Enumeration for no-trivial spanning forests of complete bipartite graphs *

Bolian Liu[a] † and Fengying Huang[b]

[a]School of Mathematical Sciences, South China Normal University,

[b]School of Computer Science, Guangdong Polytechnic Normal University,

Guangzhou, 510631, P.R. China

Abstract

In this paper we give another proof for labeled spanning forests of the complete bipartite graph $K_{m,n}$ and obtain two Abel type polynomials. And then we investigate the enumeration of no-trivial rooted labeled spanning forests of the complete bipartite graph $K_{m,n}$.

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1 Introduction

Let $K_{m,n}$ be a labeled complete bipartite graph with vertex set $V(K_{m,n}) = A \cup B$, $|A| = m$, $|B| = n$. A forest of $l + k$ labeled rooted trees as spanning subgraphs of $K_{m,n}$ with l roots in A and k roots in B is denoted by $[m, l; n, k] - forest$ $(l \leq m, k \leq n)$ while the number of $[m, l; n, k]$-forests is denoted by $f(m, l; n, k)$.

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†Corresponding author's e-mail address: liubl@scnu.edu.cn

In [1], Y. Jin and C. Liu obtained the following results.

Theorem A *For $m \geq 0, n > 1$ and $k \geq 1$*

$$f(m,0;n,k) = k\binom{n}{k}m^{n-k}n^{m-1} = \binom{n-1}{k-1}m^{n-k}n^{m},$$

where $f(0,0;1,1)$ is defined to be 1.

Theorem B *For $1 \leq l \leq m$ and $1 \leq k \leq n$*

$$f(m,l;n,k) = \binom{m}{l}\binom{n}{k}n^{m-l-1}m^{n-k-1}(km + ln - kl).$$

Let $[m,l;n,k]^* - forest$ denote $[m,l;n,k]$-forest with l fixed roots in A and k fixed roots in B. Similarly, $f^*(m,l;n,k)$ denotes the number of $[m,l;n,k]^*$-forests.

It is easy to know that

$$f(m,l;n,k) = \binom{m}{l}\binom{n}{k}f^*(m,l;n,k). \tag{1}$$

From Theorem A, B and (1), we have

$$f^*(m,0;n,k) = km^{n-k}n^{m-1} \tag{2}$$

$$f^*(m,l;n,k) = n^{m-l-1}m^{n-l-1}(km + ln - kl) \tag{3}$$

In fact, we have the following recurrences

$$f^*(m,0;n,k) = \sum_{i=0}^{n-k}\sum_{j=0}^{m}\binom{n-k}{i}\binom{m}{j}f^*(j,0;i+1,1)f^*(m-j,0;n-i-1,k-1) \tag{4}$$

$$\begin{aligned} f^*(m,l;n,k) &= \sum_{i=0}^{n-k}\sum_{j=0}^{m-l}\tbinom{n-k}{i}\tbinom{m-l}{j}f^*(j,0;k+i,k)f^*(m-j,l;n-k-i,0) \\ &= \sum_{i=0}^{n-k}\sum_{j=0}^{m-l}\tbinom{n-k}{i}\tbinom{m-l}{j}f^*(j,0;k+i,k)f^*(n-k-i,0;m-j,l) \end{aligned} \tag{5}$$

We consider only formula (4). Notice that k trees with fixed roots in B can be decomposed into one tree with fixed root and $k-1$ trees with fixed roots. The formula (4) can follow. Thus combining formula (2) and (3). We obtain an identity as follows

$$\sum_{i=0}^{n-k}\sum_{j=0}^{m}\binom{n-k}{i}\binom{m}{j}j^i(i+1)^{j-1}(k-1)(m-j)^{n-i-k}(n-i-1)^{m-j-1}$$
$$= km^{n-k}n^{m-1}, \tag{6}$$

where we define $0^0=1$.

Similarly we can deal with formula (5) through the same method. Then we obtain the following equation

$$\sum_{i=0}^{n-k}\sum_{j=0}^{m-l}\binom{n-k}{i}\binom{m-l}{j}k(k+i)^{j-1}j^i l(m-j)^{n-i-k-1}(n-k-i)^{m-j-l}$$
$$= n^{m-l-1}m^{n-l-1}(km+ln-kl). \tag{7}$$

Conversely, if we first proved identities (6) and (7) then using induction and formulas (6) and (7), we can prove formulas (2) and (3). Then Theorem A and Theorem B are proved by another method.

A component of forest consisting of only a vertex is also viewed as a rooted tree in [1]. Such rooted tree is called trivial tree while spanning forest without trivial tree is called no-trivial spanning forest. A natural problem is how to count the number of no-trivial spanning forests for a labeled complete bipartite graph. In this paper we will settle the problem.

All of first, we will introduce Foata's method for enumeration of the subset of $[n]^{[n]}$ and then prove (6) and (7) by applying this method in the next section. In Section 3 an inverse relation will be proved. Then applying the inverse relation, we obtain some enumerations for no-trivial spanning forests of complete bipartite graph in final section.

2 Another proof for labeled spanning forests of the complete bipartite graph

First of all, we will introduce the enumeration of the subset of $[n]^{[n]}$, due to Foata (§1.18 of [4]), where $[n]^{[n]}$ denotes all mappings from $[n]$ onto $[n]$ and $[n] = \{1, 2, \dots, n\}$.

Given $E \subseteq [n]^{[n]}$, consider the enumeration of E, i.e. the (commutative) polynomial $\mathcal{T} = \mathcal{T}_E = \sum_{f \in E} t(f)$. Take $E \subseteq [3]^{[3]}$ for example, where $E = \{f_1, f_2, f_3, f_4\}$ with $f_1(i) = 1$, for $i = 1, 2, 3$; $f_2(1) = 2$, $f_2(2) = 2$, $f_2(3) = 1$; $f_3(1) = 2$, $f_3(2) = 3$, $f_3(3) = 1$; and $f_4(1) = 2$, $f_4(2) = 1$, $f_4(3) = 2$. We have $t(f_1) = t_1^3$, $t(f_2) = t(f_4) = t_1 t_2^2$ and $t(f_3) = t_1 t_2 t_3$. And thus $\mathcal{T}_E = t_1^3 + 2t_1 t_2^2 + t_1 t_2 t_3$.

We can give more examples here. (1) Set $E = [n]^{[n]}$. Then $\mathcal{T}_E = (t_1 + t_2 + \cdots + t_n)^n$. (2) If E is the set containing all functions fixed at $1, 2, \dots, k$, $\mathcal{T}_E = t_1 t_2 \dots t_k (t_1 + t_2 + \cdots + t_n)^{n-k}$. (3) If E is the set which contains all acyclic functions rooted or fixed at $1, 2, \dots, k$, then $\mathcal{T}_E = t_1 t_2 \dots t_k (t_1 + t_2 + \cdots + t_k)(t_1 + t_2 + \cdots + t_n)^{n-k-1}$. Evidently, $\mathcal{T}_E(1, 1, \dots) = |E|$. Therefore, we have (1) $|[n]^{[n]}| = n^n$; (2) the number of functions fixed at k elements is n^{n-k}; (3) the number of forests rooted at k given vertices is $k \cdot n^{n-k-1}$.

We can deduce some properties of $\mathcal{T}_E$. The coefficient of $t_1^{\alpha_1} t_2^{\alpha_2} \dots$ in $\mathcal{T}_E(t_1, t_2, \dots)$ is the number of $f \in E$ in which there are α_1 1, α_2 2, ... If E can be classified into some types $E_1, E_2, \dots$, written as $E = E_1 + E_2 + \dots$, then $\mathcal{T}_E = \mathcal{T}_{E_1} + \mathcal{T}_{E_2} + \dots$. If for any $f \in E$ there exist $f_i \in E_i (i = 1, 2, \dots)$ such that $f = f_1 f_2 \dots$, i.e. $E = E_1 E_2 \dots$, then $\mathcal{T}_E = \mathcal{T}_{E_1} \mathcal{T}_{E_2} \dots$.

We now consider the enumeration of a subset of $[n + m + 2]^{[n+m+2]}$.

