EFFICIENT COUNTING AND ASYMPTOTICS OF k-NONCROSSING TANGLED-DIAGRAMS

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Abstract. In this paper we enumerate k-noncrossing tangled-diagrams. A tangled-diagram is a labeled graph whose vertices are $1, \ldots, n$ have degree ≤ 2, and are arranged in increasing order in a horizontal line. Its arcs are drawn in the upper halfplane with a particular notion of crossings and nestings. Our main result is the asymptotic formula for the number of k-noncrossing tangled-diagrams $T_k(n) \sim c_k\, n^{-((k-1)^2+(k-1)/2)}\, (4(k-1)^2 + 2(k-1) + 1)^n$ for some $c_k > 0$.

1. Tangled diagrams as molecules or walks

In this paper we show how to compute the numbers of k-noncrossing tangled-diagrams and prove the asymptotic formula

$$T_k(n) \sim c_k\, n^{-((k-1)^2+(k-1)/2)}\, (4(k-1)^2 + 2(k-1) + 1)^n, \qquad c_k > 0\ . \tag{1.1}$$

This article is accompanied by a Maple package `TANGLE`, downloadable from the webpage

`http://www.math.rutgers.edu/~zeilberg/mamarim/mamarimhtml/tangled.html` .

k-noncrossing tangled-diagrams are motivated by studies of RNA molecules. They serve as combinatorial frames for searching molecular configurations and were recently studied [5] by the first three authors. Tangled-diagrams are labeled graphs over the vertices $1, \ldots, n$, drawn in a horizontal line in increasing order. Their arcs are drawn in the upper halfplane having the following types

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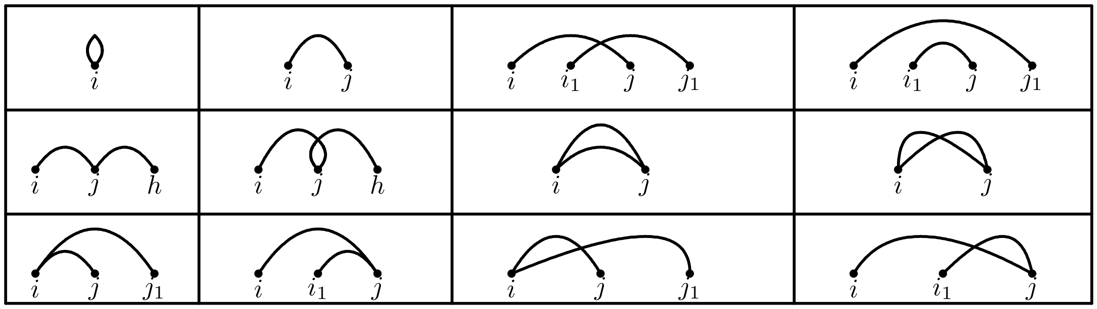
of arcs



Tangled diagrams have possibly isolated points, for instance, the tangled diagram displayed in Figure 1 has the isolated point 12. Details on tangled-diagrams can be found in [5]. It is interesting

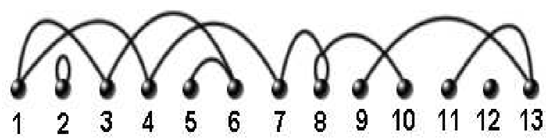


FIGURE 1. A tangled-diagram over 13 vertices.

to observe that tangled-diagrams are in correspondence to the following types of walks:

Observation 1: The number of k-noncrossing tangled-diagrams over $[n]$, without isolated points, equals the number of simple lattice walks in $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, from the origin back to the origin, taking n days, where at each day the walker can either make *one* unit step in any (legal) direction, or else feel energetic and make any *two* consecutive steps (chosen randomly).

Observation 2: The number of k-noncrossing tangled-diagrams over $[n]$, (allowing isolated points), equals the number of simple lattice walks in $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, from the origin back to the origin, taking n days, where at each day the walker can either feel lazy and stay in place, or make *one* unit step in any (legal) direction, or else feel energetic and make any *two* consecutive steps (chosen randomly).

These follow easily from the consideration in [5], and are left as amusing exercises for the readers. The paper is organized as follows: in Section 2 we consider enumeration and computation using the holonomic framework [14]. In Section 3 we validate that the formula, proved in Section 2 for $k = 2, 3, 4$, holds for arbitrary k.

