Counting the average size of Markov graphs

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ABSTRACT. We calculate the average size (i.e. number of arcs) of Markov graphs for several classes of vertex maps on finite trees. These are include arbitrary maps, permutations, cyclic permutations and the so-called neighbourhood maps. In the latter case we obtain an explicit formula for the size of corresponding Markov graphs and then provide sharp bounds for it in terms of the underlying trees.

1. Introduction

Let X be a finite undirected tree (i.e. connected acyclic graph) and $\sigma : V(X) \to V(X)$ be some map from the vertex set of X to itself. The Markov graph $\Gamma = \Gamma(X, \sigma)$ is a directed graph with the vertex set $V(\Gamma) = E(X)$ and the arc set $A(\Gamma) = \{(u_1 v_1, u_2 v_2) \in V(\Gamma) \times V(\Gamma) : u_2, v_2 \in [\sigma(u_1), \sigma(v_1)]_X\}$, where $[u, v]_X$ denotes the set of vertices on a unique shortest path between u and v in X. In other words, vertices in $\Gamma(X, \sigma)$ correspond to the edges of X and there is an arc $e_1 \to e_2$ in Γ if e_1 "covers" e_2 under σ.

One particular class of Markov graphs can be used to obtain an elegant combinatorial proof of Sharkovsky's theorem [**4, 13**]. Namely, for a continuous map $f : [0, 1] \to [0, 1]$ and its n-periodic point $x \in [0, 1]$ we can consider the orbit $orb_f(x) = \{x, f(x), \ldots, f^{n-1}(x)\}$ which is a finite subset of $[0, 1]$. Let $orb_f(x) = \{x_1 < \cdots < x_n\}$ be its natural ordering. The periodic graph has the vertex set $\{1, \ldots, n-1\}$ and the arc set $\{(i, j) : \min\{f(x_i), f(x_{i+1})\} \leqslant x_j < \max\{f(x_i), f(x_{i+1})\}\}$. Since the restriction of f to $orb_f(x)$ is a cyclic permutation, we can conclude that periodic graphs are exactly Markov graphs $\Gamma(X, \sigma)$ for paths X and their cyclic permutations σ.

In this paper we calculate the average size (i.e. number of arcs) of Markov graphs for several classes of vertex maps on trees using topological indices which

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arise from Chemical Graph Theory. These are include Wiener, Narumi-Katayama, Hosoya, general Randic and first general Zagreb indices. The maps that we consider are arbitrary maps, permutations, cyclic permutations and the so-called neighbourhood maps. In the latter case we obtain an explicit formula for the size of corresponding Markov graphs and then provide sharp bounds for it in terms of the underlying trees.

2. Preliminaries

We consider undirected as well as directed graphs (these are may contain loops). All our graphs will be simple and finite. An *undirected graph*, or just a *graph* is a pair $G = (V, E)$, where $V = V(G)$ is the set of its *vertices* and $E = E(G)$ is the set of its *edges* which are unordered pairs of vertices. Two vertices $u, v \in V(G)$ are *adjacent* in G if there is an edge $e = uv \in E(G)$. In this case, the edge e is *incident* to u as well as to v in G. Similarly, two edges are *adjacent* if they share a common vertex. The set $N_G(u) = \{v \in V(G) : uv \in E(G)\}$ is called the *neighbourhood* of a vertex $u \in V(G)$. Also, $N_G[u] = N_G(u) \cup \{u\}$ is the *closed neighbourhood* of u. The *degree* of u is the number $d_G(u) = |N_G(u)|$. A well-known *Handshaking Lemma* states that $\sum_{u \in V(G)} d_G(u) = 2|E(G)|$ for any graph G.

A vertex of degree one is called a *leaf vertex*. An edge is called a *leaf edge* if it is incident to a leaf vertex. The edge which is not a leaf edge will be called an *inner edge*.

Having a pair of graphs G_1 and G_2 we define their *join* as a graph $G_1 + G_2$ with the vertex set $V(G_1) \sqcup V(G_2)$ and the edge set $E(G_1) \sqcup E(G_2) \sqcup \{uv : u \in V(G_1), v \in V(G_2)\}$.

A graph is *connected* if there is a path between every pair of its vertices. The *connected component* of a graph is its maximal connected subgraph. By $k(G)$ we denote the number of connected components of G. The *distance* $d_G(u, v)$ between two vertices $u, v \in V(G)$ in a connected graph G is the number of edges on a shortest path joining u and v in G. The number $diam\, G = \max_{u,v \in V(G)} d_G(u, v)$ is called the *diameter* of G. For any set of vertices $A \subset V(G)$ we put $diam\, A = diam\, G[A]$, where $G[A]$ denotes the subgraph of G induced by A. Also, put $[u, v]_G = \{w \in V(G) : d_G(u, w) + d_G(w, v) = d_G(u, v)\}$ for any pair of vertices $u, v \in V(G)$ in a connected graph G.

A *tree* is a connected acyclic graph. Paths P_n and stars $K_{1,n-1}$ with n vertices provide natural examples of trees. For each edge $uv \in E(X)$ in a tree X we put $A_X(u, v) = \{w \in V(X) : d_X(w, u) < d_X(w, v)\}$. Clearly, $V(X) = A_X(u, v) \sqcup A_X(v, u)$ for any $uv \in E(X)$.

A *matching* is a set of pairwise non-adjacent edges. A matching $E' \subset E(G)$ is *perfect* if $V(G[E']) = V(G)$, i.e. if every vertex from $V(G)$ is incident to some edge from E'. It is easy to see that each graph which has a perfect matching necessarily has an even number of vertices. It is also well known that every tree has at most one perfect matching.

LEMMA 2.1. *For every tree X with $|V(X)| \geqslant 2$ there exists a set of leaf vertices $A \subset L(X)$ such that $X - A$ has a perfect matching.*

PROOF. We use induction on $|V(X)|$. If $|V(X)| = 2$, then $X \simeq P_2$ and thus X has a perfect matching consisting of one edge (in this case $A = \emptyset$).

Now let $|V(X)| \geqslant 3$. Consider the following two cases.

Case 1: There exists $u \in L(X)$ such that $L(X - \{u\}) = L(X) - \{u\}$.

By induction assumption there exists a set $A' \subset L(X - \{u\})$ such that $(X - \{u\}) - A'$ has a perfect matching. Putting $A = A' \cup \{u\}$ we obtain that $X - A = X - (A' \cup \{u\}) = (X - \{u\}) - A'$ has a perfect matching.