Let $E \subseteq [n + m + 2]^{[n+m+2]}$ be a set containing all acyclic functions rooted or fixed at $n + 1$ and $n + 2$ such that for any $f \in E$, $f([n])$ is $[n + m + 2] - [n + 2]$ while $f([n + m + 2] - [n + 2])$ is $[n + 2]$. Then we have

$$\mathcal{T}_E$$

$$= t_{n+1}t_{n+2}(t_{n+3}+t_{n+4}+\cdots+t_{n+m+2})^n(t_{n+1}+t_{n+2})(t_1+t_2+\cdots+t_{n+2})^{m-1} \tag{8}$$

On the other hand, E can be divided into two parts, one rooted at $n+1$ and the other at $n+2$. Let $X \subset [n]$, $Y \subset [n+m+2]-[n+2]$, $|X| = i$ and $|Y| = j$. Set $\overline{X} = [n]-X$, $\overline{Y} = ([n+m+2]-[n+2])-Y$ and $A_1 = X \cup \{n+1\} \cup Y$. Consequently, $0 \le i \le n$, $0 \le j \le m$, $|\overline{X}| = n-i$ and $\overline{Y} = m-j$. Let $E_i \subset E(i=1,2)$ be the set containing all acyclic functions rooted at $n+i$ and for any $f_i \in E_i$, $f_1(X) = Y$ and $f_1(Y) = X \cup \{n+1\}$ while $f_2(\overline{X}) = \overline{Y}$ and $f_2(\overline{Y}) = \overline{X} \cup \{n+2\}$. Obviously, we have $E = E_1E_2$. Thus

$$\mathcal{T}_{E(X,Y)} = \mathcal{T}_{E_1(X,Y)}\mathcal{T}_{E_2(X,Y)}$$

$$= t_{n+1}(\sum_{q\in Y} t_q)^{|X|}t_{n+1}(t_{n+1}+\sum_{p\in X} t_p)^{|Y|-1}t_{n+2}(\sum_{q\in \overline{Y}} t_q)^{|\overline{X}|}t_{n+2}(t_{n+2}+\sum_{p\in \overline{X}} t_p)^{|\overline{Y}|-1} \tag{9}$$

By Eqs.(8) and (9), we obtain the following identity

$$(t_{n+1}+t_{n+2})(t_1+t_2+\cdots+t_{n+2})^{m-1}(t_{n+3}+t_{n+4}+\cdots+t_{n+m+2})^n$$

$$= \sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}t_{n+1}t_{n+2}(t_{n+1}+\sum_{p\in X}t_p)^{j-1}(t_{n+2}+\sum_{p\in\overline{X}}t_p)^{m-j-1}(\sum_{q\in Y}t_q)^i(\sum_{q\in\overline{Y}}t_q)^{n-i} \tag{10}$$

Set $t_{n+1} = x$, $t_{n+2} = y+nz$, $t_i = -z$ $(i \in [n+m+2]-\{n+1,n+2\})$ in (10). We obtain an Abel type polynomial as follows

Theorem 2.1 *For any real numbers x, y and real integer z, we have*

$$(x+y+nz)(x+y)^{m-1}(-mz)^n$$

$$=\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}x(y+nz)(x-iz)^{j-1}(y+iz)^{m-j-1}(-jz)^i[-(m-j)z]^{n-i}$$

In the following we will enumerate a subset of $[n+m+4]^{[n+m+4]}$.

Suppose that $E \subset [n+m+4]^{[n+m+4]}$ is a set containing all acyclic functions rooted or fixed at $n+1, n+2, n+m+3$ and $n+m+4$ and for any function $f \in E$, f maps from $[n]$ onto $[n+m+4]-[n+2]$ and from $[n+m+2]-[n+2]$ onto $[n+2]$.

If there exists no elements mapping onto a root, then the root is an isolated point. By the definition of E, for any $f \in E$, the possible isolated point set of f is one of the sets $\emptyset$, $\{n+1\}$, $\{n+2\}$, $\{n+m+3\}$, $\{n+m+4\}$ $\{n+1, n+m+3\}$, $\{n+1, n+m+4\}$, $\{n+2, n+m+3\}$, $\{n+2, n+m+4\}$, $\{n+1, n+2, n+m+3\}$, $\{n+1, n+2, n+m+4\}$, $\{n+1, n+m+3, n+m+4\}$ and $\{n+2, n+m+3, n+m+4\}$.

Let E_1, E_2 and E_3 be subsets of E, where the isolated point sets of E_1 are $\{n+1\}$, $\{n+2\}$ $\{n+1, n+m+3\}$, $\{n+1, n+m+4\}$, $\{n+2, n+m+3\}$, $\{n+2, n+m+4\}$, $\{n+1, n+m+3, n+m+4\}$, $\{n+2, n+m+3, n+m+4\}$ and $\emptyset$, E_2 contains $\{n+m+3\}$, $\{n+m+4\}$ $\{n+1, n+m+3\}$, $\{n+1, n+m+4\}$, $\{n+2, n+m+3\}$, $\{n+2, n+m+4\}$, $\{n+1, n+2, n+m+3\}$, $\{n+1, n+2, n+m+4\}$ and $\emptyset$ as isolated point sets and the isolated point sets of E_3 are $\{n+1, n+m+3\}$, $\{n+1, n+m+4\}$, $\{n+2, n+m+3\}$, $\{n+2, n+m+4\}$ and $\emptyset$. Then we obtain

$$\mathcal{T}_E = \mathcal{T}_{E_1} + \mathcal{T}_{E_2} - \mathcal{T}_{E_3},$$

where

$$\begin{aligned}\mathcal{T}_{E_1} = \; & t_{n+m+3}t_{n+m+4}(t_{n+1}+t_{n+2})(t_1+t_2+\cdots+t_{n+2})^{m-1}t_{n+1}t_{n+2} \\ & \times(t_{n+3}+t_{n+4}+\cdots+t_{n+m+4})^n,\end{aligned}$$

$$\begin{aligned}\mathcal{T}_{E_2} = \; & t_{n+1}t_{n+2}(t_{n+m+3}+t_{n+m+4})(t_{n+3}+t_{n+4}+\cdots+t_{n+m+4})^{n-1} \\ & \times t_{n+m+3}t_{n+m+4}(t_1+t_2+\cdots+t_{n+2})^m\end{aligned}$$

and

$$\mathcal{T}_{E_3} = t_{n+1}t_{n+2}(t_{n+m+3}+t_{n+m+4})(t_1+t_2+\cdots+t_{n+2})^{m-1}t_{n+m+3} \times t_{n+m+4}(t_{n+1}+t_{n+2})(t_{n+3}+t_{n+4}+\cdots+t_{n+m+4})^{n-1}$$

E can be separated into two groups, one rooted at $n+1$ and $n+2$ while the other at $n+m+3$ and $n+m+4$. Let $X \subset [n]$ and $Y \subset [n+m+2]-[n+2]$. Suppose $|X|=i$ and $|Y|=j$. And then set $\overline{X}=[n]-X$ and $\overline{Y}=([n+m+2]-[n+2])-Y$. Following the similar discussion as to obtaining Eq.(9), we have

$$\begin{aligned}&\mathcal{T}_{E(X,Y)}\\ = \;& t_{n+1}t_{n+2}(\sum_{q\in Y} t_q)^{|X|}(t_{n+1}+t_{n+2})(t_{n+1}+t_{n+2}+\sum_{p\in X} t_p)^{|Y|-1}t_{n+m+3}\\ &\times t_{n+m+4}(\sum_{p\in\overline{X}} t_p)^{|\overline{Y}|}(t_{n+m+3}+t_{n+m+4})(t_{n+m+3}+t_{n+m+4}+\sum_{q\in\overline{Y}} t_q)^{|\overline{X}|-1}\end{aligned}$$

Thus we obtain the following equation.

$$\begin{aligned}&(t_{n+1}+t_{n+2})(t_1+\cdots+t_{n+2})^{m-1}(t_{n+3}+\cdots+t_{n+m+4})^{n-1}(t_{n+5}+\ldots\\ &+t_{n+m+4})+(t_{n+m+3}+t_{n+m+4})(t_{n+3}+\cdots+t_{n+m+4})^{n-1}(t_1+\cdots+t_{n+2})^m\\ &=\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}\{(t_{n+1}+t_{n+2})(t_{n+1}+t_{n+2}+\sum_{p\in X}t_p)^{j-1}(\sum_{p\in\overline{X}}t_p)^{m-j}\\ &\times(t_{n+m+3}+t_{n+m+4})(\sum_{q\in Y}t_q)^i(t_{n+m+3}+t_{n+m+4}+\sum_{q\in\overline{Y}}t_q)^{n-i-1}\}\end{aligned} \tag{11}$$

Set $t_{n+1}=x, t_{n+2}=y+nz, t_{n+m+3}=u, t_{n+m+4}=w+mz$ and $t_i=-z$ $(i\in([n+m+4]-n+1,n+2,n+m+3,n+m+4))$ in (11). We can deduce another Abel type polynomial.

Theorem 2.2 *For any real numbers x,y,u,w and z, the following identity holds.*

$$\begin{aligned}&\{(x+y)(u+w)-nmz^2\}(x+y)^{m-1}(u+w)^{n-1}\\ &=\sum_{i=0}^{n}\sum_{j=0}^{m}\binom{n}{i}\binom{m}{j}\{(x+y+nz)(x+y+nz-iz)^{j-1}(-nz+iz)^{m-j}\\ &\times(u+w+mz)(-jz)^i(u+w+jz)^{n-i-1}\}.\end{aligned}$$

Applying Theorem 2.1 and Theorem 2.2, we can prove Theorem A and Theorem B in another way, respectively.

If we replace n by $n-k$ in Theorem 2.1 and set $x=1$ $y=n-1$ and $z=-1$, we obtain identity (6). Replace n and m by $n-k$ and $m-l$ in Theorem 2.2, respectively and then set $x+y=n$, $u+w=m$ and $z=-1$, we obtain identity (7). By (1), we have Theorem A and Theorem B. Actually, if substitute n for $n-k$ and set $t_{n+1}=1$, $t_{n+2}=k-1$ and $t_i=1$ in (10), we also can obtain identity (6). Similar method can be applied to deduce identity (7).

