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 with vertices $1, \ldots, n$, having degree at most two, which are arranged in increasing order in a horizontal line. The 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 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 the Maple package `TANGLE`, which is available at

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

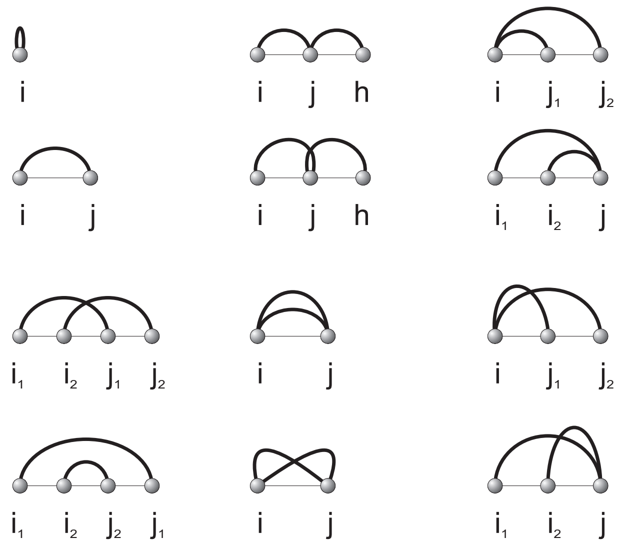

Figure 1: Arcs in tangled diagrams: a list of all possible arc-configurations.

K-noncrossing tangled diagrams are motivated by the studies of RNA molecules. They serve as a combinatorial model for searching molecular configurations and were recently studied [5] by the first three authors. Let us recall that a tangled diagram, or a tangle, is a labeled graph on the vertex set $[n] = \{1, \ldots, n\}$, with vertices of degree at most two, drawn in increasing order in a horizontal line. The arcs are drawn in the upper halfplane. In general, a tangled diagram has isolated vertices and its types of nonisolated vertices are given in Fig. 1. Tangled diagrams have possibly isolated vertices, for instance, the tangled diagram displayed in Fig. 1 has the isolated vertices 2 and 12.

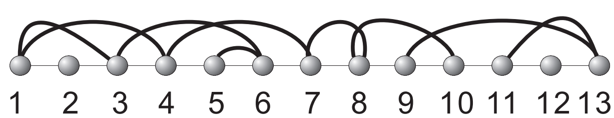

Figure 2: A tangled diagram with 13 vertices.

In order to describe the geometric crossings in tangled diagrams, we map a tangled diagram into a partial matching. This mapping is called inflation and intuitively "splits" each vertex of degree two, j, into two vertices j and j' having degree one, see Fig. 3. Accordingly, a tangle with ℓ vertices of degree two is expanded into a diagram on $n + \ell$ vertices. Clearly, the inflation map has a unique inverse, obtained by identifying the vertices j, j'. A set of k arcs (i_{r_s}, j_{r_s}), $1 \leq s \leq k$, is called a k-crossing if $i_{r_1} < i_{r_2} < \cdots < i_{r_k} < j_{r_1} < j_{r_2} < \cdots < j_{r_k}$ and k-nesting if $i_{r_1} < i_{r_2} < \cdots < i_{r_k} < j_{r_k} < j_{r_{k-1}} < \cdots < j_{r_1}$. A partial matching is called k-noncrossing (k-nonnesting) [4], if it does not contain any k-crossing (k-nesting). A tangle is k-noncrossing (k-nonnesting) if its inflation is a k-

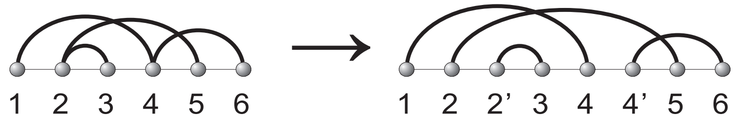

Figure 3: The inflation of a tangled diagram into a partial matching with 8 vertices.