Case 2: For all leaf vertices $u \in L(X)$ we have $L(X - \{u\}) \neq L(X) - \{u\}$.

Note that in this case X is not a star $K_{1,n}, n \geqslant 2$. Also, X is not a star $K_{1,1}$ as $|V(X)| \geqslant 3$. For every leaf vertex $u \in L(X)$ let x_u denotes the unique vertex adjacent to u in X, i.e. let $N_X(u) = \{x_u\}$. Thus, $L(X - L(X)) = \{x_u : u \in L(X)\}$.

Since X is not a star, $|V(X - L(X))| \geqslant 2$ and therefore by induction assumption there exists $A' \subset L(X - L(X))$ such that $(X - L(X)) - A'$ has a perfect matching $E' \subset E((X - L(X)) - A')$. Put $A = \{u \in L(X) : x_u \notin A'\}$. Then $E'' = E' \cup \{ux_u : x_u \in A'\}$ is a perfect matching in $X - A$. $\qquad\square$

A *directed graph*, or just a *digraph* is a pair $D = (V, A)$, where $V = V(D)$ is the set of its *vertices* and $A = A(D) \subset V \times V$ is the set of its *arcs*. The existence of an arc $(u, v) \in A(D)$ will be also denoted as $u \to v$ in D. The arc of the form $u \to u$ is called a *loop* at the vertex u. For every vertex $u \in V(D)$ put $N_D^+(u) = \{v \in V(D) : u \to v \text{ in } D\}$ and $N_D^-(u) = \{v \in V(D) : v \to u \text{ in } D\}$. The cardinalities $d_D^+(u) = |N_D^+(u)|$ and $d_D^-(u) = |N_D^-(u)|$ are called the *outdegree* and the *indegree* of the vertex u, respectively. The *size* of a digraph D is the number of its arcs, i.e. the value $|A(D)|$. Clearly, $|A(D)| = \sum_{u \in V(D)} d_D^+(u) = \sum_{u \in V(D)} d_D^-(u)$ for every digraph D. The digraph is called *weakly connected* if its underlying graph (which is obtained by ignoring orientation of arcs and loops) is connected.

A *map* is just a function. By $Im\,\sigma$ and $fix\,\sigma$ we denote the image and the set of all fixed points of a map σ, respectively. An *orientation* of an undirected graph G is a map $\tau : E(G) \to V(G)$ such that $\tau(e)$ is incident to e for all edges $e \in E(G)$.

For a given tree X by $\mathcal{T}(X), \mathcal{P}(X)$ and $\mathcal{C}(X)$ we denote the classes of maps, permutations and cyclic permutations of the vertex set $V(X)$, respectively.

DEFINITION 2.1. Let X be a tree and $\sigma : V(X) \to V(X)$ be some map. The *Markov graph* $\Gamma = \Gamma(X, \sigma)$ is a digraph with the vertex set $V(\Gamma) = E(X)$ and $N_\Gamma^+(uv) = E([\sigma(u), \sigma(v)]_X)$ for all edges $uv \in E(X)$. In other words, for a pair of edges $e_1, e_2 \in E(G)$ there is an arc $e_1 \to e_2$ in Γ if e_1 "covers" e_2 under σ.
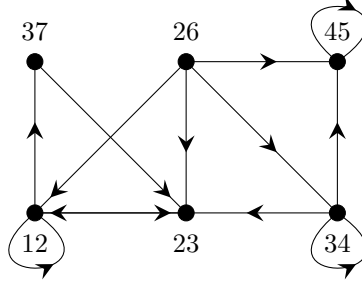
EXAMPLE 2.1. Consider a tree X with the vertex set $V(X) = \{1, \ldots, 7\}$ and the edge set $E(X) = \{12, 23, 34, 45, 26, 37\}$. For the vertex map

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 7 & 1 & 2 & 5 & 4 & 5 & 3 \end{pmatrix}$$

the Markov graph $\Gamma(X, \sigma)$ is shown in Figure 1.

LEMMA 2.2. [6] *Let X be a tree, $\sigma : V(X) \to V(X)$ be a map and $\Gamma = \Gamma(X, \sigma)$ be the corresponding Markov graph. Then for every edge $uv \in E(X)$ it holds*

(1) $d_\Gamma^+(uv) = d_X(\sigma(u), \sigma(v));$

FIGURE 1. Markov graph $\Gamma(X, \sigma)$ for the pair (X, σ).

(2) $d_\Gamma^-(uv) = k(\sigma^{-1}(A_X(u,v))) + k(\sigma^{-1}(A_X(v,u))) - 1.$

From Lemma 2.2 one can deduce the following bounds on the size of Markov graphs for arbitrary vertex maps on trees.

PROPOSITION 2.1. [**6**] *For any tree X and its map $\sigma : V(X) \to V(X)$ we have*

$$|Im\,\sigma| - 1 \leqslant |A(\Gamma(X,\sigma))| \leqslant (n-1) \cdot diam\,Im\,\sigma.$$

3. Arbitrary maps, permutations and cyclic permutations

In order to calculate the average size of Markov graphs for arbitrary maps, permutations and cyclic permutations we must consider the oldest and the most famous topological index. Namely, for every connected graph G the number

$$W(G) = \sum_{\{u,v\} \subset V(G)} d_X(u,v) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d_X(u,v)$$

is called its *Wiener index* [**16**]. For example, $W(K_{1,n-1}) = (n-1)^2$ and $W(P_n) = \frac{1}{6}n(n-1)(n+1)$. In [**2**] it was proved that for all n-vertex trees X the next inequalities hold: $W(K_{1,n-1}) \leqslant W(X) \leqslant W(P_n)$. Moreover, the Wiener index of trees can be calculated more efficiently than simply enumerating all possible distances between pairs of vertices.

LEMMA 3.1. [**10, 16**] *For any tree X we have the following equality:*

$$W(X) = \sum_{uv \in E(X)} |A_X(u,v)| \cdot |A_X(v,u)|.$$

For every connected graph G the number $Sz(G) = \sum_{uv \in E(G)} |A_G(u,v)| \cdot |A_G(v,u)|$ is called its *Szeged index* [**3**]. In [**5**] it is proved that $Sz(G) \geqslant W(G)$ for every connected graph G. Wherein, for trees X we have the equality $Sz(X) = W(X)$.