3 An Inverse Relation for Multiple Variations

It is well-known (see [2]) that the inverse relation

$$a_n=\sum_{j\geq 0}\binom{n}{j}b_{n-j}\alpha^j \iff b_n=\sum_{j\geq 0}\binom{n}{j}a_{n-j}(-\alpha)^j, \tag{12}$$

where α is constant.

Let $\alpha=1$. It is the famous binomial inverse relation as follows.

$$a_n=\sum_{j\geq 0}\binom{n}{j}b_{n-j} \iff b_n=\sum_{j\geq 0}\binom{n}{j}a_{n-j}(-1)^j. \tag{13}$$

Applying binomial inverse relation k times, we obtain binomial inverse relation for k variations.

$$\begin{aligned} a_{n_1,n_2,\ldots,n_k} &= \sum_{\substack{t_i\geq 0\\ 1\leq i\leq k}}\prod_{i=1}^{k}\binom{n_i}{t_i}b_{t_1,t_2,\ldots,t_k}\\ \iff b_{n_1,n_2,\ldots,n_k} &= \sum_{\substack{t_i\geq 0\\ 1\leq i\leq k}}(-1)^{\sum n_i-\sum t_i}\prod_{i=1}^{k}\binom{n_i}{t_i}a_{t_1,t_2,\ldots,t_k}.\end{aligned}$$

Now we will generalize formula (13) to another inverse relation for multiple variations as follows.

For some r, $1 \leq r \leq k$,

$$a_{n_1,n_2,\ldots,n_k} = \sum_{j\geq 0} \binom{n_r}{j} b_{n_1-j,n_2-j,\ldots,n_k-j}$$

$$\iff \quad b_{n_1,n_2,\ldots,n_k} = \sum_{j\geq 0} (-1)^j \binom{n_r}{j} a_{n_1-j,n_2-j,\ldots,n_k-j}, \tag{14}$$

where $j \leq min(n_1, n_2, \ldots, n_k)$.

Without loss of generality, we change form (14) to its equivalent form (15) as follows.

$$a_{n_1,n_2,\ldots,n_k} = \sum_{j\geq 0} \binom{n_1}{j} b_{n_1-j,n_2-j,\ldots,n_k-j} \qquad (15.1)$$

$$\iff \quad b_{n_1,n_2,\ldots,n_k} = \sum_{j\geq 0} (-1)^j \binom{n_1}{j} a_{n_1-j,n_2-j,\ldots,n_k-j}, \qquad (15.2) \tag{15}$$

where $min(n_1, n_2, \ldots, n_k) \geq j$.

Now we use generating function to prove inverse relation (15).

Proof. Let

$$A_{n_1}(t_2, t_3, \ldots, t_k) = \sum_{n_i\geq 0,\ 2\leq i\leq k} a_{n_1,n_2,\ldots,n_k} t_2^{n_2} t_3^{n_3} \ldots t_k^{n_k}$$

$$B_{n_1}(t_2, t_3, \ldots, t_k) = \sum_{n_i\geq 0,\ 2\leq i\leq k} b_{n_1,n_2,\ldots,n_k} t_2^{n_2} t_3^{n_3} \ldots t_k^{n_k}$$

We will prove (15.2) $\Longrightarrow$ (15.1).

$$B_{n_1}(t_2, t_3, \ldots, t_k)$$

$$= \sum_{\substack{n_i\geq 0\\ 2\leq i\leq k}} \Big(\sum_{j\geq 0} (-1)^j \binom{n_1}{j} a_{n_1-j,n_2-j,\ldots,n_k-j}\Big) t_2^{n_2} t_3^{n_3} \ldots t_k^{n_k}$$

$$= \sum_{j\geq 0} (-1)^j \binom{n_1}{j} t_2^j t_3^j \ldots t_k^j \sum a_{n_1-j,n_2-j,\ldots,n_k-j} t_2^{n_2-j} t_3^{n_3-j} \ldots t_k^{n_k-j}$$

$$= \sum_{j\geq 0} \binom{n_1}{j} A_{n_1-j}(t_2, t_3, \ldots, t_k)(-t_2 t_3 \ldots t_k)^j.$$

Since $t_i (i = 2, 3, \ldots, k)$ doesn't depend on j, by inverse relation (12)

$$\begin{aligned}
A_{n_1}(t_2, t_3, \ldots, t_k) &= \sum_{j\geq 0} \binom{n_1}{j} B_{n_1-j}(t_2, t_3, \ldots, t_k)(t_2 t_3 \ldots t_k)^j \\
&= \sum_{j\geq 0} \binom{n_1}{j} \sum_{\substack{v_i \geq 0 \\ 2\leq i\leq k}} b_{n_1-j, v_2, \ldots, v_k} t_2^{v_2} \ldots t_k^{v_k} (t_2 t_3 \ldots t_k)^j \\
&= \sum_{j\geq 0} \sum_{\substack{v_i \geq 0 \\ 2\leq i\leq k}} \binom{n_1}{j} b_{n_1-j, v_2, \ldots, v_k} t_2^{v_2+j} \ldots t_k^{v_k+j} \\
&= \sum_{\substack{n_i \geq j \\ 2\leq i\leq k}} \sum_{j\geq 0} \binom{n_1}{j} b_{n_1-j, n_2-j, \ldots, n_k-j} t_2^{n_2} \ldots t_k^{n_k}.
\end{aligned}$$

Then

$$a_{n_1, n_2, \ldots, n_k} = \sum_{j\geq 0} \binom{n_1}{j} b_{n_1-j, n_2-j, \ldots, n_k-j} t_2^{n_2} \ldots t_k^{n_k},$$

where $min(n_1, n_2, \ldots, n_k) \geq j$.

Similarly, we can prove (15.1) $\Longrightarrow$ (15.2). ∎

If $k = 2$ in (14), we have

$$\begin{aligned}
a(n, m) &= \sum_{j\geq 0}^{min(n,m)} \binom{n}{j} b(n-j, m-j) \\
\Longleftrightarrow \quad b(n, m) &= \sum_{j\geq 0}^{min(n,m)} (-1)^j \binom{n}{j} a(n-j, m-j).
\end{aligned} \tag{16}$$

4 Counting No-trivial Spanning Forests of Complete Bipartite Graphs

Let $F(m, l; n, k)$ denote the number of no-trivial spanning $[m, l; n, k]$-forests of labeled complete bipartite graph $K_{m,n}$. We obtain the following enumerations for $F(m, l; n, k)$. It is easy to know $F(0, 0; 1, 1) = 0$ and $F(m, 0; n, k) = 0$ if $k > min(n, m)$.

Theorem 4.1 *For $min(n,m) \geq k \geq 1$,*

$$F(m,0;n,k) = m^{n-k} n \binom{n-1}{k-1} \sum_{q\geq 0} (-1)^q \binom{k-1}{q} (n-q)^{m-1}.$$

Proof. According to the definitions of $f(m,0;n,k)$ and $F(m,0;n,k)$, we have

$$\sum_{q\geq 0} \binom{n}{q} F(m,0;n-q,k-q) = f(m,0;n,k).$$

By the inverse relation (12) and Theorem A, we have

$$\begin{aligned} F(m,0;n,k) &= \sum_{q\geq 0} (-1)^q \tbinom{n}{q} f(m,0;n-q,k-q) \\ &= \sum_{q\geq 0} (-1)^q \tbinom{n}{q} \tbinom{n-q-1}{k-q-1} m^{n-k} (n-q)^m \\ &= m^{n-k} n \tbinom{n-1}{k-1} \sum_{q\geq 0} (-1)^q \tbinom{k-1}{q} (n-q)^{m-1}. \end{aligned}$$

∎

Theorem 4.2 *For $min(n,m) \geq l \geq 1$, $min(n,m) \geq k \geq 1$,*

$$\begin{aligned} F(m,l;n,k) = \; & \tbinom{m}{l} \tbinom{n}{k} \sum_{\substack{p\geq 0 \\ q\geq 0}} (-1)^{m+n-p-q} \tbinom{l}{p} \tbinom{k}{q} (n-q)^{m-l-1} \\ & \times (m-p)^{n-k-1} [m(k-q) + n(l-p) + pq - kl]. \end{aligned}$$

Proof. Since

$$\sum_{\substack{p\geq 0 \\ q\geq 0}} \binom{m}{p} \binom{n}{q} F(m-p,l-p;n-q,k-q) = f(m,l;n,k),$$

by the inverse relation and Theorem B, we have

$$F(m,l;n,k)$$
$$=\sum_{\substack{p\geq 0\\ q\geq 0}}(-1)^{m+n-p-q}\binom{m}{p}\binom{n}{q}f(m-p,l-p;n-q,k-q)$$

$$=\sum_{\substack{p\geq 0\\ q\geq 0}}(-1)^{m+n-p-q}\binom{m}{p}\binom{n}{q}\binom{m-p}{l-p}\binom{n-q}{k-q}(n-q)^{m-l-1}(m-p)^{n-k-1}$$

$$\times((k-q)(m-p)+(l-p)(n-q)-(k-q)(l-p))$$

$$=\binom{m}{l}\binom{n}{k}\sum_{\substack{p\geq 0\\ q\geq 0}}(-1)^{m+n-p-q}\binom{l}{p}\binom{k}{q}(n-q)^{m-l-1}$$

$$\times(m-p)^{n-k-1}(m(k-q)+n(l-p)+pq-kl).$$

∎

In fact, using inverse method and the result in [3], we also can obtain enumeration of no-trivial forests for a complete graph K_n.