2. Efficient enumeration

Let $t_k(n)$ and $\tilde{t}_k(n)$ denote the numbers of k-noncrossing tangled-diagrams with and without isolated points, respectively. Furthermore let $f_k(m)$ denote the number of k-noncrossing matchings over m vertices or equivalently be the number of ways of walking n steps in $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, from the origin back to the origin. Then, as shown in [5], $\tilde{t}_k(n)$ and $t_k(n)$ are given by:

$$\tilde{t}_k(n) = \sum_{i=0}^{n} \binom{n}{i} f_k(2n-i) \quad \text{and} \quad t_k(n) = \sum_{i=0}^{n} \binom{n}{i} \tilde{t}_k(n-i) \quad . \tag{2.1}$$

Grabiner and Magyar proved an explicit determinant formula, [9] (see also [4], eq. 9) that expresses the exponential generating function of $f_k(n)$, for fixed k, as a $(k-1) \times (k-1)$ determinant

$$\sum_{n \geq 0} f_k(2n) \cdot \frac{x^{2n}}{(2n)!} \quad = \quad \det[I_{i-j}(2x) - I_{i+j}(2x)]|_{i,j=1}^{k-1} \ , \tag{2.2}$$

where $I_m(2x)$ is the hyperbolic Bessel function:

$$I_m(2x) = \sum_{j=0}^{\infty} \frac{x^{m+2j}}{j!(m+j)!} \quad . \tag{2.3}$$

Recall that a formal power series $G(x)$ is D-finite if it satisfies a linear differential equation with polynomial coefficients. For any m the hyperbolic Bessel functions are D-finite [11], which is also called P-finite in [14]. By general considerations, that we omit here, it is easy to establish a priori bounds for the order of the recurrence, and for the degrees of its polynomial coefficients, any *empirically* derived recurrence (using the command `listtorec` in the Salvy-Zimmerman Maple package `gfun`, that we adapted to our own needs in our own package `TANGLE`), is *ipso facto* rigorous. We derived explicit recurrences for $k = 2, 3, 4$, and they can be found in the webpage of this article. Also, once recurrences are found, they are very efficient in extending the counting sequences. In the same page one can find the sequences for $T_k(n)$ for $1 \leq n \leq 1000$, for $k = 2, 3, 4$, and the sequences for $1 \leq n \leq 50$ for $k = 5, 6$ (using a variant of the Grabiner-Magyar formula implemented in our Maple package `TANGLE`).

Once the existence of a recursion is established, we can, for $k = 2, 3, 4$, employ the Birkhoff-Tritzinsky theory [2, 13] and non-rigorous "series analysis" due to Zinn-Justin [3, 15]. This allows us to safely conjecture that, for any fixed k, we have the following asymptotic formula:

$$t_k(n) \quad \sim \quad c_k \cdot n^{-((k-1)^2+(k-1)/2)} \, (4(k-1)^2 + 2(k-1) + 1)^n \quad \text{for some } c_k > 0. \tag{2.4}$$

In the next Section we shall prove eq. (2.4) for arbitrary k.

3. Asymptotics of tangled-diagrams for arbitrary k

In Lemma 1 we relate the generating functions of k-noncrossing tangled diagrams $T_k(z) = \sum_n t_k(n) z^n$ and k-noncrossing matchings [4] $F_k(z) = \sum_n f_k(2n)\, z^{2n}$. The functional equation derived will be instrumental to prove eq. (2.4) for arbitrary k. For this purpose we shall employ Cauchy's integral formula: let D be a simply connected domain and let C be a simple closed positively oriented contour that lies in D. If f is analytic inside C and on C, except at the points $z_1, z_2, \ldots, z_n$ that the interior of C, then we have Cauchy's integral formula

$$\int_C f(z)dz = 2\pi i \sum_{k=1}^{n} Res[f, z_k] \ . \tag{3.1}$$

In particular, if f has a simple pole at z_0, then $Res[f, z_0] = \lim_{z \longrightarrow z_0} (z - z_0) f(z)$.

Lemma 1. *Let $k \in \mathbb{N}$, $k \geq 2$ and $|z| < 2$. Then we have*

$$T_k\left(\frac{z^2}{1+z+z^2}\right) = \frac{1+z+z^2}{z+2}\, F_k(z)\,. \tag{3.2}$$

Proof. The relation between the number of k-noncrossing tangled-diagrams, $t_k(n)$ and k-noncrossing matchings, $f_k(2m)$ given in eq. (2.1) implies $t_k(n) = \sum_{r,\ell} \binom{n}{r}\binom{n-r}{\ell} f_k(2n - 2r - \ell)$. Expressing the combinatorial terms by contour integrals we obtain

$$\begin{aligned}
\binom{n}{r} &= \frac{1}{2\pi i}\oint_{|u|=\alpha}(1+u)^n u^{-r-1}du \\
f_k(2n-2r-\ell) &= \frac{1}{2\pi i}\oint_{|z|=\beta_3} F_k(z) z^{-(2n-2r-\ell)-1}dz \\
t_k(n) &= \sum_{r,\ell}\binom{n}{r}\binom{n-r}{\ell} f_k(2n-2r-\ell) \\
&= \frac{1}{(2\pi i)^3}\sum_{r,\ell}\oint_{\substack{|v|=\beta_1\\|z|=\beta_2\\|u|=\beta_3}}(1+u)^n u^{-r-1}(1+v)^{n-r}v^{-\ell-1} \ \times \\
&\qquad F_k(z)\, z^{-(2n-2r-\ell)-1}dv\, du\, dz,
\end{aligned}$$