THEOREM 3.1. *For every tree X with $n \geqslant 3$ vertices it holds*

$$\frac{1}{n^n} \sum_{\sigma \in \mathcal{T}(X)} |A(\Gamma(X,\sigma))| = \frac{2(n-1)}{n^2} \cdot W(X),$$

$$\frac{1}{n!} \sum_{\sigma \in \mathcal{P}(X)} |A(\Gamma(X,\sigma))| = \frac{2}{n} \cdot W(X),$$

$$\frac{1}{(n-1)!} \sum_{\sigma \in \mathcal{C}(X)} |A(\Gamma(X,\sigma))| = \frac{2(n-3)}{(n-1)(n-2)} \cdot W(X) + \frac{n}{n-2}.$$

PROOF. For each pair of (not necessarily distinct) edges $e, e' \in E(X)$ define the class of maps $\mathcal{T}_{e',e}(X) = \{\sigma \in \mathcal{T}(X) : e' \to e \text{ in } \Gamma(X,\sigma)\}$. Clearly,

$$\sum_{\sigma \in \mathcal{T}(X)} |A(\Gamma(X,\sigma))| = \sum_{e,e' \in E(X)} |\mathcal{T}_{e',e}(X)| = \sum_{e \in E(X)} \sum_{e' \in E(X)} |\mathcal{T}_{e',e}(X)|.$$

If for an edge $e' = u'v' \in E(X)$ there is an arc $e' \to e$ in $\Gamma(X,\sigma)$, then $\sigma(u') \in A_X(u,v)$ and $\sigma(v') \in A_X(v,u)$, or $\sigma(u') \in A_X(v,u)$ and $\sigma(v') \in A_X(u,v)$. The number of maps σ with $\sigma(u') \in A_X(u,v)$ and $\sigma(v') \in A_X(v,u)$ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2}$. Similarly, the number of maps σ with $\sigma(u') \in A_X(v,u)$ and $\sigma(v') \in A_X(u,v)$ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2}$. Therefore,

$$\sum_{e' \in E(X)} |\mathcal{T}_{e',e}(X)| = 2(n-1) \cdot |A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2}$$

for all edges $e = uv \in E(X)$.

Using Lemma 3.1, we obtain the desired equality

$$\frac{1}{n^n} \sum_{\sigma \in \mathcal{T}(X)} |A(\Gamma(X,\sigma))| = \frac{1}{n^n} \sum_{e \in E(X)} 2(n-1) \cdot |A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2}$$

$$= \frac{2(n-1)}{n^2} \sum_{e \in E(X)} |A_X(u,v)| \cdot |A_X(v,u)|$$

$$= \frac{2(n-1)}{n^2} \cdot W(X).$$

In a similar way to arbitrary maps, for each pair of edges $e, e' \in E(X)$ consider the class of permutations $\mathcal{P}_{e',e}(X) = \{\sigma \in \mathcal{P}(X) : e' \to e \text{ in } \Gamma(X,\sigma)\}$. Then

$$\sum_{\sigma \in \mathcal{P}(X)} |A(\Gamma(X,\sigma))| = \sum_{e \in E(X)} \sum_{e' \in E(X)} |\mathcal{P}_{e',e}(X)|.$$

For every edge $e' = u'v' \in E(X)$ the number of permutations σ with $\sigma(u') \in A_X(u,v)$ and $\sigma(v') \in A_X(v,u)$ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot (n-2)!$. Similarly, the number of permutations σ with $\sigma(u') \in A_X(v,u)$ and $\sigma(v') \in A_X(u,v)$ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot (n-2)!$. This means that

$$\sum_{e' \in E(X)} |\mathcal{P}_{e',e}(X)| = 2(n-1) \cdot |A_X(u,v)| \cdot |A_X(v,u)| \cdot (n-2)!$$

for each $e = uv \in E(X)$.

Thus, we obtain the equality

$$\frac{1}{n!}\sum_{\sigma\in\mathcal{P}(X)}|A(\Gamma(X,\sigma))| = \frac{1}{n!}\sum_{e\in E(X)}2(n-1)\cdot|A_X(u,v)|\cdot|A_X(v,u)|\cdot(n-2)!$$

$$= \frac{2}{n}\sum_{e\in E(X)}|A_X(u,v)|\cdot|A_X(v,u)|$$

$$= \frac{2}{n}\cdot W(X).$$

Finally, for each pair $e, e' \in E(X)$ consider the class of cyclic permutations $\mathcal{C}_{e',e}(X) = \{\sigma \in \mathcal{C}(X) : e' \to e \text{ in } \Gamma(X,\sigma)\}$. Similarly to the above cases, we have the equality

$$\sum_{\sigma\in\mathcal{C}(X)}|A(\Gamma(X,\sigma))| = \sum_{e\in E(X)}\sum_{e'\in E(X)}|\mathcal{C}_{e',e}(X)|.$$

In order to calculate the sum $\sum_{e'\in E(X)}|\mathcal{C}_{e',e}(X)|$ for each edge $e = uv \in E(X)$ consider the following triplet of sets:

$$\bigcup_{e'\in E(A_X(u,v))}\mathcal{C}_{e,e'}(X),\ \bigcup_{e'\in E(A_X(v,u))}\mathcal{C}_{e,e'}(X) \text{ and } \mathcal{C}_{e,e}(X).$$

For every edge $e' = u'v' \in E(A_X(u,v))$ the number of cyclic permutations σ with $\sigma(u') \in A_X(u,v)$ and $\sigma(v') \in A_X(v,u)$ equals $(|A_X(u,v)|-1)|A_X(v,u)|\cdot(n-3)!$. Similarly, the number of cyclic permutations σ with $\sigma(u') \in A_X(v,u)$ and $\sigma(v') \in A_X(u,v)$ equals $(|A_X(u,v)|-1)|A_X(v,u)|\cdot(n-3)!$. Therefore,

$$|\bigcup_{e'\in E(A_X(u,v))}\mathcal{C}_{e,e'}(X)| = \sum_{e'\in E(A_X(u,v))}2\left(|A_X(u,v)|-1\right)\cdot|A_X(v,u)|\cdot(n-3)!$$

$$= 2(n-3)!\sum_{e'\in E(A_X(u,v))}\left(|A_X(u,v)|-1\right)^2\cdot|A_X(v,u)|.$$

Similarly, we obtain the equality

$$|\bigcup_{e'\in E(A_X(v,u))}\mathcal{C}_{e,e'}(X)| = 2(n-3)!\sum_{e'\in E(A_X(v,u))}\left(|A_X(v,u)|-1\right)^2\cdot|A_X(u,v)|.$$