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ON THE COMPLEXITY OF UNIQUE LIST COLOURABILITY AND THE FIXING NUMBER OF GRAPHS

Amir Daneshgar
Department of Mathematical Sciences
Sharif University of Technology
P.O. Box 11365–9415, *Tehran, Iran*
daneshgar@sharif.ac.ir

Hossein Hajiabolhassan
Department of Mathematical Sciences
Shahid Beheshti University
P.O. Box 19834, *Tehran, Iran*
hhaji@sbu.ac.ir

Siamak Taati
Department of Mathematical Sciences
Sharif University of Technology
P.O. Box 11365–9415, *Tehran, Iran*

Abstract

Let G be a finite simple χ-chromatic graph and $\mathcal{L} = \{L_u\}_{u\in V(G)}$ be a list assignment to its vertices with $L_u \subseteq \{1,\ldots,\chi\}$. A list colouring problem $(G,\mathcal{L})$ with a unique solution for which the sum $\sum_{u\in V(G)} |L_u|$ is maximized, is called a *maximum χ-list assignment* of G. In this paper, we prove a *Circuit Simulation Lemma* that, strictly speaking, makes it possible to simulate any Boolean function by *effective* 3-colourings of a graph that is *polynomial-time constructable* from the Boolean function itself. We use the lemma to simply prove some old results as corollaries, and also we prove that the following decision problem, related to the computation of the fixing number of a graph [Daneshgar 1997, Daneshgar and Naserasr, Ars Combin. 69 (2003)], is Σ_2^P-complete.

PROBLEM FIXGRPHCOL
Given A graph G and two integers k and m.
Question Does G have a maximum k-list assignment, $\mathcal{L}$, with

$$\sum_{u\in V(G)} |L_u| \geq m?$$

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1 Introduction

Consider a list colouring problem $(\mathrm{G}, \mathcal{L})$ where $\mathcal{L} = \{L_u\}_{u \in V(G)}$ is a list assignment to the vertices of the graph G. If $s \stackrel{\text{def}}{=} \sum_{u \in V(G)} |L_u|$ then one may naturally ask about the maximum value of the number s if one is restricted to the list assignments for which the list colouring problem $(\mathrm{G}, \mathcal{L})$ has a unique solution.

In this paper we consider this problem for the maximum χ-list assignments of a χ-chromatic graph G for which the list colouring problem has a unique solution and the parameter s is maximized. Also, we show that the extremal case in which the list of a vertex is the set $\{1, \ldots, \chi\}$ in any such maximum list assignment, is feasible, by a direct construction (Section 2).

It turns out that such vertices, in a sense, can be used as isolating vertices in a construction that introduces a reduction which shows that the problem FIXGRPHCOL (introduced in the abstract) is Σ_2^{P}-complete. The second part of the paper introduces a general type of reduction that suits best when one deals with decision problems concerning unique colourability of graph (Section 3.1). Then by applying this reduction (Theorem 2) and the existence result on isolated vertices (Theorem 1) we prove our Σ_2^{P}-completeness theorem in Section 3.2 (Theorem 3).

Throughout the paper the word *graph* stands for the concept of a *finite undirected graph*. For any such graph G, the vertex set and the edge set are denoted by $V(\mathrm{G})$ and $E(\mathrm{G})$, respectively. Also, a graph *homomorphism* $\sigma \in \mathrm{Hom}(\mathrm{G}, \mathrm{H})$ is a map $\sigma : V(\mathrm{G}) \longrightarrow V(\mathrm{H})$ such that

$$uv \in E(\mathrm{G}) \quad \Rightarrow \sigma(u)\sigma(v) \in E(\mathrm{H}).$$

It is easy to see that *graphs* and their *homomorphisms* form a category. Also, a homomorphism from a graph G to the complete graph K_t is called a *proper* t-colouring or a t-colouring of G for short.

Given a graph G, consider a set $\mathcal{L} = \{L_v\}_{v \in V(G)}$ with $L_v \subseteq \{1, \ldots, t\}$ such that $t \geq \chi(\mathrm{G})$ is a fixed integer. A graph G is called uniquely $\mathcal{L}$-list colourable, if the list colouring problem, $(\mathrm{G}, \mathcal{L}, t)$, on G with lists $\mathcal{L} = \{L_v\}_{v \in V(G)}$ has a unique solution. A graph G is a uniquely t-colourable graph if the ordinary proper t-colouring problem on G has a unique solution, up to a permutation of colours (for more on uniquely list colourable graphs see [5, 9]).

To see that this can also be viewed as an embedding problem, assume that the list colouring problem $(\mathrm{G}, \mathcal{L}, t)$ is given, and let $\mathrm{H} = \mathrm{G} \cup \mathrm{K}_t$ with $V(\mathrm{K}_t) = \{v_1, \ldots, v_t\}$. Also, assume that (without loss of generality) we have fixed the colours of vertices $V(\mathrm{K}_t) = \{v_1, \ldots, v_t\}$ such that v_i has taken the colour i for all $i \in \{1, \ldots, t\}$. Now, one may construct a new graph, $\tilde{\mathrm{H}}_{\mathrm{G}, \Phi, t}$, such that for each $u \in V(\mathrm{G})$ and $L_u \in \mathcal{L}$ we add new edges

$\Phi_u = \{uv_i \mid i \notin L_u\}$ to the graph H. If

$$\Phi \stackrel{\text{def}}{=} \bigcup_{u \in V(G)} \Phi_u,$$

then it is clear that $\tilde{H}_{G,\Phi,t}$ with the vertex set $V(H)$ and the edge set $E(H) \cup \Phi$ is a uniquely t-colourable graph (or a t-UCG for short) if and only if the list colouring problem $(G, \mathcal{L}, t)$ has a unique solution i.e. G is a uniquely $\mathcal{L}$-list colourable graph. Hereafter, we will freely switch between the embedding setup and the list colouring approach.
When $\tilde{H}_{G,\Phi,t}$ is a t-UCG, this set of new edges, Φ, is called a *fixing set* (of edges) for G (with respect to K_t) and it is easy to see that

$$|\Phi| = t|V(G)| - \sum_{u \in V(G)} |L_u|.$$

An element of a fixing set is called a *fixing edge*. On the other hand, one is mainly interested in the minimal case, for which $(G, \mathcal{L}, t)$ has a unique solution and the sum $\sum_{u \in V(G)} |L_u|$ is maximized. Hence, $\phi_0(G, t)$ (for any fixed $t \geq \chi(G)$) is defined as

$$\phi_0(G,t) \stackrel{\text{def}}{=} \min\{|\Phi| \mid \Phi \text{ is a fixing set for G with respect to } K_t\}. \quad (1)$$

Also, $\phi(G,t) \stackrel{\text{def}}{=} \phi_0(G,t) - \binom{t}{2}$ is called the *fixing number* of G with respect to K_t (see [2, 3, 4, 10]).

Theorem A. [4] *For any k-chromatic graph* G, $\phi_0(G,k) \geq \binom{k}{2}$ *and equality holds if and only if* G *is a k-UCG.*

Accordingly, any list colouring problem $(G, \mathcal{L}, t)$ with a unique solution for which the sum $\sum_{u \in V(G)} |L_u|$ is maximized, is called a *maximum t-list assignment* for G, and the corresponding t-colouring of G for which the minimum in (1) is attained, is called a *minimum t-colouring* of G. By definition it is clear that minimum t-colourings of G are induced by the unique t-colouring of the extensions $\tilde{H}_{G,\Phi,t}$ in cases that Φ is a minimum-size fixing set of edges for G with respect to K_t.
Let $i \neq j$, σ be a t-colouring of G, and $\omega_{ij}(G,\sigma)$ denote the number of components of the subgraph of G induced on the vertices whose colours are in $\{i, j\}$. We define,

$$\Omega(G,\sigma) \stackrel{\text{def}}{=} \sum_{1 \leq i < j \leq t} \omega_{ij}(G,\sigma).$$

Also, let

$$\Omega^{min}(G,t) \stackrel{\text{def}}{=} \min_{\sigma}\Big(\sum_{1 \le i < j \le t} \omega_{ij}(G,\sigma)\Big),$$

in which the minimum is taken over all t-colourings, σ, of G. We recall the following result,

Theorem B. [3] *For any k-chromatic graph* G *and $t \geq k$, if Φ is a fixing set of* G *with respect to* K_t *and σ_0 is the corresponding colouring of* G*, then* $\Omega(G,\sigma_0) \leq |\Phi|$. *Moreover,* $\Omega^{min}(G,t) \leq \phi_0(G,t)$.

2 Isolated vertices

In this section we introduce the concept of an *isolated vertex*. Strictly speaking, an isolated vertex is a vertex that does not contribute to any minimum-size fixing set, i.e. such a vertex has a list of size χ in any maximum χ-list assignment.

