A COMBINATORIAL VIEW ON STAR MOMENTS OF REGULAR DIRECTED GRAPHS AND TREES

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Abstract. We investigate the method of moments for d-regular digraphs and the limiting d-regular directed tree T_d as the number of vertices tends to infinity, in the same spirit as McKay [11] for the undirected setting. In particular, we provide a combinatorial derivation of the formula for the star moments (from a root vertex $o \in T_d$)

$$M_d(w) \quad := \sum_{\substack{v_0,v_1\dots,v_{k-1},v_k\in T_d\\ v_0=v_k=o}} A_d^{w_1}(v_0,v_1)A_d^{w_2}(v_1,v_2)\cdots A_d^{w_k}(v_{k-1},v_k)$$

with A_d the adjacency matrix of T_d, where $w := w_1\cdots w_k$ is any word on the alphabet $\{1,*\}$ and A_d^* is the adjoint matrix of A_d. Our analysis highlights a connection between the non-zero summands of $M_d(w)$ and the non-crossing partitions of $\{1,\dots,k\}$ which are in some sense compatible with w.

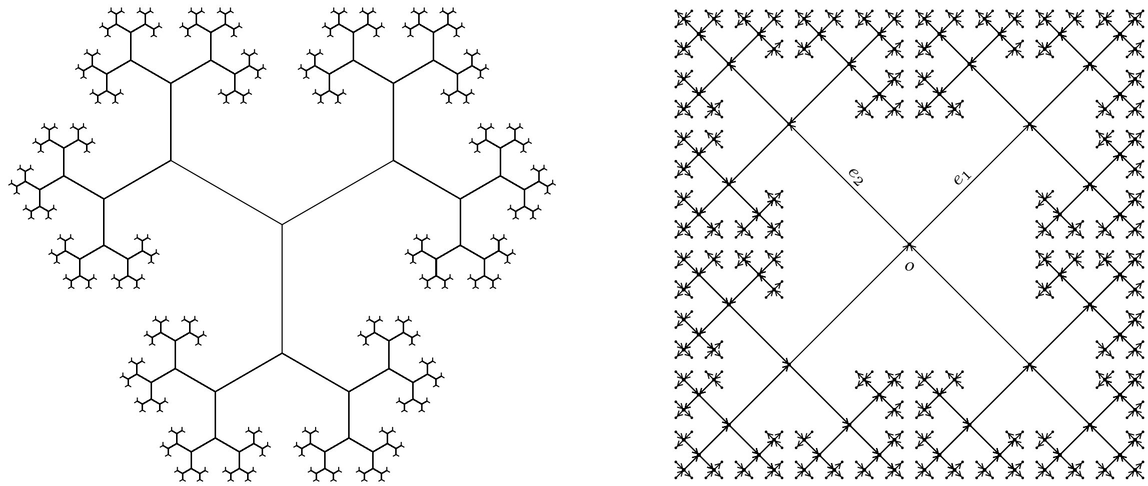
1. Introduction

Counting paths in graphs and other discrete structures is a standard question with applications to many areas of mathematics, see [10, 2, 18, 17] or the book [4]. In random matrix theory, this question is typically raised when studying the convergence of empirical spectral distributions (ESDs) through the method of moments, of which Wigner's original proof of the semicircular law [16] is a renowned example. Essentially, for random Hermitian matrices $W_n := (W_n(i,j))_{1\le i,j\le n}$ whose coefficients on and above the diagonal are i.i.d. with mean 0 and variance 1 (so called Wigner matrices), the different summands $\mathbb{E}\, W_n(i_1,i_2)\cdots W_n(i_k,i_1)$ occurring in the expansion of the states $\mathbb{E}\operatorname{Tr} W_n^k$, $k\ge 1$, can be related to certain cycles $i_1\to\cdots\to i_k\to i_1$ in a graph with vertex set $[n] := \{1,\dots,n\}$, and understanding the combinatorics of these cycles helps to determine how each of those summands contributes to the k-th moment of the limiting spectral distribution (the semicircle distribution).

In contrast, when $\mathbb{A}_{d,n}\in\{0,1\}^{n\times n}$ is the adjacency matrix of a uniformly sampled graph $\mathbb{G}_{d,n}$ with n vertices and constant degree $d\ge 2$ (that is, $\mathbb{G}_{d,n}$ is a uniform d-regular graph on $[n]$ and $\mathbb{A}_{d,n}(i,j)=1$ if and only if $\{i,j\}$ is an edge in $\mathbb{G}_{d,n}$), McKay [11] showed using the same method that the mean ESD $\mathbb{E}\,\frac{1}{n}\sum_{i=1}^n \delta_{\lambda_i(\mathbb{A}_{d,n})}$ associated with $\mathbb{A}_{d,n}$'s eigenvalues $\lambda_1(\mathbb{A}_{d,n}),\dots,\lambda_n(\mathbb{A}_{d,n})$ converges weakly (and in moments) towards a certain probability measure $\mu_{\mathbb{T}_d}$ which is now known as the Kesten–McKay distribution, in the sense that

$$\frac{1}{n}\,\mathbb{E}\sum_{i=1}^n f\big(\lambda_i(\mathbb{A}_{d,n})\big) \xrightarrow[n\to\infty]{} \int f(x)\,\mu_{\mathbb{T}_d}(\mathrm{d}x) \tag{1}$$

holds for any polynomial or continuous bounded function $f:\mathbb{R}\to\mathbb{R}$. When $f(x) := x^k$ for some positive integer k, the left-hand side of (1), which can also be written $\frac{1}{n}\,\mathbb{E}\operatorname{Tr}\mathbb{A}_{d,n}^k$, coincides with the expected total number of excursions of length k from a uniformly chosen vertex in $\mathbb{G}_{d,n}$, while the



(A) (B)

FIGURE 1. (A) The undirected tree $\mathbb{T}_3$ and (B) the directed tree T_2.

right-hand side of (1) counts the number of such excursions (from a fixed vertex) in the (infinite) d-regular tree $\mathbb{T}_d$, which is the Cayley graph of the free group with presentation $\langle e_1, \dots, e_d \mid e_i^2 = 1\rangle$, see Figure 1A. In fact, since the graphs $\mathbb{G}_{d,n}$ converge locally to the tree $\mathbb{T}_d$ as $n \to \infty$ (i.e., with respect to the Benjamini–Schramm topology [3]), the convergence (1) of their mean ESDs can be recovered from Bordenave–Lelarge's criterion [6].