Now we need to calculate the cardinality of $\mathcal{C}_{e,e'}(X)$. At first, note that the number of cyclic permutations σ for which there is a loop $e \to e$ in $\Gamma(X,\sigma)$ and $\sigma(u) \neq v, \sigma(v) \neq u$ clearly equals $2(|A_X(u,v)|-1)(|A_X(v,u)|-1)$. On the other hand, the number of cyclic permutations σ for which $e \to e$ in $\Gamma(X,\sigma)$ and $\sigma(u) = v$ or $\sigma(v) = u$ equals $(|A_X(u,v)|-1+|A_X(v,u)|-1)\cdot(n-3)! = (n-2)\cdot(n-3)!$. Thus,

$$|\mathcal{C}_{e,e}(X)| = (2(|A_X(u,v)|-1)\cdot(|A_X(v,u)|-1)+n-2)\cdot(n-3)!.$$

Combining the above equalities, we obtain

$$\sum_{e' \in E(X)} |\mathcal{C}_{e',e}(X)| = |\bigcup_{e' \in E(A_X(u,v))} \mathcal{C}_{e,e'}(X)| + |\bigcup_{e' \in E(A_X(v,u))} \mathcal{C}_{e,e'}(X)| + |\mathcal{C}_{e,e}(X)|$$

$$= 2(n-3)! \sum_{e' \in E(A_X(u,v))} (|A_X(u,v)| - 1)^2 \cdot |A_X(v,u)|$$

$$+ 2(n-3)! \sum_{e' \in E(A_X(v,u))} (|A_X(v,u)| - 1)^2 \cdot |A_X(u,v)|$$

$$+ (2(|A_X(u,v)| - 1) \cdot (|A_X(v,u)| - 1) + n - 2) \cdot (n-3)!$$

$$= (2|A_X(u,v)|^2 \cdot |A_X(v,u)| + 2|A_X(v,u)|^2 \cdot |A_X(u,v)|$$

$$- 6|A_X(u,v)| \cdot |A_X(v,u)| + n) \cdot (n-3)!$$

$$= ((2n-6)|A_X(u,v)| \cdot |A_X(v,u)| + n) \cdot (n-3)!.$$

Finally,

$$\frac{1}{(n-1)!} \sum_{\sigma \in \mathcal{C}(X)} |A(\Gamma(X,\sigma))| = \frac{1}{(n-1)!} \sum_{e \in E(X)} \sum_{e' \in E(X)} |\mathcal{C}_{e',e}(X)|$$

$$= \frac{2(n-3)}{(n-1)(n-2)} \cdot W(X) + \frac{n}{n-2}.$$

$\square$

4. Edge labellings and neighbourhood maps

DEFINITION 4.1. For a tree X and a map $\sigma : V(X) \to V(X)$ define its *edge labelling* $\tau_\sigma : E(X) \to V(X) \cup \{1, -1\}$ in the following way:

$$\tau_\sigma(e) = \begin{cases} u \text{ if } \sigma(u), \sigma(v) \in A_X(u,v), \\ v \text{ if } \sigma(u), \sigma(v) \in A_X(v,u), \\ 1 \text{ if } \sigma(u) \in A_X(u,v) \text{ and } \sigma(v) \in A_X(v,u), \\ -1 \text{ if } \sigma(u) \in A_X(v,u) \text{ and } \sigma(v) \in A_X(u,v) \end{cases}$$

for all $e = uv \in E(X)$. Thus, if $\tau_\sigma(e) = u$, then the edge e gets an orientation $u \to v$. Otherwise, the edge e is σ-*positive* or σ-*negative* depending on the sign of $\tau_\sigma(e)$. By $X(\tau_\sigma)$ we denote the mixed tree which corresponds to the pair (X, σ).

EXAMPLE 4.1. Consider the pair (X, σ) from Example 2.1. Then the corresponding mixed tree $X(\tau_\sigma)$ is shown in Figure 2 (signs $+$ and $-$ denote σ-positive and σ-negative edges, respectively).

Edge labelling $\tau : E(X) \to V(X) \cup \{1, -1\}$ on a tree X is called *admissible* if there exists a map $\sigma : V(X) \to V(X)$ with $\sigma_\tau = \sigma$. The set of all admissible edge labellings of X is denoted by $\mathcal{D}(X)$.

THEOREM 4.1. [7] *Let X be a tree and $\tau : E(X) \to V(X) \cup \{1, -1\}$ be an edge labelling such that the restriction $\tau|_{\tau^{-1}(V(X))}$ is an orientation of X. Then τ is admissible if and only if*
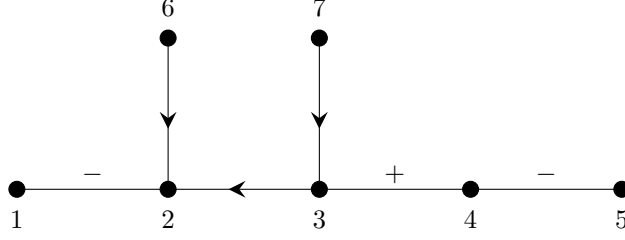
FIGURE 2. Mixed tree $X(\tau_\sigma)$ for the pair (X, σ).

(1) *each vertex from $X(\tau)$ has an outdegree at most one;*
(2) *each vertex from $X(\tau)$ is incident to at most one τ-negative edge;*
(3) *if the vertex from $X(\tau)$ is incident to some τ-negative edge, then it has zero outdegree in $X(\tau)$.*

With every admissible edge labelling τ on X we can associate the map

$$\sigma_\tau(u) = \begin{cases} v \text{ if } v \in N_X(u) \text{ and } \tau(uv) = v \text{ or } \tau(uv) = -1, \\ u \text{ otherwise} \end{cases}$$

for all $u \in V(X)$. Observe that for any pair $\tau_1, \tau_2 \in \mathcal{D}(X)$ we have $\sigma_{\tau_1} = \sigma_{\tau_2}$ if and only if $\tau_1 = \tau_2$.

A map $\sigma : V(G) \to V(G)$ from the vertex set of a graph G to itself is called a *neighbourhood map* if $\sigma(u) \in N_G[u]$ for all vertices $u \in V(G)$. Clearly, for connected graphs G (in particular, for trees) the map σ is a neighbourhood map if and only if $d_G(u, \sigma(u)) \leqslant 1$ for all $u \in V(G)$. The class of all neighbourhood maps on a graph G is denoted by $\mathcal{N}(G)$.