Definition 1. A *k-isolated vertex* for the fixing sets of the χ-colourings of a χ-chromatic graph G, is a vertex $v \in V(G)$ such that

- The vertex v is incident to at most k edges of any minimum-size fixing set of G.
- There exists at least one minimum-size fixing set of G in which v is incident to exactly k edges.

A 0-isolated vertex is called an *isolated vertex* for short. ♠

By considering graphs of small order and the fact that an isolated vertex must have a list of maximum size in *any* χ-list assignment with a unique solution, one may guess that such vertices does not exist at all. However, in the sequel we will prove that such vertices exist.
In the following proposition K[⓪,①,⊛] denotes a 3-clique on the vertex set {⓪,①,⊛} (see Figure 3(a)).

Proposition 1. *The graph* F *depicted in Figure* 1 *has the following properties,*

a) *The set* {b①, b⊛, e⓪, h⊛} *is a fixing set of size* 4 *for* F *with respect to* K[⓪,①,⊛].
b) *If $\sigma : V(F) \longrightarrow \{0, 1, *\}$ is a minimum* 3*-colouring, then we have,*

$$\sigma(a) = \sigma(b) \neq \sigma(e).$$

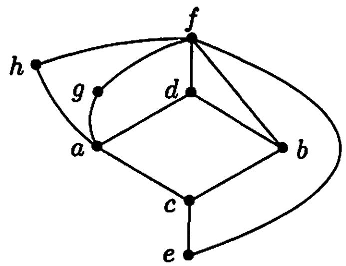


Figure 1: The graph F (see Proposition 1).

c) *The minimum* 3*-colouring of* F *is uniquely described as follows, up to a permutation of colours,*

$$\sigma(a) = \sigma(b) = 0, \;\; \sigma(d) = \sigma(e) = \sigma(g) = \sigma(h) = 1 \text{ and } \sigma(c) = \sigma(f) = *.$$

d) *The vertex* h *is a* 1*-isolated vertex of* F.

Proof.

(a) It is easy to check that $\{b①, b⊛, e⓪, h⊛\}$ is a fixing set of size 4 with respect to K[⓪, ①, ⊛] (note that the vertex f can not take the colour 1 in the corresponding list colouring problem).

(b) If $\sigma(a) \neq \sigma(b)$, without loss of generality, we may assume that $\sigma(a) = 0$ and $\sigma(b) = 1$. This implies that $\sigma(c) = \sigma(d) = *$ and $\sigma(e) = 1$. Hence,

$$\omega_{01}(\mathrm{F}, \sigma) \geq 1, \;\; \omega_{0*}(\mathrm{F}, \sigma) \geq 1, \;\; \omega_{1*}(\mathrm{F}, \sigma) = 3,$$

and by applying Theorem B we should have $\phi_0(\mathrm{F}, \sigma) \geq \Omega^{min}(\mathrm{F}, 3) \geq 5$, which is impossible.

On the other hand, if $\sigma(a) = \sigma(e)$, without loss of generality, we may assume that $\sigma(a) = \sigma(b) = \sigma(e) = 0$. Hence, $\sigma(v) \neq 0$ for any such vertex $v \in \{c, d, f, g, h\}$, and consequently, the graph $\mathrm{F} - \{a, b, e\}$ is the subgraph induced on the colours 1 and $*$. Therefore, we have

$$\omega_{01}(\mathrm{F}, \sigma) + \omega_{0*}(\mathrm{F}, \sigma) \geq 3, \;\; \omega_{1*}(\mathrm{F}, \sigma) = 2,$$

and by applying Theorem B we should have $\phi_0(\mathrm{F}, \sigma) \geq \Omega^{min}(\mathrm{F}, 3) \geq 5$, which is impossible.

(*c*) Let $\sigma : V(\mathrm{F}) \longrightarrow \{0, 1, *\}$ be a minimum 3-colouring of F and let Φ be a fixing set of σ such that $|\Phi| = 4$. By part (*b*), without loss of generality, we may assume that

$$\sigma(a) = \sigma(b) = 0 \quad \text{and} \quad \sigma(e) = 1.$$

It is easy to see that this partial conditions uniquely characterize the colouring σ as,

$$\sigma(d) = \sigma(g) = \sigma(h) = 1 \quad \text{and} \quad \sigma(c) = \sigma(f) = *,$$

up to a permutation of colours.

(*d*) Let $\sigma : V(\mathrm{F}) \longrightarrow \{0, 1, *\}$ be the minimum 3-colouring of F (introduced in part (*c*)) and let Φ be a fixing set of σ such that $|\Phi| = 4$. Assume that two edges in Φ are incident to h and fix the colour of h as 1. Then,

- *There is an edge in Φ that connects vertices e and* ⓪.

  This is clear since any neighbour of e takes the colour $*$ in σ.

- *There is an edge in Φ that connects vertices b and* ⊛.

  To prove this, first, assume that the colours of all vertices except b, d and f are fixed. Then the extension problem is equivalent to a list colouring problem on the triangle $\mathrm{K}[b, d, f]$ in which the size of the lists assigned to any one of these three vertices are 2. But since a triangle is not a U2LC [5, 9] we deduce that the extension problem has two feasible solutions. This proves that there should be at least one fixing edge in Φ that is incident to one of the vertices b, d or f.
  On the other hand, we may consider a similar situation in which the colours of all vertices except a, b, c and d are fixed. By a similar argument since the 4-cycle C_4 is not a U2LC [5, 9] we deduce that the extension problem has two feasible solutions, and consequently, there should be at least one fixing edge in Φ that is incident to one of the vertices a, b, c or d.
  Since we have assumed that $|\Phi| = 4$ and that we already have two fixing edges incident to h and one fixing edge incident to e, there should be a fixing edge incident to $\{b, d, f\} \cap \{a, b, c, d\} = \{b, d\}$.
  However, since $\sigma(h) = \sigma(e) = 1$, the fourth fixing edge must be incident to a vertex whose colour is in $\{0, *\}$. This implies that this fixing edge must be incident to b and ⊛.

These facts imply that $\Phi = \{h\textcircled{0}, h\textcircled{*}, e\textcircled{0}, b\textcircled{*}\}$. But it is easy to check that the colouring $\tilde{\sigma}$ defined as

$$\tilde{\sigma}(a) = \tilde{\sigma}(f) = 0, \quad \tilde{\sigma}(b) = \tilde{\sigma}(e) = \tilde{\sigma}(g) = \tilde{\sigma}(h) = 1, \quad \tilde{\sigma}(c) = \tilde{\sigma}(d) = *,$$

is also compatible with Φ, which is the desired contradiction.
Also, part (a) shows that there exists a minimum-size fixing set in which there is a fixing edge incident to h.

■

Let h be a 1-isolated vertex of a graph H. Consider two copies of the graph H, namely H_1 and H_2, in which the vertices h_1 and h_2 are 1-isolated, respectively. Construct the graph $T_{H[h]}[w]$ on the vertex set $V(H_1) \cup V(H_2) \cup \{w\}$ by adding three new edges $\{h_1h_2, h_1w, h_2w\}$ along with all edges in $E(H_1) \cup E(H_2)$ (see Figure 2).
At first it may seem intuitively natural to deduce that the vertex w in $T_{H[h]}[w]$ is an isolated vertex, however, we would like to note that it does not seem to be easy to exclude the existence of a minimum fixing set in which there is only one fixing edge incident to w, since one could consider a case in which, $\chi(H) = 3$, H has a minimum fixing set of size k and also a fixing set of size $k + 1$ in which there are two fixing edges incident to h. Now, one may use k fixing edges to fix the colours in H_1, and one more fixing edge incident to w in order to fix the colour of w along with $(k + 1) - 2 = k - 1$ more fixing edges on H_2 to fix the rest of the colours. The following theorem shows that such cases can not happen.

Theorem 1. *Let h be a 1-isolated vertex and k be the size of a minimum-size fixing set of the graph* H. *Then, any minimum-size fixing set of* $T_{H[h]}[w]$ *contains exactly $2k - 1$ fixing edges. Moreover, the vertex w is an isolated vertex of this graph.*

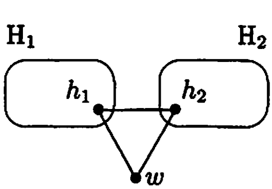


Figure 2: The graph $T_{H[h]}[w]$ (see Theorem 1).