In the present note, we adapt McKay's approach to the asymmetric (i.e., oriented) case. Although the local convergence as $n \to \infty$ of uniform d-regular digraphs $G_{d,n}$ towards the d-regular directed tree T_d does hold in a similar fashion (w.r.t. the "oriented" Benjamini–Schramm topology), it does not imply the convergence of ESDs anymore, and the analogue of (1) for oriented regular graphs is still an open question, known as the *oriented Kesten–McKay conjecture* [5]: the ESD of $G_{d,n}$ should converge towards a probability distribution on $\mathbb{C}$ corresponding in some sense to the spectral measure of T_d. One difficulty for this conjecture is that, because the adjacency matrix $A_{d,n}$ of $G_{d,n}$ is no longer Hermitian, the tracial moments $\mathbb{E}\operatorname{Tr} A_{d,n}^k$, $k \geq 0$, do not continuously determine the (now complex-valued) mean ESD of $A_{d,n}$. In fact, as $A_{d,n}$ is not even normal, neither do the star moments $\mathbb{E}\operatorname{Tr} A_{d,n}^w$ defined for any bit string $w := w_1 \cdots w_k$ on the alphabet $\Sigma := \{1, *\}$, where $A_{d,n}^w := A_{d,n}^{w_1} \cdots A_{d,n}^{w_k}$, and $A_{d,n}^*$ stands for the adjoint matrix of $A_{d,n} =: A_{d,n}^1$ (said differently, $A_{d,n}^*$ is the adjacency matrix of the graph $G_{d,n}^*$ obtained from $G_{d,n}$ by reversing each of its arcs). Nonetheless, investigating the star moments of regular digraphs remains interesting from a combinatorial perspective, and their convergence towards the corresponding star moments of the regular directed tree suggests that the conjecture holds true.

By definition, the d-regular directed tree T_d is the unique infinite, connected, and acyclic digraph in which every vertex has constant in- and out-degree $d \geq 2$. In other words, T_d is the Cayley graph of the free group $F_d := \langle e_1, \dots, e_d\rangle$ where unlike its symmetric version, the generators have no relations (see Figure 1B). We identify the vertex set of T_d with F_d, the root vertex $o \in T_d$ corresponding to the identity element, and we let A_d denote the adjacency matrix.

Theorem 1 (Convergence of star moments for uniform d-regular digraphs)**.** *For every $k \geq 0$ and every $w \in \Sigma^k$,*

$$\frac{1}{n}\mathbb{E}\operatorname{Tr} A_{d,n}^w \xrightarrow[n\to\infty]{} M_d(w) := A_d^w(o,o),$$

where $A_d^w(v,v')$ is defined for any pair of vertices $v, v' \in T_d$ by

$$A_d^w(v,v') \qquad := \sum_{\substack{v_0,v_1\dots,v_{k-1},v_k \in T_d \\ v_0=v,\ v_k=v'}} A_d^{w_1}(v_0,v_1)A_d^{w_2}(v_1,v_2)\cdots A_d^{w_k}(v_{k-1},v_k).$$

Note that $A_d^w(v,v') = \mathbb{1}_{\{v=v'\}}$ if $w = \varnothing \in \Sigma^0$ is the empty word. In any case, all summands of $A_d(v,v')$ are either 0 or 1, and each non-zero summand corresponds to a solution $(i_1,\dots,i_k) \in [d]^k$ to the word problem

$$v \cdot e_{i_1}^{w_1} \cdots e_{i_k}^{w_k} = v'$$

in the free group F_d, where e_i^* denotes the inverse of $e_i =: e_i^1$. We call such a solution $(i_1,\dots,i_k)$ a w-path from v to v', which we can also picture as

$$v =: v_0 \xrightarrow{w_1} v_1 \xrightarrow{w_2} \cdots \xrightarrow{w_{k-1}} v_{k-1} \xrightarrow{w_k} v_k := v',$$

where $v_j := v \cdot e_{i_1}^{w_1} \cdots e_{i_j}^{w_j}$ for all $0 \leq j \leq k$. In plain words, $M_d(w)$ is the cardinal of the set $\mathcal{P}(w)$ of all w-paths from o to o (or from any other vertex to itself, by transitivity of the Cayley graph T_d). We stress that we do not consider any randomness on T_d: in this respect, our purpose is different from Kesten [10], who studied spectral properties of random walks on the undirected regular tree $\mathbb{T}_d$.

In fact, Theorem 1 is a consequence of the following general criterion, similar to [11, Theorem 1.1]: under a growth assumption on the number of short cycles, we show that the star moments of deterministic d-regular digraphs converge to the star moments of the d-regular directed tree T_d.

Theorem 2 (Convergence of star moments for deterministic d-regular digraphs)**.** *Let G_n, $n \geq 1$, be a d-regular digraph with adjacency matrix A_n on a vertex set V_n. Let $k \geq 1$ and suppose that for every $j \in [k]$, the number $c_j(G_n)$ of cycles with length j in G_n (see (4)) fulfills*

$$\frac{c_j(G_n)}{|V_n|} \xrightarrow[n\to\infty]{} 0. \tag{2}$$

Then for every word $w \in \Sigma^k$,

$$\frac{1}{|V_n|}\operatorname{Tr} A_n^w \xrightarrow[n\to\infty]{} M_d(w). \tag{3}$$

Our last result is a combinatorial derivation of a formula for $M_d(w)$, which requires some notation. Recall that a partition π of $[k]$ can also be seen as the equivalence relation $\sim_\pi$ on $[k]$ such that $i \sim_\pi j \iff \exists V \in \pi,\ \{i,j\} \subseteq V$ for all $i,j \in [k]$. We say that π is *non-crossing*, written $\pi \in \mathrm{NC}(k)$, if $i_1 \sim_\pi j_1,\ i_2 \sim_\pi j_2 \implies j_1 \sim_\pi i_2$ for all $1 \leq i_1 < i_2 < j_1 < j_2 \leq k$. The cardinal $|\mathrm{NC}(k)|$ is equal to the ubiquitous Catalan number $C_k := \frac{1}{k+1}\binom{2k}{k}$, which is also [15] the cardinal $|\mathrm{NC}_2(2k)|$ of the non-crossing *pair* partitions of $[2k]$ (where each block has size 2). We further say that π is an *alternating non-crossing partition* of w ($\pi \in \mathrm{ANC}(w)$) if for every block $V := \{i_1 < \ldots < i_m\} \in \pi$, the subword $w|_V := w_{i_1} \cdots w_{i_m}$ of w is *alternating*, that is either of the form $w|_V = 1{*}\cdots1{*}$ or $w|_V = {*}1\cdots{*}1$ (so w and all blocks of π must have even size).