REMARK 4.1. For trees X the class $\mathcal{P}(X) \cap \mathcal{N}(X)$ of neighbourhood permutations has been studied in [**14, 15**] under the name of *compatible permutations*. For example, it is easy to see that each edge transposition $(uv), uv \in E(X)$ on a tree X is a compatible permutation. This implies that the class of compatible permutations of X is a generating set for the group of all permutations $\mathcal{P}(X)$. Moreover, the minimum number k such that each permutation of an n-vertex tree can be decomposed into a product of k compatible permutations, is at least n [**15**] (the equality $k = n$ holds for n-vertex paths P_n [**14**]).

PROPOSITION 4.1. *A map $\sigma : V(X) \to V(X)$ from the vertex set of a tree X to itself is a neighbourhood map if and only if there exists an admissible edge labelling $\tau \in \mathcal{D}(X)$ such that $\sigma = \sigma_\tau$.*

PROOF. From the definition it clearly follows that σ_τ is a neighbourhood map for any $\tau \in \mathcal{D}(X)$. Conversely, suppose that σ is a neighbourhood map. Putting $\tau = \tau_\sigma$ we obtain $\sigma = \sigma_\tau$.   □

Therefore, there is one-to-one correspondence between neighbourhood maps and admissible edge labellings on trees.

For a given graph G its *Narumi-Katayama index* [11] defined as the product $NK(G) = \prod_{u \in V(G)} d_G(u)$ of degrees over all vertices in G. Using this topological index we can calculate the number of admissible edge labellings on any given tree.

COROLLARY 4.1. *For every n-vertex tree X we have*

$$|\mathcal{D}(X)| = \frac{1}{n} \cdot NK(K_1 + X).$$

PROOF. Obviously, the number of admissible edge labellings τ equals the number of maps σ_τ. By Proposition 4.1 the last number equals the number of neighbourhood maps. Thus,

$$|\mathcal{D}(X)| = |\mathcal{N}(X)| = \prod_{u \in V(X)} |N_X[u]| = \prod_{u \in V(X)} (d_X(u) + 1) = \frac{1}{n} \cdot NK(K_1 + X).$$

$\square$

EXAMPLE 4.2. For $n \geqslant 2$ the star $K_{1,n-1}$ contains precisely $2^{n-1}n$ different admissible edge labellings. For $n = 3$ there is twelve admissible edge labellings on $K_{1,2} \simeq P_3$ (see Figure 3).
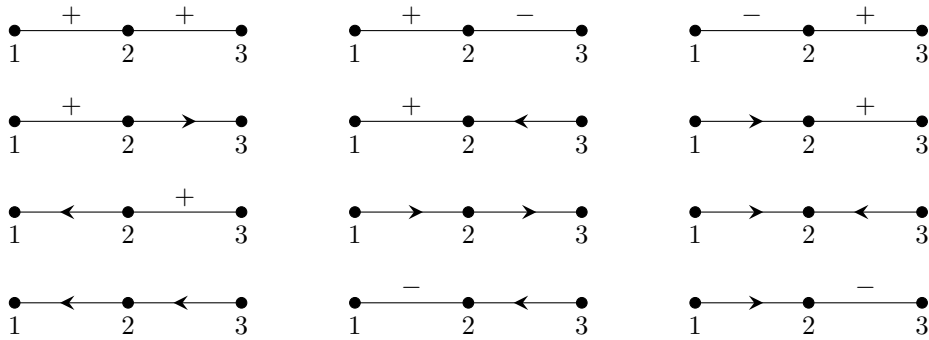

FIGURE 3. Twelve mixed trees $X(\tau)$ for $\tau \in \mathcal{D}(K_{1,2})$.

Given a tree X and a map $\sigma : V(X) \to V(X)$ by $n(X, \sigma)$ and $p(X, \sigma)$ we denote the number of σ-negative and σ-positive edges in X, respectively.

THEOREM 4.2. [7] *For every tree X and a map $\sigma : V(X) \to V(X)$ we have*

$$n(X, \sigma) + |fix\,\sigma| = p(X, \sigma) + 1.$$

COROLLARY 4.2. *Suppose that a map $\sigma : V(X) \to V(X)$ on a tree X does not have fixed points. Then X contains a σ-negative edge.*

Similarly to the average size of Markov graphs we can calculate the average number of σ-positive and σ-negative edges in trees for arbitrary maps, permutations and cyclic permutations.

PROPOSITION 4.2. *For every tree X with $n \geqslant 3$ vertices the following equalities hold:*

$$\frac{1}{n^n} \sum_{\sigma \in \mathcal{T}(X)} p(X, \sigma) = \sum_{\sigma \in \mathcal{T}(X)} n(X, \sigma) = \frac{W(X)}{n^2},$$

$$\frac{1}{n!} \sum_{\sigma \in \mathcal{P}(X)} p(X, \sigma) = \sum_{\sigma \in \mathcal{P}(X)} n(X, \sigma) = \frac{W(X)}{n(n-1)},$$

$$\frac{1}{(n-1)!} \sum_{\sigma \in \mathcal{C}(X)} p(X, \sigma) = \frac{W(X)}{(n-1)(n-2)} - \frac{n-1}{n-2},$$

$$\frac{1}{(n-1)!} \sum_{\sigma \in \mathcal{C}(X)} n(X, \sigma) = \frac{W(X)}{(n-1)(n-2)} - \frac{1}{n-2}.$$

PROOF. The proof is similar to the one of Theorem 3.1.

For any map $\sigma : V(X) \to V(X)$ an edge $e = uv \in E(X)$ is σ-positive if $\sigma(u) \in A_X(u,v)$ and $\sigma(v) \in A_X(v,u)$. The number of such maps σ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2}$. Thus,

$$\sum_{\sigma \in \mathcal{T}(X)} p(X, \sigma) = \sum_{uv \in E(X)} |A_X(u,v)| \cdot |A_X(v,u)| \cdot n^{n-2} = W(X) \cdot n^{n-2}.$$

Similarly one can prove that $\sum_{\sigma \in \mathcal{T}(X)} n(X, \sigma) = W(X) \cdot n^{n-2}$.

Further, the number of permutations σ with $\sigma(u) \in A_X(u,v)$ and $\sigma(v) \in A_X(v,u)$ equals $|A_X(u,v)| \cdot |A_X(v,u)| \cdot (n-2)!$. This means that

$$\sum_{\sigma \in \mathcal{P}(X)} p(X, \sigma) = \sum_{uv \in E(X)} |A_X(u,v)| \cdot |A_X(v,u)| \cdot (n-2)! = W(X) \cdot (n-2)!.$$

In a similar way we obtain the equality $\sum_{\sigma \in \mathcal{P}(X)} n(X, \sigma) = W(X) \cdot (n-2)!$.