Proof. To show that any minimum-size fixing set is of size $2k-1$, note that since h is a 1-isolated vertex of H, there exists a minimum-size fixing set $\Phi = \Psi \cup \{h⊛\}$ for H. Now, fix the colouring σ_1 of H_1 using the fixing set Φ such that $\sigma_1(h_1) = *$ (possibly by applying a permutation of colours). On the other hand, it is also possible to use the set Ψ to fix the colouring σ_2 of H_2 such that $\sigma_2(h_2) = 1$ since there is an edge between the vertices h_1 and h_2. Then it is easy to see that the union of the colourings σ_1 and σ_2 has only a unique extension to a colouring σ of the graph $T_{H[h]}[w]$ and moreover we have $\sigma(w) = 0$. This shows that for any minimum-size fixing set Θ of $T_{H[h]}[w]$ we have $|\Theta| \leq 2k-1$.
On the other hand, let Θ be a minimum-size fixing set of $T_{H[h]}[w]$ such that $|\Theta| < 2k-1$. Since h is a 1-isolated vertex of H, the subset $A \subseteq \Theta$ of fixing edges incident to $V(H_1) - \{h_1\}$ contains at least $k-1$ fixing edges. Also, since a similar statement is true for the subset $B \subseteq \Theta$ of fixing edges incident to $V(H_2) - \{h_2\}$, we deduce that $\Theta = A \cup B$ and, moreover, $|A| = |B| = k-1$.
Now, since the size of any minimum-size fixing set of H is equal to k, and moreover, $\Theta = A \cup B$ is a fixing set of $T_{H[h]}[w]$, there exist two colourings σ_A and γ_A for H_1 which are compatible with A and $\sigma_A(h_1) \neq \gamma_A(h_1)$. Also, with the same reasoning, there exist two colourings σ_B and γ_B for H_2 which are compatible with B and $\sigma_B(h_2) \neq \gamma_B(h_2)$. Hence, it is easy to see that by using the P. Hall's theorem on the triangle $K[h_1, h_2, w]$, one can construct two different colourings σ and γ for $T_{H[h]}[w]$ which are compatible with Θ. This is a contradiction, and consequently, for any minimum-size fixing set of $T_{H[h]}[w]$ as Θ we have $|\Theta| = 2k-1$.
Using a similar reasoning, one may note that for any minimum-size fixing set of $T_{H[h]}[w]$ as Θ, it is impossible to have only one fixing-edge in Θ that is incident to w.
Also, it is clear that the number of fixing-edges in Θ incident to w can not be equal to 2, because in that case, the number of fixing-edges in Θ incident to H_1 or H_2 must be less than $k-1$ which is not possible. ∎

3 Algorithmic considerations

3.1 A circuit simulation lemma

Let C be a Boolean circuit computing an n-variable function[2] f. Our goal in this section is to construct a graph G on the vertex set $X \cup W \cup Y$, where $X = \{x_1, x_2, \ldots, x_n\}$, $R = \{⓪, ①, ⊛\} \subseteq W$ and $Y = \{y\}$, in such a way

[2]We loosely do not distinguish between a Boolean expression and the corresponding Boolean circuit.

that,

i) $\chi(\mathrm{G}) = 3$.

ii) In any 3-colouring of G with three colours $\{0, 1, *\}$, the elements of R are forced to take different colours, and the elements of X cannot take the same colour as the vertex ⊛.

iii) Any arbitrary function $\sigma_0 : X \cup R \rightarrow \{0, 1, *\}$ with $\sigma_0(ⓘ) = i$, $(i = 0, 1, *)$ and $\sigma_0(X) \subseteq \{0, 1\}$, is *uniquely* extendable to a proper 3-colouring σ of G in an efficient and computable way.

iv) We have $\sigma(y) = f(\sigma(x_1), \sigma(x_2), \ldots, \sigma(x_n))$.

v) The size of G is linearly bounded by the size of C.

Since in what follows we need to construct graphs using amalgams, we introduce the concept of a *marked graph* and we use the corresponding formal constructions to present the necessary amalgam constructions in an efficient and precise form. (Although what follows is a concrete formulation which is more or less classical, e.g. as in the theory of graph grammars [6], or amalgamated products of groups [12], a reader who is not familiar with the basic concepts of category theory may intuitively think of constructions as amalgams by disjoint union and identification of vertices. Examples 1 and 2 are sufficient to grasp the essence of the definition necessary to follow the main results of the paper.)
Let $X = \{x_1, x_2, \ldots, x_k\}$ and G be a set and a graph, respectively, and also, consider a one-to-one map $\varrho : X \longrightarrow V(\mathrm{G})$. Evidently, one can consider ϱ as a graph monomorphism from the empty graph X on the vertex set X to the graph G, where in this setting we interpret the situation as a *labeling* of some vertices of G by the elements of X. The data introduced by (X, G, ϱ) is called a *marked graph* G marked by the set X through the map ϱ. Note that (by abuse of language) we may introduce the corresponding marked graph as $\mathrm{G}[x_1, x_2, \ldots, x_k]$ when the definition of ϱ (especially its range) is clear from the context. Also, (by abuse of language) we may refer to *the vertex* x_i as the vertex $\varrho(x_i) \in V(\mathrm{G})$. This is most natural when $X \subseteq V(G)$ and vertices in X are marked by the corresponding elements in $V(G)$ through the identity mapping. As an example, Figure 3(a) shows a graph, K_3, marked by the set $X = \{⓪, ①, ⊛\}$.
If $\varsigma : X \longrightarrow Y$ is an onto (but not necessarily one-to-one) map, then one can obtain a new marked graph (Y, H, τ) by considering the push-out of the diagram

$$\mathrm{Y} \xleftarrow{\varsigma} \mathrm{X} \xrightarrow{\varrho} \mathrm{G}$$

in the category of graphs. It is easy to check that the push-out exists and is a monomorphism. Also, it is easy to see that the new marked graph

(Y, H, τ) can be obtained from (X, G, ϱ) by identifying the vertices in each inverse-image of ς. Hence, again (by abuse of language) we may denote (Y, H, τ) as $\mathrm{G}[\varsigma(x_1), \varsigma(x_2), \ldots, \varsigma(x_k)]$ where we allow repetition in the list appearing in the brackets. Note that with this notation one may interpret x_i's as a set of *variables* in the *graph structure* $\mathrm{G}[x_1, x_2, \ldots, x_k]$, such that when one assigns other (new and not necessarily distinct) *values* to these variables one can obtain some other graphs (by identification of vertices).
On the other hand, given two marked graphs (X, G, ϱ) and (Y, H, τ) with $X = \{x_1, x_2, \ldots, x_k\}$ and $Y = \{y_1, y_2, \ldots, y_l\}$, one can construct their amalgam $(X, \mathrm{G}, \varrho) + (Y, \mathrm{H}, \tau)$ by forming the push-out of the following diagram,

$$\mathrm{H} \xleftarrow{\tilde{\tau}} \mathrm{X} \cap \mathrm{Y} \xrightarrow{\tilde{\varrho}} \mathrm{G},$$

in which $\tilde{\tau} \stackrel{\text{def}}{=} \tau|_{X \cap Y}$ and $\tilde{\varrho} \stackrel{\text{def}}{=} \varrho|_{X \cap Y}$. Following our previous notations we may denote the new structure by

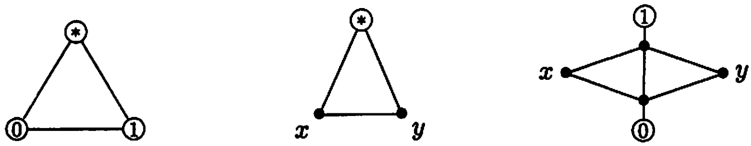
$$\mathrm{G}[x_1, x_2, \ldots, x_k] + \mathrm{H}[y_1, y_2, \ldots, y_l]$$

if there is no confusion about the definition of mappings. Note that when $\mathrm{X} \cap \mathrm{Y}$ is the empty set, then the amalgam is the *disjoint union* of the two marked graphs. Also, by the universal property of the push-out diagram, the amalgam can be considered as marked graphs marked by X, Y, $X \cup Y$ or $X \cap Y$.
Sometimes it is preferred to partition the list of variables in a graph structure as,

$$\mathrm{G}[x_1, x_2, \ldots, x_k; y_1, y_2, \ldots, y_l; z_1, z_2, \ldots, z_m]. \tag{2}$$

In these cases we may either follow this extended notation, or use bold symbols for an ordered list of variables and write this graph structure as $\mathrm{G}[\mathbf{x}; \mathbf{y}; \mathbf{z}]$ (if there is no confusion about the size of the lists). Moreover, it is understood that a repeated appearance of a graph structure in an expression as $\mathrm{G}[v] + \mathrm{G}[v, w]$ is always considered as different isomorphic copies of the structure marked properly by the indicated labels (e.g. $\mathrm{G}[v] + \mathrm{G}[v, w]$ is an amalgam constructed by two different isomorphic copies of G identified on the vertex v where the vertex w in one of these copies is marked).
By $\mathrm{K}[v_1, v_2, \ldots, v_k]$ we mean a k-clique on $\{v_1, v_2, \ldots, v_k\}$ marked by its own set of vertices. Specially, a single edge is denoted by $\varepsilon[v_1, v_2]$ (i.e., $\varepsilon[v_1, v_2] = \mathrm{K}[v_1, v_2]$). In our constructions we use three specific vertices ⓪, ① and ⊛ as *references*, in the sense that, the colours of ⓪ and ① play the role of 0 and 1 signals that correspond to *false* and *true* truth values. In this setup usually a 3-clique K[⓪,①,⊛] is used to ensure that ⓪, ① and ⊛ take pairwise different colours (Figure 3(a)).
Assumption: Since we will only be considering *simple* graphs throughout

the paper, whenever we consider amalgams, it is assumed that we are considering the base simple graph in which all loops are excluded.