Theorem 3 (Combinatorial formula for $M_d(w)$)**.** *For every $k \geq 0$ and every $w \in \Sigma^k$,*

$$M_d(w) \quad = \sum_{\pi \in \mathrm{ANC}(w)} \left(\prod_{V \in \pi} (-1)^{\frac{|V|}{2}-1} C_{\frac{|V|}{2}-1} \right) d^{|\pi|}.$$

Notably, our proof shows that the w-paths may be counted by an inclusion-exclusion principle involving non-crossing pair partitions, thus explaining the presence of signs and Catalan numbers.

We mention that Theorems 1 and 3 may be recovered by taking a detour to free probability from a theorem of Nica [12], see Section 3, where we also put the oriented Kesten–McKay conjecture in more context. Our main motivation for this work is to provide direct combinatorial proofs, which we do in Section 2.

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2. Direct combinatorial proofs

2.1. **Convergence of star moments.** In this section, we prove Theorem 2 and its corollary, Theorem 1. Let G be a multigraph with adjacency matrix A and vertex set V. We call a sequence of $j \geq 1$ distinct arcs $\varepsilon_1, \ldots, \varepsilon_j$ (read in any cyclic order) a *plain cycle of length j in G* if each of the pairs $\{\varepsilon_1, \varepsilon_2\}, \ldots, \{\varepsilon_{j-1}, \varepsilon_j\}, \{\varepsilon_j, \varepsilon_1\}$ has a common vertex (we disregard the arc orientations). Discounting the cyclic orderings, the number of plain cycles with length j in G is then given by

$$c_j(G) := \frac{1}{2j} \sum_{w \in \Sigma^j} \sum_{\mathbf{v}} A^{w_1}(v_0, v_1) \cdots A^{w_j}(v_{j-1}, v_j), \tag{4}$$

the second summation ranging over every $\mathbf{v} := (v_0, \ldots, v_{j-1}, v_j = v_0) \in V^{j+1}$ such that the sequence $\left((v_{i-1}, v_i)^{w_i}\right)_{1 \leq i \leq j}$ is injective, where $(v, v')^1 := (v, v')$ and $(v, v')^* := (v', v)$ for all $v, v' \in V$.

Proof of Theorem 2. Write $v \in \mathcal{C}_{n,k}$ if there exists a vertex $v' \in V_n$ at distance at most k from v (i.e., $A_n^{w'}(v, v') > 0$ for some $w' \in \Sigma^j$, with $j \leq k$) and belonging to a cycle of length at most k in G_n. Note that, by union bound,

$$|\mathcal{C}_{n,k}| \leq \sum_{i=1}^{k} (2d)^i \sum_{j=1}^{k} j\, c_j(G_n) \leq k^2 (2d)^k \sum_{j=1}^{k} c_j(G_n).$$

Thus, on the one hand,

$$\frac{1}{|V_n|} \sum_{v \in \mathcal{C}_{n,k}} A_n^w(v, v) \leq k^2 (2d^2)^k \, \frac{\sum_{j=1}^k c_j(G_n)}{|V_n|} \xrightarrow[n \to \infty]{} 0, \tag{5}$$

using the trivial upper bound $A_n^w(v, v) \leq d^k$ and (2). On the other hand, for $v \notin \mathcal{C}_{n,k}$, no vertex accessible in at most k steps from v belongs to a cycle of length at most k. Since G_n is d-regular, the ball $B_{G_n}(v, k)$ of radius k around v must then look exactly like the ball $B_{T_d}(o, k)$. In particular, $A_n^w(v, v) = A_d^w(o, o)$ for all $v \in V_n \setminus \mathcal{C}_{n,k}$, and thus

$$\frac{1}{|V_n|} \sum_{v \notin \mathcal{C}_{n,k}} A_n^w(v, v) = \frac{|V_n| - |\mathcal{C}_{n,k}|}{|V_n|} \, A_d^w(o, o) \xrightarrow[n \to \infty]{} M_d(w). \tag{6}$$

Adding (5) and (6) then shows as stated that

$$\frac{1}{|V_n|}\operatorname{Tr} A_n^w = \frac{1}{|V_n|}\sum_{v\in\mathcal{C}_{n,k}} A_n^w(v,v) + \frac{1}{|V_n|}\sum_{v\notin\mathcal{C}_{n,k}} A_n^w(v,v) \xrightarrow[n\to\infty]{} M_d(w). \qquad \square$$

Remark 2.1. *As we can see from the proof, the condition* (2) *implies more generally that* $G_n \to T_d$ *with respect to the "oriented" Benjamini–Schramm topology: for every* $k \geq 1$*, the balls of radius* k *in* G_n *are eventually isomorphic to the ball of radius* k *in* T_d*. As such, Theorem 2 constitutes the non-symmetric version of* [1, Proposition 14].

Next, we show that the growth condition (2) of Theorem 2 holds in expectation for the uniform d-regular digraph $G_{d,n}$.