Finally, the number of cyclic permutations σ for which the edge $e = uv$ is σ-positive equals $(|A_X(u,v)| - 1) \cdot (|A_X(v,u)| - 1) \cdot (n-3)!$. Thus,

$$\sum_{\sigma \in \mathcal{C}(X)} p(X, \sigma) = \sum_{uv \in E(X)} (|A_X(u,v)| - 1) \cdot (|A_X(v,u)| - 1) \cdot (n-3)!$$

$$= \sum_{uv \in E(X)} (|A_X(u,v)| \cdot |A_X(v,u)| - n + 1) \cdot (n-3)!$$

$$= (W(X) - (n-1)^2) \cdot (n-3)!.$$

The number of cyclic permutations σ for which the edge $e = uv$ is σ-negative equals $((|A_X(u,v)| - 1) \cdot (|A_X(v,u)| - 1) + n - 2) \cdot (n-3)!$. Therefore,

$$\sum_{\sigma \in \mathcal{C}(X)} n(X, \sigma) = \sum_{uv \in E(X)} ((|A_X(u,v)| - 1) \cdot (|A_X(v,u)| - 1) + n - 2) \cdot (n-3)!$$

$$= \sum_{uv \in E(X)} (|A_X(u,v)| \cdot |A_X(v,u)| - n + 1 + n - 2) \cdot (n-3)!$$

$$= (W(X) - n + 1) \cdot (n-3)!.$$

$\square$

In particular, Proposition 4.2 implies that

$$\frac{1}{(n-1)!}\sum_{\sigma\in\mathcal{C}(X)}n(X,\sigma) = \frac{W(X)}{(n-1)(n-2)} - \frac{1}{n-2} \geqslant \frac{W(K_{1,n-1})}{(n-1)(n-2)} - \frac{1}{n-2} = 1.$$

This means that the Markov graph $\Gamma(X,\sigma)$ of any cyclic permutation $\sigma \in \mathcal{C}(X)$ on average has at least one σ-negative edge, which is consistent with Corollary 4.2.

The following theorem contains an explicit formula for the size of Markov graphs for neighbourhood maps.

THEOREM 4.3. *For a tree X and its neighbourhood map $\sigma : V(X) \to V(X)$ we have*

$$|A(\Gamma(X,\sigma))| = |E(X)| + 2p(X,\sigma) - \sum_{u \in fix\,\sigma} d_X(u).$$

PROOF. Put $\Gamma = \Gamma(X,\sigma)$. Fix an arbitrary edge $e = uv \in E(X)$. If e is σ-negative, then clearly $d_\Gamma^-(e) = d_X(u) + d_X(v) - 1$. If e is σ-positive, then $d_\Gamma^-(e) = 1$. Finally, if $\tau_\sigma(e) = v$, then $d_\Gamma^-(e) = d_X(u) - 1$. It now follows that

$$|A(\Gamma)| = \sum_{e \in E(X)} d_\Gamma^+(e) = \sum_{\substack{uv \in E(X), \\ \tau_\sigma(uv)=-1}}(d_X(u) + d_X(v) - 1) + p(X,\sigma)$$

$$+ \sum_{\substack{\exists v \in N_X(u): \\ \tau_\sigma(uv)=v}}(d_X(u) - 1) = \sum_{\substack{uv \in E(X), \\ \tau_\sigma(uv)=-1}}(d_X(u) + d_X(v)) - n(X,\sigma) + p(X,\sigma)$$

$$+ \sum_{\substack{\exists v \in N_X(u): \\ \tau_\sigma(uv)=v}}d_X(u) - |\{u \in V(X) : \tau_\sigma(uv) = v \text{ for some } v \in N_X(u)\}|.$$

Combining Theorem 4.1 with Handshaking Lemma, we obtain

$$\sum_{\substack{uv \in E(X), \\ \tau_\sigma(uv)=-1}}(d_X(u) + d_X(v)) + \sum_{\substack{\exists v \in N_X(u): \\ \tau_\sigma(uv)=v}}d_X(u) = 2|E(X)| - \sum_{u \in fix\,\sigma}d_X(u).$$

In addition, the number of vertices $u \in V(X)$ for which there exists $v \in N_X(u)$ with $\tau_\sigma(uv) = v$ equals the number of arcs in $X(\tau_\sigma)$. The last number clearly equals $|E(X)| - n(X,\sigma) - p(X,\sigma)$. Combining these facts, we obtain the desired equality

$$|A(\Gamma)| = 2|E(X)| - \sum_{u \in fix\,\sigma}d_X(u) - n(X,\sigma) + p(X,\sigma) - |E(X)| + n(X,\sigma) + p(X,\sigma)$$

$$= |E(X)| + 2p(X,\sigma) - \sum_{u \in fix\,\sigma}d_X(u).$$

$\square$

A map $\sigma : V(X) \to V(X)$ on a tree X is called *expansive* if each vertex from $\Gamma(X,\sigma)$ has a loop. In other words, σ is expansive if $|\tau_\sigma(e)| = 1$ for all $e \in E(X)$. Having a matching $E' \subset E(X)$ put $\tau_{E'}(e) = -1$ for all $e \in E'$ and $\tau_{E'}(e) = 1$ for all $e \in E(X) - E'$. It is easy to see that $\tau_{E'} \in \mathcal{D}(X)$ and thus the map $\sigma_{E'} = \sigma_{\tau_{E'}}$ is correctly defined. Similarly, σ is *anti-expansive* provided $\Gamma(X,\sigma)$ does not have

any loops. In other words, σ is anti-expansive if $n(X, \sigma) = p(X, \sigma) = 0$. From Theorem 4.2 it follows that each anti-expansive map has a unique fixed point.

COROLLARY 4.3. *For every tree X and its anti-expansive neighbourhood map $\sigma : V(X) \to V(X)$ it holds $|A(\Gamma(X, \sigma))| = |E(X)| - d_X(u_0)$, where $fix\,\sigma = \{u_0\}$.*

Using Theorem 4.3, we can obtain sharp bounds on the size of Markov graphs for neighbourhood maps in terms of the corresponding trees.

THEOREM 4.4. *For every tree X with $|V(X)| \geqslant 2$ and its neighbourhood map σ the following sharp bounds hold:*

$$|E(X)| - |L(X)| \leqslant |A(\Gamma(X, \sigma))| \leqslant 2|E(X)| - 1.$$

PROOF. At first we prove the upper bound. Combining Theorem 4.2 with Theorem 4.3, we can conclude that

$$
\begin{aligned}
|A(\Gamma(X, \sigma))| &= |E(X)| + 2p(X, \sigma) - \sum_{u \in fix\,\sigma} d_X(u) \\
&\leqslant |E(X)| + 2p(X, \sigma) - |fix\,\sigma| \\
&= |E(X)| + p(X, \sigma) - n(X, \sigma) - 1 \\
&\leqslant 2|E(X)| - 1
\end{aligned}
$$

for all neighbourhood maps $\sigma \in \mathcal{N}(X)$.