where $\alpha, \beta_1, \beta_2, \beta_3$ are arbitrary small positive numbers. Due to absolute convergence of the series we derive

$$\begin{aligned}
t_k(n) &= \frac{1}{(2\pi i)^3}\sum_{r}\oint_{\substack{|v|=\beta_1\\|z|=\beta_2\\|u|=\beta_3}}(1+u)^n u^{-r-1}F_k(z)\, z^{-2n+2r-1}(1+v)^{n-r}v^{-1} \ \times \\
&\qquad \sum_{\ell}\left(\frac{z}{v}\right)^{\ell} dv\, du\, dz,
\end{aligned}$$

which is equivalent to

$$\begin{aligned}
t_k(n) &= \frac{1}{(2\pi i)^3}\sum_{r}\oint_{\substack{|u|=\beta_3\\|z|=\beta_2}}(1+u)^n u^{-r-1}F_k(z)\, z^{-2n+2r-1} \ \times \\
&\qquad \left(\oint_{|v|=\beta_1}\frac{(1+v)^{n-r}}{v-z}dv\right) du\, dz\ .
\end{aligned}$$

Since $v=z$ is the only (simple) pole in the integration domain, eq. (3.1) implies

$$\oint_{|v|=\beta_1}\frac{(1+v)^{n-r}}{v-z}dv = 2\pi i\,(1+z)^{n-r}\ .$$

We accordingly obtain

$$t_k(n) = \frac{1}{(2\pi i)^2}\sum_{r}\oint_{\substack{|u|=\beta_3\\|z|=\beta_2}}(1+u)^n u^{-r-1}F_k(z)\, z^{-2n+2r-1}(1+z)^{n-r}du\, dz. \tag{3.3}$$

Proceeding analogously w.r.t. the summation over r yields

$$\begin{aligned} t_k(n) &= \frac{1}{(2\pi i)^2} \oint_{\substack{|u|=\beta_3 \\ |z|=\beta_2}} (1+u)^n F_k(z)\, z^{-2n-1}(1+z)^n u^{-1} \sum_r \frac{z^{2r}}{u^r(1+z)^r} du\, dz \\ &= \frac{1}{(2\pi i)^2} \oint_{|z|=\beta_2} F_k(z)\, z^{-2n-1}(1+z)^n \left(\oint_{|u|=\beta_3} (1+u)^n \frac{1}{u-\frac{z^2}{1+z}} du \right) dz \ . \end{aligned}$$

Since $u = \frac{z^2}{1+z}$ is the only pole in the integration domain, Cauchy's integral formula implies $\oint_{|u|=\beta_3} (1+u)^n \frac{1}{u-\frac{z^2}{1+z}} du = 2\pi i\, (1+\frac{z^2}{1+z})^n$. We finally compute

$$\begin{aligned} t_k(n) &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} F_k(z)\, z^{-1} z^{-2n} (1+z)^n (1+\frac{z^2}{1+z})^n dz \\ &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} F_k(z)\, z^{-1} \left(\frac{1+z+z^2}{z^2}\right)^n dz \\ &= \frac{1}{2\pi i} \oint_{|z|=\beta_2} \frac{1+z+z^2}{z+2} F_k(z) \left(\frac{z^2}{1+z+z^2}\right)^{-n-1} d\left(\frac{z^2}{1+z+z^2}\right) \end{aligned}$$

and the lemma follows from Cauchy's integral formula

$$T_k\left(\frac{z^2}{1+z+z^2}\right) = \frac{1+z+z^2}{z+2} F_k(z) \ . \tag{3.4}$$

□

Theorem 1. *For arbitrary $k \in \mathbb{N}$, $k \geq 2$ the number of tangled-diagrams is asymptotically given by*

$$t_k(n) \sim c_k\, n^{-((k-1)^2+\frac{k-1}{2})} \left(4(k-1)^2 + 2(k-1) + 1\right)^n \quad \textit{where } c_k > 0 \ . \tag{3.5}$$

Proof. According to [11, 14], $F_k(x) = \sum_n f_k(2n)\, x^{2n}$ and $T_k(x)$ are both D-finite. Therefore both have a respective singular expansion [7]. We consider the following asymptotic formula for $f_k(2n)$ [10]: for arbitrary $k \geq 2$

$$f_k(2n) \sim n^{-((k-1)^2+\frac{k-1}{2})} \ (2(k-1))^n \ . \tag{3.6}$$

Eq. (3.6) allows us to make two observations. First $F_k(x)$ has the positive, real, dominant singularity, $\rho_k = (2(k-1))^{-1}$ and secondly, in view of the subexponential factor $n^{-((k-1)^2+\frac{k-1}{2})}$:

$$F_k(z) = O\left((z-\rho_k)^{((k-1)^2+\frac{k-1}{2})-1}\right), \qquad \text{as } z \longrightarrow \rho_k. \tag{3.7}$$