Lemma 2.2 ($G_{d,n}$ has few short cycles on average)**.** *For every* $k \geq 1$*,*

$$\frac{1}{n}\,\mathbb{E}\, c_k(G_{d,n}) \xrightarrow[n\to\infty]{} 0.$$

Proof. To estimate this expectation, it is convenient to work with the so called *configuration model* $\mathbf{CM}_{d,n}$, whose construction we briefly recall. First, to each vertex $i \in [n]$ we attach d unique incoming half-arcs $\varepsilon^+_{i+(p-1)n}$, $p \in [d]$, and another d unique outgoing half-arcs $\varepsilon^-_{i+(q-1)n}$, $q \in [d]$. Second, we choose uniformly at random a bijection $f_{d,n}$ joining each of the nd outgoing half-arcs to one of the nd incoming half-arcs (so there are $(nd)!$ possible choices for the bijection $f_{d,n}$). This gives rise to a random multigraph $\mathbf{CM}_{d,n}$ on $[n]$ in which the number of arcs $\mathbf{A}_{d,n}(i,j)$ from i to j equals the number of pairs $(p,q) \in [d]^2$ such that $f\big(\varepsilon^+_{i+(p-1)n}\big) = \varepsilon^-_{j+(q-1)n}$. Also, the distribution of $\mathbf{CM}_{d,n}$ conditional on the event

$$\mathcal{S}_{d,n} : \text{“}\mathbf{CM}_{d,n} \text{ is simple”} = \Big\{\mathbf{A}_{d,n}(i,i) = 0 \text{ and } \mathbf{A}_{d,n}(i,j) \leq 1 \text{ for all } i \neq j \in [n]\Big\}$$

coincides with the law of $G_{d,n}$: $\mathcal{L}(G_{d,n}) = \mathcal{L}(\mathbf{CM}_{d,n} \mid \mathcal{S}_{d,n})$. Now, the expected number $\mathbb{E}\, c_k\big(\mathbf{CM}_{d,n}\big)$ of cycles with length k is easy to estimate from (4):

$$\begin{aligned}
\mathbb{E}\, c_k(\mathbf{CM}_{d,n}) &\leq \frac{1}{2k}\cdot 2^k \cdot n^k \cdot d^k\, \mathbb{P}\big(f_{d,n}(\varepsilon_1^+) = \varepsilon_2^-, \ldots, f_{d,n}(\varepsilon_{k-1}^+) = \varepsilon_k^-, f_{d,n}(\varepsilon_k^+) = \varepsilon_1^-\big)\\
&= \frac{(2nd)^k\,(nd-k)!}{2k\,(nd)!}\\
&\sim \frac{2^{k-1}}{k},
\end{aligned}$$

by Stirling's formula. Furthermore, the probability $\mathbb{P}(\mathcal{S}_{d,n})$ of $\mathbf{CM}_{d,n}$ being simple was computed in [9] and is known [7] to be bounded away from zero as $n \to \infty$. Hence

$$\frac{1}{n}\,\mathbb{E}\, c_k(G_{d,n}) = \frac{1}{n}\,\mathbb{E}[c_k(\mathbf{CM}_{d,n}) \mid \mathcal{S}_{d,n}] \leq \frac{\mathbb{E}\, c_k(\mathbf{CM}_{d,n})}{n\,\mathbb{P}(\mathcal{S}_{d,n})} \xrightarrow[n\to\infty]{} 0,$$

which concludes the proof. $\square$

We are now ready to prove Theorem 1.

Proof of Theorem 1. Let $(n_p)_{p\geq 1}$ be an increasing sequence of integers tending to ∞. By Lemma 2.2, the convergence

$$\frac{1}{n_p}\, c_k\big(G_{d,n_p}\big) \xrightarrow[p\to\infty]{} 0$$

holds in expectation, and thus also in probability. A classical application of the Borel–Cantelli lemma shows that it further holds almost surely along a subsequence: there exists $(n'_p)_{p\geq 1} \subseteq (n_p)_{p\geq 1}$ such that

$$\frac{1}{n'_p}\, c_k\Big(G_{d,n'_p}\Big) \xrightarrow[p\to\infty]{} 0$$

almost surely. Then Theorem 2 entails that

$$\frac{1}{n'_p}\operatorname{Tr} A^w_{d,n'_p} \xrightarrow[p\to\infty]{} M_d(w)$$

holds almost surely. Since $\operatorname{Tr} A^w_{d,n'_p} \leq n'_p\, d^k$, the dominated convergence theorem then yields

$$\frac{1}{n'_p}\,\mathbb{E}\operatorname{Tr} A^w_{d,n'_p} \xrightarrow[p\to\infty]{} M_d(w).$$

We have just showed that every subsequence of $\frac{1}{n}\,\mathbb{E}\operatorname{Tr} A^w_{d,n}$, $n\geq 1$, admits a further subsequence converging to $M_d(w)$, so Theorem 1 is proved. □

2.2. **Combinatorial formula for $M_d(w)$.** Before establishing Theorem 3, let us warm up with a simple necessary condition for the set $\mathcal{P}(w)$ of w-paths from o to o to be non-empty.

Lemma 2.3. *If $w := w_1\cdots w_k$ is a word on Σ such that $\mathcal{P}(w)\neq\emptyset$, then w is balanced: $w\in\{1{*},{*}1\}^p$ with $k=2p$.*

Proof. We proceed by induction on k. The lemma holds trivially if $k=0$. Suppose $k\neq 0$. By assumption, there exists a w-path $\mathbf{p} := (i_1,\dots,i_k)$ from $v_0 := o$ to itself:

$$\mathbf{p} \;=\; v_0 \overset{w_1}{\text{---}} v_1 \overset{w_2}{\text{---}} \cdots \overset{w_k}{\text{---}} v_k = v_0,$$

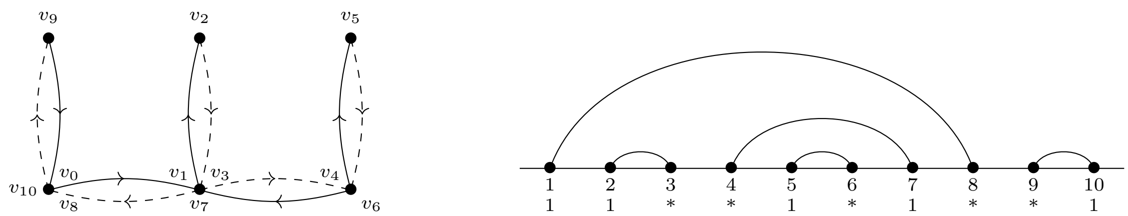
with $v_j := e_{i_1}^{w_1}\cdots e_{i_j}^{w_j}$, $0\leq j\leq k$, where we recall that the generators $e_1,\dots,e_d$ have no relations. In particular $v_1\neq v_0$ (because $e_{i_1}\neq o$), and thus $k\geq 2$. Let $2\leq r\leq k$ be the smallest index for which $v_r = v_0$, so

$$o = v_0 = v_r := e_{i_1}^{w_1}\Big(e_{i_2}^{w_2}\cdots e_{i_{r-1}}^{w_{r-1}}\Big)e_{i_r}^{w_r}, \qquad \text{that is,}\quad e_{i_r}^{w_r}e_{i_1}^{w_1} = \Big(e_{i_2}^{w_2}\cdots e_{i_{r-1}}^{w_{r-1}}\Big)^{-1}.$$