Now we prove that the upper bound is sharp. By Lemma 2.1 there exists a set of leaf vertices $A \subset L(X)$ such that the tree $X - A$ has a perfect matching $E' \subset E(X - A)$. Clearly, E' is a matching in X. Consider the map $\sigma = \sigma_{E'}$ on $V(X)$. Obviously, $fix\,\sigma = A \subset L(X)$ which implies $\sum_{u \in fix\,\sigma} d_X(u) = |fix\,\sigma| = |A|$. Since σ is expansive, then

$$
\begin{aligned}
p(X, \sigma) = |E(X)| - n(X, \sigma) = |E(X)| - |E'| &= |E(X)| - \frac{|V(X - A)|}{2} \\
&= |E(X)| - \frac{|E(X)| + 1 - |A|}{2} = \frac{|E(X)| - 1 + |A|}{2}.
\end{aligned}
$$

Hence,

$$
\begin{aligned}
|A(\Gamma(X, \sigma))| &= |E(X)| + 2p(X, \sigma) - \sum_{u \in fix\,\sigma} d_X(u) \\
&= |E(X)| + 2 \cdot \frac{|E(X)| - 1 + |A|}{2} - |A| \\
&= 2|E(X)| - 1.
\end{aligned}
$$

Now let $\sigma \in \mathcal{N}(X)$ be an arbitrary neighbourhood map and $\Gamma = \Gamma(X, \sigma)$ be its Markov graph. Note that the inequality $d_\Gamma^+(e) \geqslant 1$ holds for all edges $e \in E(X)$ with $|\tau_\sigma(e)| = 1$. Thus, for every edge $e = uv \in E(X)$ with $d_\Gamma^+(e) = 0$ we necessarily have $\tau_\sigma(e) \in V(X)$. Without loss of generality, suppose $\tau_\sigma(e) = v$. Then $d_\Gamma^+(e) = d_X(u) - 1$, i.e. $d_X(u) = 1$. Therefore, for each inner edge $e \in E(X)$ we have $d_\Gamma^+(e) \geqslant 1$. This implies the lower bound $|A(\Gamma)| \geqslant |E(X)| - |L(X)|$.

Now we prove that the lower bound is sharp. If $|V(X)| = 2$, then $X \simeq P_2$ is a path with two vertices. For each of the two possible constant maps $\sigma : V(X) \to V(X)$ we clearly have $|A(\Gamma(X, \sigma))| = 0 = |E(X)| - |L(X)|$. Thus, suppose that $|V(X)| \geqslant 3$. Consider the following edge labelling:

$$\tau(e) = \begin{cases} 1 \text{ if } e \text{ is an inner edge in } X, \\ v \text{ if } e = uv \text{ for } u \in L(X) \end{cases}$$

for all $e \in E(X)$. It is easy to see that $\tau \in \mathcal{D}(X)$. Put $\sigma = \sigma_\tau$. Then $p(X, \sigma) = |E(X)| - |L(X)|$ and $fix\,\sigma = V(X) - L(X)$ which implies $\sum_{u \in fix\,\sigma} d_X(u) = 2|E(X)| - |L(X)|$. Hence, we obtain the desired equality

$$|A(\Gamma(X, \sigma))| = |E(X)| + 2p(X, \sigma) - \sum_{u \in fix\,\sigma} d_X(u)$$
$$= |E(X)| + 2(|E(X)| - |L(X)|) - 2|E(X)| + |L(X)|$$
$$= |E(X)| - |L(X)|.$$

$\square$

EXAMPLE 4.3. Consider the tree X from Example 2.1 and the following pair of sets of its leaf vertices: $A_1 = \{6\}, A_2 = \{1, 6, 7\}$. Then subtrees $X - A_1$ and $X - A_2$ contain perfect matchings $E_1 = \{12, 37, 45\}$ and $E_2 = \{23, 45\}$, respectively. Thus, for two neighbourhood maps $\sigma_1 = \sigma_{E_1} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 2 & 1 & 7 & 5 & 4 & 6 & 3 \end{pmatrix}$ and $\sigma_2 = \sigma_{E_2} = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 3 & 2 & 5 & 4 & 6 & 7 \end{pmatrix}$ we have $|A(\Gamma(X, \sigma_1))| = |A(\Gamma(X, \sigma_2))| = 11 = 2|E(X)| - 1$.

For every number $\alpha \in \mathbb{R} - \{0\}$ the *general Randic index* [1] of a graph G is the value $R^\alpha(G) = \sum_{uv \in E(G)} (d_G(u)d_G(v))^\alpha$. The number $R(G) = R^{-\frac{1}{2}}(G)$ is called the *Randic index* of G.

Similarly, for any number $\alpha \in \mathbb{R} - \{0, 1\}$ the *first general Zagreb index* [8, 9] of G defined as the value $Z_1^\alpha(G) = \sum_{u \in V(G)} d_G^\alpha(u)$. The number $Z_1(G) = Z_1^2(G)$ is called the *first Zagreb index* of G.

LEMMA 4.1. *For every n-vertex graph G the following equalities hold:*

$$\sum_{u \in V(G)} \frac{1}{d_G(u) + 1} = Z_1^{-1}(K_1 + G) - \frac{1}{n},$$

$$\sum_{uv \in E(G)} \frac{1}{(d_G(u) + 1)(d_G(v) + 1)} = R^{-1}(K_1 + G) - \frac{Z_1^{-1}(K_1 + G)}{n} + \frac{1}{n^2}.$$

PROOF. Let $H = K_1 + G$ and the vertex $v_0 \in V(H)$ corresponds to K_1. Clearly, $d_H(v_0) = |V(H)| - 1 = |V(G)| = n$ and $d_H(u) = d_G(u) + 1$ for all vertices $u \in V(H) - \{v_0\} = V(G)$. This implies the equality

$$Z_1^{-1}(H) = \sum_{u \in V(H)} \frac{1}{d_H(u)} = \frac{1}{n} + \sum_{u \in V(G)} \frac{1}{d_G(u) + 1}.$$