noncrossing (k-nonnesting) partial matching [5]. It is interesting to note that tangled diagrams are in correspondence with the following types of walks:

Observation 1. The number of k-noncrossing tangled diagrams on $[n]$, without isolated vertices, equals the number of simple lattice walks in the region $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, 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 on $[n]$, (allowing isolated vertices), equals the number of simple lattice walks in the region $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, 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 observations follow easily from the consideration in [5]. 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 vertices, respectively. Furthermore let $f_k(m)$ denote the number of k-noncrossing matchings on m vertices or equivalently be the number of ways of walking n steps in the region $x_1 \geq x_2 \geq \cdots \geq x_{k-1} \geq 0$, from the origin back to the origin. Then, as shown in [5], $\tilde{t}_k(n)$ and $t_k(n)$ are given by:

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

As for $f_k(n)$, Grabiner and Magyar proved an explicit determinant formula, [9] (see also [4], (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:

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

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 $1 \le n \le 1000$, for $k = 2, 3, 4$, and the sequences for $1 \le n \le 50$ 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 (2.4) for arbitrary k.

3 Tangled diagrams for arbitrary k

In Lemma 3.1 we relate the generating functions for 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 (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 vertices $z_1, z_2, \dots, z_n$ that are in 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 $Res[f, z_0] = \lim_{z \to z_0} (z - z_0) f(z)$.

Lemma 3.1. *Let $k \in \mathbb{N}$, $k \ge 2$ 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 the number of k-noncrossing matchings, $f_k(2m)$, given in (2.1) implies

$$t_k(n) = \sum_{r,\ell} \binom{n}{r} \binom{n-r}{\ell} f_k(2n-2r-\ell).$$

Expressing the binomial coefficients by contour integrals we obtain

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

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

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

which is equivalent to

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

Since $v = z$ is the only (simple) pole in the integration domain, (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 with respect to 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

$$\oint_{|u|=\beta_3} (1+u)^n \frac{1}{u - \frac{z^2}{1+z}} du = 2\pi i \left(1 + \frac{z^2}{1+z}\right)^n .$$

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

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

This completes the proof. ∎

Theorem 3.2. *For any $k \geq 2$, the number of k-noncrossing 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 any $k \geq 2$

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

(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 second, in view of the subexponential factor $n^{-((k-1)^2 + \frac{k-1}{2})}$, we have

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

According to Lemma 3.1 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. Using Bender's method ($F_k(z)$ satisfies the "ratio test") [1], the relations (3.8) and (3.6) imply

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

It follows 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 $x\mapsto\vartheta(x)$ is strictly increasing and continuous, whence $\tau_k=\vartheta(\zeta)$ for some $0<\zeta\le 1$. We shall proceed by analyzing the dominat singularities of $T_k(z)$. We observe that any such dominant singularity v can be written as $v=\vartheta(\zeta)$. Suppose $\vartheta(\zeta)$ is an additional dominant singularity of $T_k(\vartheta(z))$. We note that

$$\forall\,\zeta\in\mathbb{C}\setminus\mathbb{R};\qquad |\vartheta(\zeta)|=\tau_k \quad\Longrightarrow\quad |\zeta|<\rho_k, \tag{3.10}$$

from which we conclude that τ_k is the unique dominant singularity of $T_k(z)$. It remains to show that the subexponential factors of $T_k(\vartheta(z))$ and $T_k(z)$ coincide. 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

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

The equation (3.8) leads to the following interpretation for $T_k(\vartheta(z))$ at $z=\zeta$:

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

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 accordingly derive

$$[z^n]\,T_k(z)\sim c_k\, n^{-((k-1)^2+\frac{k-1}{2})}\left(\frac{\rho_k^2}{\rho_k^2+\rho_k+1}\right)^n \quad \text{for some } c_k>0 \tag{3.11}$$

and the theorem follows. ∎

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