Since the generators have no relations, this forces $i_1 = i_r$ and $w_1\neq w_r$ (in other words, T_d has no cycle so the arc taken in $v_0 \overset{w_1}{\text{---}} v_1$ must match the one in $v_{r-1} \overset{w_r}{\text{---}} v_r = v_0$). Thus w is of the form $w = 1u{*}v$ or $w = {*}u1v$ where $u = w_2\cdots w_{r-1}$ and $v := w_{r+1}\cdots v_k$, and

$$\mathbf{p} \;=\; v_0 \overset{w_1}{\text{---}} \underbrace{v_1 \overset{w_2}{\text{---}} \cdots \overset{w_{r-1}}{\text{---}} v_{r-1}}_{u\text{-path}} \overset{w_r}{\text{---}} v_r = \underbrace{v_0 \overset{w_{r+1}}{\text{---}} v_{r+1} \overset{w_{r+2}}{\text{---}} \cdots \overset{w_k}{\text{---}} v_k}_{v\text{-path}} = v_0. \tag{7}$$

By induction, the smaller words u and v are balanced, and thus w is also balanced. □



(A) $\mathbf{p} = (i, j, j, k, \ell, \ell, k, i, m, m)$, $k \notin \{i, \ell\}$. (Arcs in T_d^* are drawn with a dashed line.)

(B) $\pi = \big\{\{1, 8\}, \{2, 3\}, \{4, 7\}, \{5, 6\}, \{9, 10\}\big\}$, with $\lhd_\pi = \{(1, 4), (4, 5)\}$ and $B(\pi) = \big\{\{4, 7\}, \{5, 6\}\big\}$.

FIGURE 2. (A) A w-path $\mathbf{p}$ and (B) its skeleton $\pi := \sigma_w(\mathbf{p})$, for $w := 11{*}{*}1{*}1{*}{*}1$.

A consequence of Lemma 2.3 is that $M_d(w) = 0$ if w is not balanced, so Theorem 3 is proved for such a word since then $\mathrm{ANC}(w) = \emptyset$. Note also that Theorem 3 holds if w is the empty word $\varnothing$, because $\mathrm{ANC}(\varnothing) := \{\emptyset\}$ is reduced to the empty partition and $\mathcal{P}(\varnothing) := \{\emptyset\}$ is reduced to the empty path. We henceforth assume $w := w_1 \cdots w_{2p}$ non-empty and balanced. The decomposition (7) of a w-path (from o to o) with respect to its first return time to the origin is clearly unambiguous. Putting aside the choice of vertices along the path, this gives rise to a "skeleton" which as we now claim can be encoded as a certain partition $\pi \in \mathrm{ANC}(w)$ whose every block $V \in \pi$ has cardinal $|V| = 2$; we write $\pi \in \mathrm{ANC}_2(w)$ and call it an *alternating non-crossing pair partition* of w. Specifically, let $\mathbf{p} := (i_1, \ldots, i_{2p}) \in \mathcal{P}(w)$ and denote by $r \in \{2, \ldots, 2p\}$ its first return time to o, that is $v_j := e_{i_1}^{w_1} \cdots e_{i_j}^{w_j} \neq o$ for every $1 \leq j < r$, and $v_r = o$. Then the skeleton of $\mathbf{p}$ is defined inductively as

$$\sigma_w(\mathbf{p}) := \Big\{\{1, r\}\Big\} \cup \Big\{V + 1 : V \in \sigma_u(i_2, \ldots, i_{r-1})\Big\} \cup \Big\{V + r : V \in \sigma_v(i_{r+1}, \ldots, i_{2p})\Big\},$$

where $u := w_2 \cdots w_{r-1}$ and $v := w_{r+1} \cdots w_{2p}$, with the base case $\sigma_\varnothing(\emptyset) := \emptyset$ for the unique $\varnothing$-path $\emptyset$. Essentially, a block $V := \{j < k\}$ in $\sigma_w(\mathbf{p})$ means that $v_j, \ldots, v_{k-1} \neq v_{j-1} = v_k$, i.e., k is the first return time to the vertex visited at time $j - 1$.

Conversely, given an alternating non-crossing *pair* partition $\pi \in \mathrm{ANC}_2(w)$ of w, what is $\sigma_w^{-1}\{\pi\}$, the subset of w-paths $\mathbf{p} := (i_1, \ldots, i_{2p}) \in \mathcal{P}(w)$ with skeleton $\sigma_w(\mathbf{p}) = \pi$? Clearly, since each block $V := \{j < k\} \in \pi$ indicates a segment of the path where it exits and first returns to the vertex v_{j-1}, we must have $i_j = i_k$, i.e., the arc taken at time j to exit v_{j-1} must be taken again at time k (but "backwards", since $w_j \neq w_k$) in order to return to v_{j-1}. This condition alone does of course not prevent a premature return $v_{j'} = v_{j-1}$ for some $j' \in \{j + 1, \ldots, k - 1\}$. A premature return at time j' can however only happen if

(i) $w_{j'} \neq w_j$ (the arc at time j' must be taken in the opposite direction as when exiting v_{j-1}), and

(ii) j' is the lower element in its block, $U := \{j' < k'\} \in \pi$, which is directly surrounded by V: $j < j' < k' < k$ and there is no other block $\{j'' < k''\} \in \pi$ with $j < j'' < j' < k' < k'' < k$.