Similarly,

$$R^{-1}(H) = \sum_{uv \in E(H)} \frac{1}{d_H(u)d_H(v)} = \sum_{uv \in E(G)} \frac{1}{d_H(u)d_H(v)} + \sum_{uv_0 \in E(H)} \frac{1}{d_H(u)d_H(v_0)}$$

$$= \sum_{uv \in E(G)} \frac{1}{(d_G(u)+1)(d_G(v)+1)} + \frac{1}{d_H(v_0)} \cdot \sum_{u \in V(H)-\{v_0\}} \frac{1}{d_H(u)}$$

$$= \sum_{uv \in E(G)} \frac{1}{(d_G(u)+1)(d_G(v)+1)} + \frac{1}{n} \cdot \left(Z_1^{-1}(H) - \frac{1}{n} \right)$$

$$= \sum_{uv \in E(G)} \frac{1}{(d_G(u)+1)(d_G(v)+1)} + \frac{Z_1^{-1}(H)}{n} - \frac{1}{n^2}.$$

$\square$

Recall, that by Corollary 4.1 the number of neighbourhood maps on any n-vertex tree X equals $\frac{1}{n} \cdot NK(K_1 + X)$.

THEOREM 4.5. *For every n-vertex tree X we have*

$$\frac{1}{|\mathcal{N}(X)|} \sum_{\sigma \in \mathcal{N}(X)} |A(\Gamma(X,\sigma))| = (3 - \frac{2}{n}) \cdot Z_1^{-1}(K_1 + X) + 2R^{-1}(K_1 + X) + \frac{2}{n^2} - \frac{3}{n} - 3.$$

PROOF. Suppose that $\sigma \in \mathcal{N}(X)$ is a neighbourhood map. By definition $d_X(u, \sigma(u)) \leqslant 1$ for all $u \in V(X)$. By Lemma 2.2 $d_{\Gamma(X,\sigma)}^+(e) = d_X(\sigma(u), \sigma(v)) \leqslant d_X(u, \sigma(u)) + d_X(u,v) + d_X(v, \sigma(v)) = 3$ for all $e = uv \in E(X)$. For each edge $e \in E(X)$ consider the triplet of classes of neighbourhood maps $\mathcal{N}_{i,e}(X) = \{\sigma \in \mathcal{N}(X) : d_{\Gamma(X,\sigma)}^+(e) = i\}$, $1 \leqslant i \leqslant 3$. Clearly,

$$\sum_{\sigma \in \mathcal{N}(X)} |A(\Gamma(X,\sigma))| = \sum_{e \in E(X)} \sum_{i=1}^{3} i \cdot |\mathcal{N}_{i,e}(X)|.$$

We proceed by calculating cardinalities $|\mathcal{N}_{i,e}(X)|, 1 \leqslant i \leqslant 3$ for any fixed edge $e = uv \in E(X)$.

If $\sigma \in \mathcal{N}_{1,e}(X)$, then $\sigma(u) = u$ and $\sigma(v) = v$, or $\sigma(u) = v$ and $\sigma(v) = u$, or $\sigma(u) = v$ and $\sigma(v) \in N_X(v) - \{u\}$, or $\sigma(u) \in N_X(u) - \{v\}$ and $\sigma(v) = u$. Whence,

$$|\mathcal{N}_{1,e}(X)| = (1 + 1 + d_X(v) - 1 + d_X - 1) \cdot \prod_{w \neq u,v} (d_X(w) + 1)$$

$$= (d_X(u) + d_X(v)) \cdot \prod_{w \neq u,v} (d_X(w) + 1).$$

If $\sigma \in \mathcal{N}_{2,e}(X)$, then $\sigma(u) = u$ and $\sigma(v) \in N_X(v) - \{u\}$, or $\sigma(u) \in N_X(u) - \{v\}$ and $\sigma(v) = v$. Hence,

$$|\mathcal{N}_{2,e}(X)| = (d_X(u) + d_X(v) - 2) \cdot \prod_{w \neq u,v} (d_X(w) + 1).$$

Finally, for any $\sigma \in \mathcal{N}_{3,e}(X)$ it holds $\sigma(u) \in N_X(u) - \{v\}$ and $\sigma(v) \in N_X(v) - \{u\}$. This means that

$$|\mathcal{N}_{3,e}(X)| = (d_X(u) - 1) \cdot (d_X(v) - 1) \cdot \prod_{w \neq u,v}(d_X(w) + 1).$$

Therefore,

$$
\begin{aligned}
\sum_{\sigma \in \mathcal{N}(X)} |A(\Gamma(X, \sigma_\tau))| &= \sum_{uv \in E(X)} (|\mathcal{N}_{1,e}(X)| + 2|\mathcal{N}_{2,e}(X)| + 3|\mathcal{N}_{3,e}(X)|) \\
&= \sum_{uv \in E(X)} (d_X(u) + d_X(v) + 2 \cdot (d_X(u) + d_X(v) - 2) \\
&\quad + 3 \cdot (d_X(u) - 1)(d_X(v) - 1)) \cdot \prod_{w \neq u,v}(d_X(w) + 1) \\
&= \sum_{uv \in E(X)} (3 \cdot d_X(u)d_X(v) - 1) \cdot \prod_{w \neq u,v}(d_X(w) + 1).
\end{aligned}
$$

Thus,

$$\frac{1}{|\mathcal{N}(X)|} \sum_{\sigma \in \mathcal{N}(X)} |A(\Gamma(X, \sigma))| = \sum_{uv \in E(X)} \frac{3 \cdot d_X(u)d_X(v) - 1}{(d_X(u) + 1)(d_X(v) + 1)}.$$

On the other hand,

$$\frac{3 \cdot d_X(u)d_X(v) - 1}{(d_X(u) + 1)(d_X(v) + 1)} = \frac{3}{d_X(u) + 1} + \frac{2}{(d_X(u) + 1)(d_X(v) + 1)} - 3.$$

Now Lemma 4.1 yields the desired equality

$$
\begin{aligned}
\frac{1}{|\mathcal{N}(X)|} \sum_{\sigma \in \mathcal{N}(X)} |A(\Gamma(X, \sigma))| &= 3 \cdot (Z_1^{-1}(K_1 + G) - \frac{1}{n}) + 2 \cdot (R^{-1}(K_1 + G) \\
&\quad - \frac{Z_1^{-1}(K_1 + G)}{n} + \frac{1}{n^2}) - 3 \\
&= (3 - \frac{2}{n}) \cdot Z_1^{-1}(K_1 + X) + 2R^{-1}(K_1 + X) \\
&\quad + \frac{2}{n^2} - \frac{3}{n} - 3.
\end{aligned}
$$

□

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