According to Lemma 1 we have

$$T_k\left(\frac{z^2}{z^2+z+1}\right) = \frac{z^2+z+1}{z+2}\, F_k(z)\ , \tag{3.8}$$

where $|z| \le \rho_k \le \frac{1}{2}+\epsilon$, $\epsilon > 0$ is arbitrarily small and the function $\vartheta(z) = \frac{z^2}{z^2+z+1}$ is regular at $z = \rho_k$. Since the composition $H(\eta(z))$ of a D-finite function H and a rational function η, where $\eta(0) = 0$ is D-finite [11], the functions $T_k(\vartheta(z))$ and $F_k(z)$ have singular expansions. Eq. (3.8) and eq. (3.6) imply using Bender's method ($F_k(z)$ satisfies the "ratio test") [1]

$$[z^n]\, T_k(\vartheta(z)) \sim \frac{\rho_k^2+\rho_k+1}{\rho_k+2}\, [z^n]\, F_k(z) \sim \frac{\rho_k^2+\rho_k+1}{\rho_k+2}\, n^{-((k-1)^2+\frac{k-1}{2})} \left(\rho_k^{-1}\right)^n\ . \tag{3.9}$$

Eq. (3.9) implies that $\tau_k = \frac{\rho_k^2}{\rho_k^2+\rho_k+1}$ is the positive, real, dominant singularity of $T_k(z)$. Indeed, Pringsheim's Theorem [12] guarantees the existence of a positive, real, dominant singularity of $T_k(z)$, denoted by τ_k. For $0 \le x \le 1$ the mapping $x \mapsto \frac{x^2}{x^2+x+1}$ is strictly increasing and continuous, whence $\tau_k = \frac{\zeta^2}{\zeta^2+\zeta+1}$ for some $0 < \zeta \le 1$. In view of eq. (3.8), ζ is the dominant, positive, real singularity of $F_k(z)$, i.e. $\zeta = \rho_k$. Accordingly,

$$[z^n]\, T_k(z) \sim \theta(n) \left(\frac{\rho_k^2}{\rho_k^2+\rho_k+1}\right)^n\ . \tag{3.10}$$

We shall proceed by analyzing $T_k(z)$ at dominant singularities. We observe that any dominant singularity v can be written as $v = \vartheta(\zeta)$. Let $S_{T_k}(z-\vartheta(\zeta))$ denote the singular expansion of $T_k(z)$ at $v = \vartheta(\zeta)$. Since $\vartheta(z)$ is regular at ζ, $T_k(\vartheta(z))$ we have the *supercritical* case of singularity analysis [7]: given $\psi(\phi(z))$, ϕ being regular at the singularity of ψ, the singularity-type of the composition is that of ψ. Indeed, we have

$$\begin{aligned} T_k(\vartheta(z)) &= O(S_{T_k}(\vartheta(z)-\vartheta(\zeta))) && \text{as } \vartheta(z) \to \vartheta(\zeta). \\ &= O(S_{T_k}(z-\zeta)) && \text{as } z \to \zeta. \end{aligned}$$

Eq. (3.8) provides the following interpretation for $T_k(\vartheta(z))$ at $z = \zeta$:

$$T_k(\vartheta(z)) = O(F_k(z)) \qquad \text{as } z \to \zeta,$$

from which we can conclude that $T_k(z)$ has at $v = \vartheta(\zeta)$ exactly the same subexponential factors as $F_k(z)$ at ζ. We next prove that τ_k is the unique dominant singularity of $T_k(z)$. Suppose $v = \vartheta(\zeta)$ is an additional dominant singularity of $T_k(z)$. The key observations is

$$\forall\, \zeta \in \mathbb{C} \setminus \mathbb{R}; \qquad \vartheta(\zeta) = \tau_k \quad \Longrightarrow \quad |\zeta| < \rho_k\ . \tag{3.11}$$

Eq. (3.11) implies that if v exists then ζ is a singularity of $F_k(z)$ of modulus strictly smaller than ρ_k, which is impossible. Therefore τ_k is unique and we derive

$$[z^n]\, T_k(z) \sim c_k\, n^{-((k-1)^2+\frac{k-1}{2})} \left(\frac{\rho_k^2}{\rho_k^2+\rho_k+1}\right)^n \quad \text{for some } c_k > 0 \tag{3.12}$$

and the theorem follows. □

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