In case (i) and (ii) hold, we write $j \lhd_\pi j'$ as well as $U \in B(\pi)$, and say that j, j' form a *bad pair* and that U is a *bad block*. See Figure 2 for an illustration. Summarizing, for a w-path $(i_1, \ldots, i_{2p})$

to have skeleton π, we must have $i_j \neq i_{j'}$ if j, j' form a bad pair (i.e., $j \lhd_\pi j'$), and $i_j = i_{j'}$ if j, j' belong to the same block ($j \sim_\pi j'$). It should be clear that these requirements are also sufficient:

Lemma 2.4. *The map $\sigma_w : \mathcal{P}(w) \to \mathrm{ANC}_2(w)$ is surjective: for every $\pi \in \mathrm{ANC}_2(w)$,*

$$\sigma_w^{-1}\{\pi\} = \left\{ (i_1, \dots, i_{2p}) \in [d]^{2p} \;\middle|\; \forall (j, j') \in [2p]^2,\ \begin{cases} j \sim_\pi j' \implies i_j = i_{j'} \\ j \lhd_\pi j' \implies i_j \neq i_{j'} \end{cases} \right\}. \tag{8}$$

Furthermore,

$$\left|\sigma_w^{-1}\{\pi\}\right| = \prod_{V \in \pi} \left(d - \mathbb{1}_{\{V \in B(\pi)\}}\right). \tag{9}$$

Proof. First, the expression given for the cardinal (9) is always positive because $d \geq 2$, and is easily derived from (8): for each block $V := \{j < k\} \in \pi$, there are d degrees of freedom for the choice of $i_j = i_k \in [d]$, except if V is a bad block, in which case there is one degree of freedom less (because $i_j = i_k$ must be different from $i_{j'}$, where $j \lhd_\pi j'$). It remains to prove (8), which we do by induction on the balanced word $w := w_1 \cdots w_{2p}$. There is nothing to prove if $p = 0$. Suppose $p \geq 1$ and consider the decomposition of π with respect to the block containing 1,

$$\pi := \big\{\{1, r\}\big\} \cup \big\{V + 1 : V \in \pi^{(u)}\big\} \cup \big\{V + r : V \in \pi^{(v)}\big\},$$

where $u := w_2 \cdots w_{r-1}$, $v := w_{r+1} \cdots w_{2p}$, and

$$\pi^{(u)} := \Big\{V - 1 : V \in \pi,\ V \subseteq \{2, \dots, r-1\}\Big\} \in \mathrm{ANC}_2(u),$$

$$\pi^{(v)} := \Big\{V - r : V \in \pi,\ V \subseteq \{r+1, \dots, 2p\}\Big\} \in \mathrm{ANC}_2(v).$$

For $j \in [r-2]$, write $j \in J$ if $w_{j+1} \neq w_1$ and the block $\{j < k\} \in \pi^{(u)}$ containing j in $\pi^{(u)}$ is not surrounded by any other block (i.e., there is no $\{j' < k'\} \in \pi^{(u)}$ with $j' < j < k < k'$). Because of the previous decomposition and the definition of $\lhd_\pi$, we then have

$$\lhd_\pi = \big\{(1, j+1) : j \in J\big\} \cup \big\{(j+1, j'+1) : j \lhd_{\pi^{(u)}} j'\big\} \cup \big\{(j+r, j'+r) : j \lhd_{\pi^{(v)}} j'\big\}.$$

Recall also that $\{1, r\} \in \pi$ indicates that the w-paths with skeleton π first return to o at time r. Thus

$$(i_1, \dots, i_{2p}) \in \sigma_w^{-1}\{\pi\} \iff \begin{cases} i_1 = i_r,\ \forall j \in J,\ i_{j+1} \neq i_1, \\ (i_2, \dots, i_{r-1}) \in \sigma_u^{-1}\big(\pi^{(u)}\big),\ (i_{r+1}, \dots, i_{2p}) \in \sigma_v^{-1}\big(\pi^{(v)}\big), \end{cases}$$

and, by the induction hypothesis,

$$(i_1, \dots, i_{2p}) \in \sigma_w^{-1}\{\pi\} \iff \begin{cases} i_1 = i_r,\ \forall j \in J,\ i_{j+1} \neq i_1, \\ \forall (j, j') \in \{2, \dots, r-1\}^2,\ \begin{cases} (j-1) \sim_{\pi^{(u)}} (j'-1) \implies i_j = i_{j'}, \\ (j-1) \lhd_{\pi^{(u)}} (j'-1) \implies i_j \neq i_{j'}, \end{cases} \\ \forall (j, j') \in \{r+1, \dots, 2p\}^2,\ \begin{cases} (j-r) \sim_{\pi^{(v)}} (j'-r) \implies i_j = i_{j'}, \\ (j-r) \lhd_{\pi^{(v)}} (j'-r) \implies i_j \neq i_{j'}, \end{cases} \end{cases}$$

$$\iff \forall (j, j') \in [2p]^2,\ \begin{cases} j \sim_\pi j' \implies i_j = i_{j'}, \\ j \lhd_\pi j' \implies i_j \neq i_{j'}. \end{cases} \qquad \square$$

We can now complete the proof of Theorem 3.

Proof of Theorem 3. Let $w := w_1 \cdots w_{2p}$ be a balanced word on Σ. It follows from Lemma 2.4 that the set $\mathcal{P}(w)$ of w-paths from o to o may be partitioned with respect to their skeleton as

$$\mathcal{P}(w) \quad = \bigsqcup_{\pi \in \mathrm{ANC}_2(w)} \sigma_w^{-1}\{\pi\},$$

and passing to the cardinal, we get

$$M_d(w) \quad = \sum_{\pi \in \mathrm{ANC}_2(w)} \prod_{V \in \pi} \left(d - \mathbb{1}_{\{V \in B(\pi)\}}\right) \quad = \sum_{\pi \in \mathrm{ANC}_2(w)} \sum_{A \subseteq B(\pi)} (-1)^{|A|}\, d^{|\pi|-|A|},$$

by expanding out the product[1]. Now, given $\pi \in \mathrm{ANC}_2(w)$ and $A \subseteq B(\pi)$, we construct a coarser partition $\pi' := \gamma(\pi, A)$ from π by merging, for each bad pair $(j, j') \in A$, the block containing j' into its surrounding block (the one containing j). In other words, $\sim_{\pi'}$ is the smallest equivalence relation on $[2p]$ containing $\sim_\pi \cup A$. For instance, if π is the partition of Figure 2B and $A := \{(4,5)\}$, then $\pi' := \gamma(\pi, A) = \big\{\{1,8\},\{2,3\},\{4,5,6,7\},\{9,10\}\big\}$. It is clear that the conditions (i) and (ii) of forming a bad pair guarantee that π' remains non-crossing and alternating w.r.t. w: $\pi' \in \mathrm{ANC}(w)$. Further, π' has exactly $|A|$ fewer blocks than π, which has p blocks, so $(-1)^{|A|}\, d^{|\pi|-|A|} = (-1)^{p-|\pi'|}\, d^{|\pi'|}$. Conversely, given $\pi' \in \mathrm{ANC}(w)$, any pair partition π which is *finer* than π' (i.e., $\sim_\pi \subseteq \sim_{\pi'}$) automatically leads to an alternating non-crossing pair partition $\pi \in \mathrm{ANC}_2(w)$ of w having a certain set of bad pairs. Therefore,