(a) $\mathrm{K}[\textcircled{0},\textcircled{1},\circledast]$ (b) $\nu[x,y;\circledast]$ (c) $\zeta[x,y;\textcircled{0},\textcircled{1}]$

Figure 3: Some basic structures

Example 1. NOT gate and WIRE
Consider the marked graph $\nu[x,y;\circledast]$ depicted in Figure 3(b) and note that the structure

$$\mathrm{NOT}[x,y;\textcircled{0},\textcircled{1},\circledast] \stackrel{\mathrm{def}}{=} \nu[x,y;\circledast] + \mathrm{K}[\textcircled{0},\textcircled{1},\circledast]$$

simulates the NOT gate ($f_\nu(x) = \neg x$) in the sense described at the beginning of this section. Using the same idea one may define

$$\mathrm{WIRE}[x,y;\textcircled{0},\textcircled{1},\circledast] \stackrel{\mathrm{def}}{=} \zeta[x,y;\textcircled{0},\textcircled{1}] + \mathrm{K}[\textcircled{0},\textcircled{1},\circledast],$$

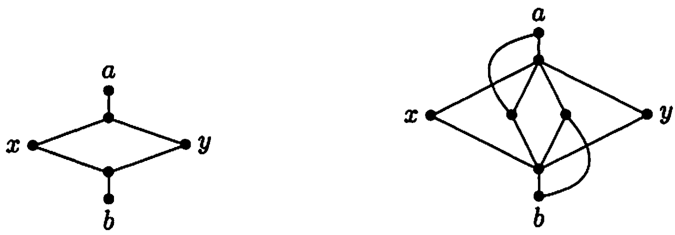
that simulates the WIRE $f_\zeta(x) = x$, in which

$$\zeta[x,y;\textcircled{0},\textcircled{1}] \stackrel{\mathrm{def}}{=} \mathrm{K}[x,v_1,v_2] + \mathrm{K}[y,v_1,v_2] + \varepsilon[\textcircled{1},v_1] + \varepsilon[v_2,\textcircled{0}],$$

is the marked graph depicted in Figure 3(c). ♣

Example 2. An interesting gadget
Our next basic structure $\bar{\kappa}[x,y;a,b]$ (Figure 4(a)) has the interesting property that, in every 3-colouring of $\bar{\kappa}[x,y;a,b] + \mathrm{K}[a,b,c]$, the vertex x takes the same colour as c if and only if the vertex y takes the same colour as c (with no other constraint). Alas, fixing the colours of x and y with respect to a,b and c does not always uniquely force the colouring of the rest of the structure.
However, by a combination of two $\bar{\kappa}$ structures as in Figure 4(b), we can construct the structure $\kappa[x,y;a,b]$ that also fulfills the unique colourability condition, i.e.

- In $\kappa[x,y;a,b] + \mathrm{K}[a,b,c]$ the vertex x takes the same colour as c if and only if the vertex y takes the same colour as c.



(a) $\bar{\kappa}[x, y; a, b]$ (b) $\kappa[x, y; a, b]$

Figure 4: Other basic structures

- If vertices x and y take their colours from the set of colours of a and b, then there is exactly one feasible extension of this partial colouring to a proper 3-colouring of $\kappa[x, y; a, b] + \mathrm{K}[a, b, c]$.
- If the colours of the vertices x and y are both the same as the colour of c, then there is exactly one feasible extension of this partial colouring to a proper 3-colouring of $\kappa[x, y; a, b] + \mathrm{K}[a, b, c]$.

♣

The next theorem is one of our main results which states that any Boolean function can be simulated by a 3-colourable graph in the sense we described at the beginning of this section. Also, in what follows we always assume that circuits are presented as generalized graphs (with different types of vertices) and we use the same type of coding for both circuits and graphs in this sense. (for more on this and the complexity background see [8, 11]).

Theorem 2. Circuit Simulation Lemma
There is a log-space algorithm $\mathcal{A}$, that given a Boolean circuit C for an n-variable Boolean function ψ, computes a graph structure

$$\overline{\mathrm{G}}_{\psi} \stackrel{\text{def}}{=} \mathrm{G}_{\psi}[x_1, x_2, \ldots, x_n; y; \textcircled{0}, \textcircled{1}, \textcircled{*}] + \mathrm{K}[\textcircled{0}, \textcircled{1}, \textcircled{*}]$$

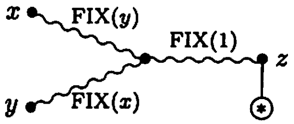
of size $O(|C|)$, such that

a) For any $1 \leq i \leq n$ and for any 3-colouring σ of $\overline{\mathrm{G}}_{\psi}$, we have $\sigma(x_i) \in \{\sigma(\textcircled{0}), \sigma(\textcircled{1})\}$.

b) For any truth assignment $A \stackrel{\text{def}}{=} (a_1, a_2, \ldots, a_n) \in \{0, 1\}^n$, there is a unique proper 3-colouring σ_A of $\overline{\mathrm{G}}_{\psi}$ satisfying

$$\sigma_A(\textcircled{i}) = i, \ (i = 0, 1, *) \quad \text{and} \quad \sigma_A(x_j) = a_j, \ (j = 1, 2, \ldots, n).$$

Moreover, for the unique colouring σ_A *we have* $\sigma_A(y) = \psi(a_1, a_2, \dots, a_n)$.



(a)

x	y		z
0	0	−	0
0	1	−	0
1	0	−	0
1	1	−	1

(b)

Figure 5: The AND gate (see Theorem 2).

Proof. First, we construct a simulator for the AND gate using the gadget of Example 2 as follows (see Figure 5). For each vertex x that can not take the same colour as ⊛, use the amalgam $\nu[x, \bar{x}, ⊛]$ (see Example 1) to construct a new vertex $\bar{x}$. Then define,

$$\mathrm{FIX}(x) \stackrel{\mathrm{def}}{=} \kappa[y, v; ⊛, \bar{x}], \quad \mathrm{FIX}(y) \stackrel{\mathrm{def}}{=} \kappa[x, v; ⊛, \bar{y}], \quad \mathrm{FIX}(1) \stackrel{\mathrm{def}}{=} \kappa[v, z; ⊛, ⓪],$$

$$\alpha[x, y; z; ⓪, ①, ⊛] \stackrel{\mathrm{def}}{=} \mathrm{FIX}(x) + \mathrm{FIX}(y) + \mathrm{FIX}(1) + \nu[x, \bar{x}, ⊛] + \nu[y, \bar{y}, ⊛] + \varepsilon[z, ⊛],$$

$$\mathrm{AND}[x, y; z; ⓪, ①, ⊛] \stackrel{\mathrm{def}}{=} \alpha[x, y; z; ⓪, ①, ⊛] + \mathrm{K}[⓪, ①, ⊛].$$

It is easy to check that the graph structures $\mathrm{NOT}[x, y; ⓪, ①, ⊛]$ (introduced in Example 1) and $\mathrm{AND}[x, y; z; ⓪, ①, ⊛]$ satisfy the properties (a) and (b) stated in the theorem, and clearly, any Boolean function ψ can be simulated by a graph structure $\mathrm{G}_\psi[x_1, x_2, \dots, x_n; y; ⓪, ①, ⊛]$ using amalgams of the graph structures $\nu[x, y; ⊛]$ and $\alpha[x, y; z; ⓪, ①, ⊛]$.
On the other hand, by the modularity of this construction, given a partial colouring of the vertices in $\{x_1, x_2, \dots, x_n\} \cup \{⓪, ①, ⊛\}$, and using the knowledge we have about the structure of G_ψ, one can complete the colouring of $\overline{\mathrm{G}}_\psi$ and find the extension in time linearly bounded by the size of the graph. To ensure this, note that the extension process can be decomposed into a (short) sequence of constant-size unique colouring problems.
Moreover, by the same argument, it is easy to see that the algorithm $\mathcal{A}$ uses a logarithmic amount of memory. ■

3.2 Some complexity results

In this section we determine the computational complexity of a number of problems related to unique colourability using the Circuit Simulation

Lemma (Theorem 2). In this regard, firstly, we show how some known results will follow easily from this lemma, and secondly, we prove the $\Sigma_2^{\mathbf{P}}$-completeness of the *fixing set problem* as the main result of this section. Since we use various versions of SAT to analyze the complexity of unique colourability problems, we define $\exists^1$ as a quantifier to mean "*there exist exactly one*". Consider the following problems,

PROBLEM $\exists^1$SAT
Given A Boolean expression ψ over a variable set $X = \{x_1, x_2, \ldots, x_n\}$.
Question Is it true that there is *exactly* one truth assignment $\eta : X \to \{0,1\}$ satisfying ψ?

It is easy to see that $\exists^1$SAT is in $\mathbf{D^P}$. Yet, it is not known or believed to be complete in this class, except that VALIANT AND VAZIRANI [13] have shown the completeness upto randomized reductions (see PAPADIMITRIOU [11]). Also, it is known that the problem is complete in **US** (see WELSH [14]).

PROBLEM $\exists^{1*}$SAT
Given A Boolean expression ψ over a variable set $X = \{x_1, x_2, \ldots, x_n\}$, and a satisfying assignment $\eta \models \psi$.
Question Is it true that there is no satisfying assignment for ψ other than η?

The problem is also trivially **coNP**-complete. Now, we consider the following unique-colouring problems,

PROBLEM $\exists^1$GRPHCOL
Given A graph G and an inteteger k.
Question Is G uniquely k-colourable?

