H be a vertex induced subgraph of G. We denote the summation $\sum_{k=0}^{n}\binom{[H\subseteq G]}{k}a^kb^{n-k}$ by $P_{[H\subseteq G]}(a,b)$. The expansion is called the *graph binomial expansion of H with respect to $[G]$*. For the case $H = G$ we simply write $P_{[G]}(a,b)$ instead of $P_{[G\subseteq G]}(a,b)$.

Proposition 4.3. *Let G be a graph with n vertices. The number of ways to color vertices of $[G]$ with two colors is $P_{[G]}(1,1)$.*

As a corollary, using Corollaries 2.1, 2.2 and 2.3, we can compute the number of ways to color $P_n, \overrightarrow{C_n}$ (a necklace with rotations but without reflections) or C_n (a necklace with rotations and reflections) with two colors. For example, we have the following.

Corollary 4.4. *Let C_n be the labelled cycle with n vertices which is clockwise directed. Then the number of ways to color vertices of C_n with two colors is*

$$1 + \sum_{k=1}^{n}\frac{1}{n}\sum_{d|\,\gcd(n,k)}\varphi(d)\binom{\frac{n}{d}}{\frac{k}{d}}.$$

Furthermore, as a corollary of Theorem 3.4, we can easily prove the following result.

Theorem 4.5. *Let G be a graph with n vertices and v be a fixed vertex of G. If $\mathrm{Tran}_G(v)$ is strongly transitive then*

$$P_{[G]}(a,b) = P_{[\mathrm{Tran}_G(v)\subseteq G]}(a,b)P_{[(\mathrm{Tran}_G(v))^c\subseteq G]}(a,b).$$

Example 4.5. Let $G=(V,E)$ be the graph with

$$V=\{1,2,3,4,5,6,7\},\quad E=\{12,23,31,34,45,56,67,74\}.$$

Then

$$P_{[G]}(a,b) = a^7+5a^6b+12a^5b^2+18a^4b^3+18a^3b^4+12a^2b^5+5ab^6+b^7.$$

Considering $u=1$ we have $\mathrm{Tran}_G(u)=\{1,2\}$ which is strongly transitive. We have

$$P_{[\mathrm{Tran}_G(u)\subseteq G]}(a,b)(a,b) = a^2+ab+b^2$$

and

$$P_{[(\mathrm{Tran}_G(u))^c\subseteq G]}(a,b) = a^5+4a^4b+7a^3b^2+7a^2b^3+4ab^4+b^5.$$

Note that

$$\begin{aligned} & a^7+5a^6b+12a^5b^2+18a^4b^3+18a^3b^4+12a^2b^5+5ab^6+b^7 \\ = \; & (a^2+ab+b^2)(a^5+4a^4b+7a^3b^2+7a^2b^3+4ab^4+b^5). \end{aligned}$$

On the other hand, considering $v=6$ we have $\mathrm{Tran}_G(v)=\{6\}$ which is strongly transitive. We have

$$P_{[\mathrm{Tran}_G(v)\subseteq G]}(a,b)(a,b) = a+b$$

and

$$P_{[(\mathrm{Tran}_G(v))^c\subseteq G]}(a,b) = a^6+4a^5b+8a^4b^2+10a^3b^3+8a^2b^4+4ab^5+b^6.$$

Note that

$$\begin{aligned} & a^7+5a^6b+12a^5b^2+18a^4b^3+18a^3b^4+12a^2b^5+5ab^6+b^7 \\ = \; & (a+b)(a^6+4a^5b+8a^4b^2+10a^3b^3+8a^2b^4+4ab^5+b^6). \end{aligned}$$

Example 4.6. Let G be the graph introduced in Example 3.4. Then

$$P_{[G]}(a,b) = a^5+3a^4b+6a^3b^2+6a^2b^3+3ab^4+b^5.$$

Considering $v=4$ we have $\mathrm{Tran}_G(v)=\{4,5\}$ which is *not* strongly transitive. We have

$$P_{[\mathrm{Tran}_G(v)\subseteq G]}(a,b)(a,b) = a^2+ab+b^2$$

and

$$P_{[(\mathrm{Tran}_G(v))^c\subseteq G]}(a,b) = a^3+2a^2b+2ab^2+b^3.$$

Note that

$$\begin{aligned} & a^5+3a^4b+6a^3b^2+6a^2b^3+3ab^4+b^5 \\ \neq \; & (a^2+ab+b^2)(a^3+2a^2b+2ab^2+b^3). \end{aligned}$$

Remark 4.1. Let G be a graph with vertices $1,2,\ldots,n$. We add i loop to vertex i of G to make a new graph G'. Then $\mathrm{Aut}(G')$ is the identity group, since no two vertices of G' are transitive to each other. This guarantees that $\binom{[G']}{k}=\binom{n}{k}$ for each $0\leqslant k\leqslant n$. Thus $P_{[G']}(a,b)=\sum_{k=0}^{n}\binom{n}{k}a^kb^{n-k}$. On the other hand, for each $v\in G'$ we have $\mathrm{Tran}_{G'}(v)=\{v\}$ which is strongly transitive and so $P_{[\mathrm{Tran}_{G'}(v)\subseteq G']}(a,b)=a+b$. Thus $P_{[G']}(a,b)=(a+b)^n$. This agrees to the famous binomial expansion.

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