$$M_d(w) \quad = \sum_{\pi' \in \mathrm{ANC}(w)} (-1)^{p-|\pi'|}\, d^{|\pi'|} \sum_{\substack{\pi \in \mathrm{ANC}_2(w) \\ \pi \preceq \pi'}} \sum_{\substack{A \subseteq B(\pi) \\ \gamma(\pi,A)=\pi'}} 1,$$

where we wrote $\pi \preceq \pi'$ for $\sim_\pi \subseteq \sim_{\pi'}$. Since

$$(-1)^{p-|\pi'|} \;=\; \prod_{V \in \pi'} (-1)^{\frac{|V|}{2}-1},$$

it remains to observe that

$$\sum_{\substack{\pi \in \mathrm{ANC}_2(w) \\ \pi \preceq \pi'}} \sum_{\substack{A \subseteq B(\pi) \\ \gamma(\pi,A)=\pi'}} 1 \quad = \quad \prod_{V \in \pi'} C_{\frac{|V|}{2}-1} \tag{10}$$

to conclude. But constructing $\pi \in \mathrm{ANC}_2(w)$ such that $\pi \preceq \pi'$ and $\gamma(\pi, A) = \pi'$ for some $A \subseteq B(\pi)$ is equivalent to partitioning each block $V := \{i_1, \ldots, i_{2m}\} \in \pi'$ using an alternating pair partition of $w|_V$ containing the block $\{1, 2m\}$. Since $w|_V$ is already alternating (because $\pi' \in \mathrm{ANC}(w)$), this amounts to choosing a non-crossing pair partition of $\{2, \ldots, 2m-1\}$, i.e., an element of $\mathrm{NC}_2(2m-2)$. Then (10) follows from the well-known fact $|\mathrm{NC}_2(2m-2)| = C_{m-1}$, see [15, Exercise 61]. $\square$

[1] At the level of sets, this amounts to writing

$$\sigma_w^{-1}\{\pi\} = \left\{(i_1, \ldots, i_{2p}) \in [d]^{2p} : \forall (j, j') \in [d]^{2p},\ j \sim_\pi j' \implies i_j = i_{j'}\right\} \setminus \bigcup_{j \lhd_\pi j'} \left\{(i_1, \ldots, i_{2p}) \in [d]^{2p} : i_j = i'_j\right\}$$

and using the inclusion-exclusion formula.

3. Free probability and the oriented Kesten–McKay conjecture

3.1. **Free probability.** Let us start this concluding section by showing how Theorems 1 and 3 may be recovered from Nica's work [12]. Free probability is a vast field initiated by Voiculescu; we only introduce the bare minimum and refer to [14] for detail. The general framework is that of non-commutative variables $x, y, \dots$ in some unital algebra $\mathfrak{A}$ endowed with an adjoint operator * and a linear form $\varphi : \mathfrak{A} \to \mathbb{C}$ such that $\varphi(1) = 1$ and $\varphi(x^* x) \geq 0$ for all $x \in \mathfrak{A}$. The pair $(\mathcal{A}, \varphi)$ is called a *non-commutative probability space*, where the *state* φ plays the rôle of an expectation. The *distribution* of x or more generally, the (joint) distribution of $(x_1, \dots, x_k)$ is given by all mixed moments $\varphi(x_{i_1} \cdots x_{i_\ell})$ for $\ell \geq 1$ and $(i_1, \dots, i_\ell) \in [k]^\ell$, which themselves may be expressed through the moment-cumulant formula [14, Lecture 11]:

$$\varphi(x_1 \cdots x_k) \;=\; \sum_{\pi \in \mathrm{NC}(k)} \prod_{\substack{V \in \pi \\ V := \{i_1 < \cdots < i_\ell\}}} \kappa_\ell(x_{i_1}, \dots, x_{i_\ell}), \tag{11}$$

where the *free cumulants* $\kappa_\ell : \mathfrak{A}^\ell \to \mathbb{C}$, $\ell \geq 1$, are defined inductively so that (11) holds for any $k \geq 1$ and any non-commutative variables $x_1, \dots, x_k \in \mathfrak{A}$. Similarly to the log-Laplace transform of classical random variables, the free cumulants of $(x_1, \dots, x_k)$ may be gathered into the so called *R-transform* [14, Lecture 16]:

$$R_{(x_1,\dots,x_k)}(z_1, \dots, z_k) := \sum_{\ell=1}^{\infty} \sum_{i_1,\dots,i_\ell \in [k]} \kappa_\ell(x_{i_1}, \dots, x_{i_\ell})\, z_{i_1} \cdots z_{i_\ell}, \tag{12}$$

which is a formal series in non-commutative indeterminates $z_1, \dots, z_k$. Analogously to independence for classical random variables, $x_1, \dots, x_k$ are *free* if $R_{(x_1,\dots,x_k)}(z_1, \dots, z_k) = R_{x_1}(z_1) + \cdots + R_{x_k}(z_k)$, which is commonly phrased by the sentence “mixed cumulants vanish” (i.e., $\kappa_\ell(x_{i_1}, \dots, x_{i_\ell}) = 0$ for every $\ell \geq 1$ and every non-constant sequence $(i_1, \dots, i_\ell) \in [k]^\ell$).