PROBLEM $\exists^{1*}$GRPHCOL
Given A graph G and a proper k-colouring $\sigma : V(\mathrm{G}) \to \{1, 2, \ldots, k\}$.
Question Is it true that G has no k-colouring other than σ (up to a permutation of colours)?

As the first consequence of the Circuit Simulation Lemma we have,

Theorem C.

a) $\exists^1$GRPHCOL *is* **US**-*complete.*

b) (P. D. DAILEY [1]) $\exists^{1*}$GRPHCOL *is* **coNP**-*complete.*

Proof.

a) It is clear that $\exists^1$GRPHCOL is in **US**. To show the completeness, we use the following reduction from $\exists^1$SAT,

$$\exists^1 \mathbf{x} \; ; \; \psi(\mathbf{x}) \quad \rightarrow \quad \langle\!\langle (\overline{G}_\psi[\mathbf{x}; y; ⓪, ①, ⊛] + \varepsilon[y, ⓪]) \, , \, k{=}3 \rangle\!\rangle,$$

where $\overline{G}_\psi$ is an implementation of the Boolean expression ψ as explained in Theorem 2.

b) The problem $\exists^{1*}$GRPHCOL is trivially in **coNP**. To prove its completeness, let $\psi(\mathbf{x})$ be a Boolean expression, and $\eta \models \psi$. Construct the graph $\overline{G}_\psi[\mathbf{x}; y; ⓪, ①, ⊛]$ as in Theorem 2, and extend the partial colouring

$$\sigma(v) = \begin{cases} \eta(v) & \text{if } v \in \{x_1, x_2, \ldots, x_n\}, \\ i & \text{if } v = ⓘ, \end{cases}$$

to the rest of the graph. The required reduction from $\exists^{1*}$SAT is as follows,

$$\langle\!\langle (\exists^1 \mathbf{x} \; ; \; \psi(\mathbf{x})) \, , \, \eta \rangle\!\rangle \quad \rightarrow \quad \langle\!\langle (\tilde{G}_\psi[\mathbf{x}; y; ; ⓪, ①, ⊛] + \varepsilon[y, ⓪]) \, , \, \sigma \rangle\!\rangle.$$

■

Again consider the following version of SAT problem,

PROBLEM $\exists\exists^1$SAT

Given A Boolean expression $\psi(\mathbf{x}, \mathbf{y})$ over a variable set $X \cup Y$.

Question Is there any assignment $\eta|_X : X \rightarrow \{0,1\}$ having *exactly* one extension to $\eta : X \cup Y \rightarrow \{0,1\}$ satisfying ψ?

The problem $\exists\exists^1$SAT is trivially in $\mathbf{\Sigma_2^P}$. To see the $\mathbf{\Sigma_2^P}$-completeness consider the following reduction from $\exists\forall$SAT,

$$\exists \mathbf{x} \forall \mathbf{y} \; ; \; \psi(\mathbf{x}, \mathbf{y}) \; \rightarrow \; \exists \mathbf{x}, \mathbf{y}_0 \exists^1 \mathbf{y} \; ; \; \psi(\mathbf{x}, \mathbf{y}_0) \wedge ((\mathbf{y} {=} \mathbf{y}_0) \vee \neg\psi(\mathbf{x}, \mathbf{y})).$$

Now, consider the *defining set problem,*

PROBLEM DEFGRPHCOL

Given A graph G and two integers k and m.

Question Does the set of k-colourings of G have a defining set of size at most m?

We have,

Theorem D. (Hatami and Maserrat [7]) DEFGRPHCOL *is* $\Sigma_2^{\mathbf{P}}$-*complete.*

Proof. The problem DEFGRPHCOL is clearly in $\Sigma_2^{\mathbf{P}}$. Also, we show that that the following map introduces a reduction from $\exists\exists^1$SAT,

$$\exists \mathbf{x} \exists^1 \mathbf{y} \; ; \; \psi(\mathbf{x}, \mathbf{y})$$

$$\downarrow$$

$$\langle \tilde{\mathrm{G}}_\psi \stackrel{\text{def}}{=} (\overline{\mathrm{G}}_\psi[\mathbf{x}, \mathbf{y}; z; ⓪, ①, ⊛] + \textstyle\sum_i \varepsilon[x_i, u_i] + \varepsilon[⊛, a] + \varepsilon[⊛, b] + \varepsilon[⓪, c] + \varepsilon[z, ⓪]) \, , \, k=3 \, , \, m=|\mathbf{x}|+3 \rangle,$$

where $\overline{\mathrm{G}}_\psi$ is as in Theorem 2.
For this, let $\psi(\mathbf{x}, \mathbf{y})$ be a positive instance of $\exists\exists^1$SAT with the corresponding assignment $\eta|_X : X \to \{0, 1\}$. Then, by Theorem 2, it is easy to see that the following partial colouring σ is a defining set of size $|\mathbf{x}| + 3$ for the set of 3-colourings of $\tilde{\mathrm{G}}_\psi$,

$$\forall \, x_i u_i \in E(\tilde{\mathrm{G}}_\psi) \;\; \sigma(u_i) \stackrel{\text{def}}{=} \neg\eta(x_i), \quad \sigma(a) \stackrel{\text{def}}{=} 0, \quad \sigma(b) \stackrel{\text{def}}{=} 1, \quad \sigma(c) \stackrel{\text{def}}{=} 1.$$

On the other hand, if $\langle \tilde{\mathrm{G}}_\psi, k = 3, m = |\mathbf{x}| + 3 \rangle$ is a positive instance of DEFGRPHCOL where $\sigma|_S$ is a defining set of size $|S| = m = |\mathbf{x}| + 3$ for $\tilde{\mathrm{G}}_\psi$, then we claim that $\{u_i \mid x_i u_i \in E(\tilde{\mathrm{G}}_\psi)\} \cup \{a, b, c\} \subseteq S$, since the colour of a vertex of degree one can be chosen from a list of size at least two, even when one fixes the colours of all the rest of vertices in a partial 3-colouring of $\tilde{\mathrm{G}}_\psi$.
This proves that $\{u_i \mid x_i u_i \in E(\tilde{\mathrm{G}}_\psi)\} \cup \{a, b, c\} = S$, and also, it is easy to see that without loss of generality one may assume,

$$\sigma(a) \stackrel{\text{def}}{=} 0, \quad \sigma(b) \stackrel{\text{def}}{=} 1, \quad \sigma(c) \stackrel{\text{def}}{=} 1.$$

Hence, by the definition of a defining set, and Theorem 2 the partial truth assignment $\eta|_X \stackrel{\text{def}}{=} \sigma|_X$ is a solution for the positive instance $\psi(\mathbf{x}, \mathbf{y})$ of $\exists\exists^1$SAT.
Moreover, it is clear by the definition that the reduction is a polynomial-time many-to-one reduction, and the theorem is proved. ■

The next problem is related to the main result of this section as follows,

PROBLEM FIXGRPHCOL

Given A graph G and two integers k and m.

Question Does $\phi_0(G,k) \leq m$ hold?
(i.e., is it possible to *fix* a k-colouring on G, using a fixing set of size at most m?)

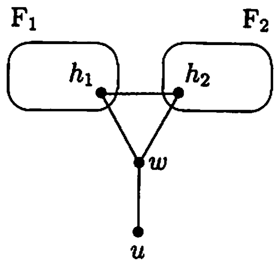


Figure 6: The graph $L[u] = T_{F[h]}[w] + \varepsilon[w,u]$ (see Theorem 3).

Theorem 3. FIXGRPHCOL *is* Σ_2^P*-complete.*

Proof. The problem FIXGRPHCOL is clearly in Σ_2^P. To show its completeness, define the graph structure $L[u]$ as follows,

$$L[u] \stackrel{\text{def}}{=} T_{F[h]}[w] + \varepsilon[w,u],$$

where $T_{F[h]}[w]$ is the graph structure introduced in Theorem 1 and F is the graph introduced in Proposition 1 (see Figures 1, 2 and 6).
Consider the following map, from $\exists\exists^1$SAT,

$$\exists \mathbf{x} \exists^1 \mathbf{y}\ ;\ \psi(\mathbf{x},\mathbf{y})$$

$$\downarrow$$

$$\langle \widehat{G}_\psi \stackrel{\text{def}}{=} (\overline{G}_\psi[\mathbf{x},\mathbf{y};z;⓪,①,⊛] + (\textstyle\sum_i L[x_i]) + L[⊛] + L[⊛] + L[⓪] + \varepsilon[z,⓪])\ ,\ k=3\ ,\ m=7(|\mathbf{x}|+3)\rangle,$$

where again $\overline{G}_\psi$ is as in Theorem 2.
Note that, if we fix the colour of u in a (partial) colouring of $L[u]$, then, by Proposition 1 and Theorem 1, still we need at least 7 fixing edges to fix a 3-colouring of $L[u]$, since w is an isolated vertex of $T_{F[h]}[w]$. This implies that $\phi_0(\overline{G}_\psi) \geq 7(|\mathbf{x}|+3)$, and consequently, similar to the proof of Theorem D, one may verify that the introduced map is a polynomial-time many-to-one reduction. ■

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