Nica [12] showed that for $P_{1,n}, \dots, P_{d,n} \in \{0,1\}^{n \times n}$ uniform, independently chosen permutation matrices, there exists a non-commutative probability space $(\mathfrak{A}, \varphi)$ and free variables $u_1, \dots, u_d \in \mathfrak{A}$ such that:

(a) There is the convergence of mixed moments

$$\frac{1}{n} \mathbb{E} \operatorname{Tr} P_{i_1,n}^{w_1} \cdots P_{i_k,n}^{w_k} \xrightarrow[n \to \infty]{} \varphi\Big(u_{i_1}^{w_1} \cdots u_{i_k}^{w_k}\Big),$$

for every $k \geq 1$, every $(i_1, \dots, i_k) \in [d]^k$, and every word $w \in \Sigma^k$.

(b) The u_i's are *Haar unitaries*, in the sense that $u_i^* u_i = u_i u_i^* = 1$ and $\varphi(u_i^k) = 0$ for every $k \geq 1$.

It follows from (a) and linearity that the star moments of $\mathbf{A}_{d,n} := P_{1,n} + \cdots + P_{d,n}$ converge to those of $a_d := u_1 + \cdots + u_d$, and it is easy to see that $\mathbf{A}_{d,n}$ is distributed like the adjacency matrix of the configuration model $\mathbf{CM}_{d,n}$ introduced in the proof of Theorem 1: then, we may again condition on $\mathbf{CM}_{d,n}$ being simple ($\mathbf{A}_{d,n}(i,i) = 0$ and $\mathbf{A}_{d,n}(i,j) \leq 1$ for all $i \neq j \in [n]$) to deduce the star-moment convergence, for every word w on Σ,

$$\frac{1}{n} \mathbb{E} \operatorname{Tr} A_{d,n}^w = \frac{1}{n} \mathbb{E}\big[\operatorname{Tr} \mathbf{A}_{d,n}^w \mid \mathbf{CM}_{d,n} \text{ is simple}\big] \xrightarrow[n \to \infty]{} \varphi(a_d^w),$$

of the uniform d-regular digraph $G_{d,n}$ with adjacency matrix $A_{d,n}$.

Finally, we check that the star moments $\varphi(a_d^w)$ coincide with the number $M_d(w)$ of w-paths in T_d. Using (b), it was derived in [13] that (for every $i \in [d]$)

$$R_{u_i,u_i^*}(z_1,z_2) = \sum_{k=1}^{\infty} (-1)^{k-1}\, C_{k-1}\Big[(z_1z_2)^k + (z_2z_1)^k\Big].$$

By freeness, $R_{a,a^*}(z_1,z_2) = R_{u_1,u_1^*}(z_1,z_2) + \cdots + R_{u_d,u_d^*}(z_1,z_2) = d\, R_{u_1,u_1^*}(z_1,z_2)$, and the structure of this R-transform shows that the free cumulants $\kappa_\ell(a_d^{w_1},\ldots,a_d^{w_\ell})$ (which we recover from (12)) vanish if $w := w_1\cdots w_\ell$ is not alternating:

$$\kappa_\ell(a_d^{w_1},\ldots,a_d^{w_\ell}) = \begin{cases} d\,(-1)^{p-1}\, C_{p-1}, & \text{if } w \text{ is alternating: } w=(1*)^p \text{ or } w=(*1)^p,\\ 0, & \text{otherwise.}\end{cases}$$

Recalling the definition of $\mathrm{ANC}(w)$, the moment-cumulant formula (11) then easily yields

$$\varphi(a_d^w) \;=\; \sum_{\pi\in \mathrm{ANC}(w)} \left(\prod_{V\in\pi} (-1)^{\frac{|V|}{2}-1}\, C_{\frac{|V|}{2}-1}\right) d^{|\pi|},$$

as in Theorem 3.

3.2. **The oriented Kesten–McKay conjecture.** Theorem 1 states that the uniform d-regular digraph $G_{d,n}$ converges in star moments to the d-regular directed tree T_d. As we saw in the previous section, the star moments of T_d agree with those of the sum $a_d := u_1+\cdots+u_d$ of d free Haar unitary elements in some non-commutative probability space $(\mathfrak{A},\varphi)$. This implies the convergence of mean empirical *singular value* distributions: for every $z\in\mathbb{C}$ and every continuous bounded function f,

$$\frac{1}{n}\,\mathbb{E}\,\mathrm{Tr}\, f\left(\sqrt{(A_{d,n}-z\mathrm{I}_n)^*(A_{d,n}-z\mathrm{I}_n)}\right) \xrightarrow[n\to\infty]{} \varphi\left(f\left(\sqrt{(a_d-z1)^*(a_d-z1)}\right)\right),$$

that is,

$$\int f(t)\,\mu_{|A_{d,n}-z|}(\mathrm{d}t) \xrightarrow[n\to\infty]{} \int f(t)\,\mu_{|a_d-z|}(\mathrm{d}t), \tag{13}$$

where $X-z$ means that we subtract z times the identity element to X, and $\mu_{|X|}$ is the spectral measure of the positive operator $|X| := \sqrt{XX^*}$ (i.e., $\mu_{|X|}$ is the unique real probability measure having the same moments as $|X|$, as given by the Riesz–Markov–Kakutani theorem).

Although $X\in\{A_{d,n},a_d\}$ is not a normal element, there still exists [8] a unique probability measure μ_X (on $\mathbb{C}$), known as the Brown measure of X, such that

$$\int \log|z-\lambda|\,\mu_X(\mathrm{d}\lambda) = \int \log(t)\,\mu_{|X-z|}(\mathrm{d}t)$$

for every $z\in\mathbb{C}$. When $X = A_{d,n}$, μ_X is nothing but the ESD $\frac{1}{n}\sum_{i=1}^n \delta_{\lambda_i(A_{d,n})}$ of $G_{d,n}$. Since the star moments of X determine $(\mu_{|X-z|})_{z\in\mathbb{C}}$ and thus μ_X, and the star moments of a_d and T_d coincide, we can also view μ_{a_d} as the spectral measure of T_d. However, we cannot directly use (13) to show

$$\frac{1}{n}\,\mathbb{E}\sum_{i=1}^n f\big(\lambda_i(A_{d,n})\big) \xrightarrow[n\to\infty]{} \int_{\mathbb{C}} f(z)\,\mu_{a_d}(\mathrm{d}z) \tag{14}$$

because the logarithm is not a bounded function. There still lacks a uniform control on the smallest singular value of $A_{d,n}-z$ to validate the oriented Kesten–McKay conjecture (14), see [5, Lemma 4.3].

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