On some primary and secondary structures in combinatorics

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Abstract. *A possible upgrade of a curriculum in undergraduate course in combinatorics is presented by giving more bijective proofs in the standard (or primary) combinatorics and by adding some topics on more refined (or secondary) combinatorics, including Dyck and Motzkin paths, Catalan, Narayana and Motzkin numbers and secondary structures coming from biology. Some log–convexity properties and asymptotics of these numbers are also presented.*

Key words: *Catalan numbers, Narayana numbers, Motzkin numbers, secondary structure, log–convexity*

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1. Introduction

Bbesides somegeneral theory, a standard undergraduate course in combinatorics of special combinatorial numbers mostly covers binomial coefficients, Stirling numbers, (sometimes) Eulerian numbers, Fibonacci and Catalan numbers and optionally a few more. Problems on global behavior of sequences in question, in particular log-concavity (or log-convexity) are hardly mentioned.

In this paper we try a) to refresh this curriculum with some bijective proofs in the standard (primary) part and b) to add some "concrete" and interesting material to it concerning Dyck and Motzkin paths and numbers, Narayana numbers and secondary structures which come from biology. Proofs dealing with this new material still stay in realms of elementary combinatorics, linear algebra and calculus.

This explains the title, and accordingly, we divide the paper in two parts: primary and secondary combinatorics.

2. Primary combinatorics

We start from scratch. Let X and N be finite sets with a number of elements $|X| = \#X = x$ and $|N| = \#N = n$. Then it is easy to see that the size of the set

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X^N of all functions $N \to X$ is equal to $|X^N| = |X|^{|N|} = x^n$, and the set $X^{\underline{N}}$ of all injections (or $1-1$ maps) $N \to X$ has the size $|X^{\underline{N}}| = x(x-1)\cdots(x-n+1) =: x^{\underline{n}}$, called the **falling power**. For any integer $k \geq 0$, let $\binom{X}{k}$ be the set of all k-subsets of X, and let $\#\binom{X}{k} = \binom{x}{k}$. In particular, denoting $[n] := \{1, 2, \ldots, n\}$, the number $\#\binom{[n]}{k} = \binom{n}{k}$ is called the **binomial coefficient**.

In the following theorem we recall (and prove) some fundamental laws of the "primary" binomial coefficients. Proofs will be mostly bijective.

Theorem 1. *For integers n, r, $k \geq 0$ and complex numbers x, y we have:*

a) $\binom{n}{r} = \frac{n^{\underline{r}}}{r!} \frac{n(n-1)\cdots(n-r+1)}{r!} = \frac{n!}{r!(n-r)!}$ (basic formula)*;*

b) $\binom{n}{r} = \binom{n}{n-r}$ (symmetry)*;*

c) $\binom{n}{r} = \frac{n}{r}\binom{n-1}{r-1}$ (absorption law)*;*

d) $\binom{n}{r} = \binom{n-1}{r-1} + \binom{n-1}{r}$ (Pascal formula)*;*

e) $\binom{n}{r}\binom{r}{k} = \binom{n}{k}\binom{n-k}{r-k}$ (product rule)*;*

f) $(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k}$ (binomial formula)*;*
(By putting $y = 1$, we get that $(x+1)^n$ is the generating function of the sequence $\binom{n}{0}$, $\binom{n}{1}$, $\ldots$)

g) $(x+y)^{\underline{n}} = \sum_{k=0}^{n} \binom{n}{k} x^{\underline{k}} y^{\underline{n-k}}$, $\quad (x+y)^{\overline{n}} = \sum_{k=0}^{n} \binom{n}{k} x^{\overline{k}} y^{\overline{n-k}}$,
*where $a^{\overline{n}} := a(a+1)\cdots(a+n-1)$ is the **rising power**;*

h) $\binom{x+y}{n} = \sum_{k=0}^{n} \binom{x}{k}\binom{y}{n-k}$ (Vandermonde's convolution)*;*

*i) A **composition** of n with k parts is an ordered k-tuple of positive integers whose sum is n. The set of all such compositions $\mathcal{C}_{n,k}$ has the size*

$$\#\mathcal{C}_{n,k} = \binom{n-1}{k-1};$$

j) $\binom{n}{k}^2 \geq \binom{n}{k-1}\binom{n}{k+1}$ (log-concavity)*;*
*Recall that a sequence $a_1, a_2, \ldots, a_n$ of (positive) real numbers is **log-concave** (resp. **log-convex**) if $a_k^2 \geq a_{k-1}a_{k+1}$ (resp. $a_k^2 \leq a_{k-1}a_{k+1}$). It is easy to see that if a sequence is log-concave then it is also **unimodal**, i.e. there is a place **(peak)** j, such that $a_1 \leq a_2 \leq \cdots \leq a_j \geq a_{j+1} \geq \cdots \geq a_n$. The peak for $\binom{n}{k}$ is at $k = \lfloor n/2 \rfloor$.*

Proof.

a) Take sets N and R with $|N| = n$, $|R| = r$. We shall prove that $r!\binom{n}{r} = n^{\underline{r}}$ by considering all injections $N^{\underline{R}}$. Any injection $f : R \to N$ can be obtained in such a way that we first choose an r-subset $A \subseteq N$ (and this can be done in $\binom{n}{r}$ ways) and then permute A with a permutation π of A (this can be done in $r!$ ways). Formally, $f \mapsto (A, \pi)$ is a bijection $N^{\underline{R}} \to \binom{N}{r} \times S_r$, and the claim follows (S_r is the symmetric group of all permutations of an r-set).

b) If $|N| = n$, then $A \mapsto N \setminus A = \overline{A}$ (complement of A in N) yields a bijection from $\binom{N}{r}$ to $\binom{N}{n-r}$.

c) It is equivalent to $r\binom{n}{r} = n\binom{n-1}{r-1}$. The left-hand side counts all ordered pairs (A, x) where $A \in \binom{[n]}{r}$ and $x \in A$, while the right-hand side counts all ordered pairs (y, B), where $y \in [n]$ and $B \in \binom{[n]\setminus\{y\}}{r-1}$. The map $(A, x) \mapsto (x, A \setminus \{x\})$ has the inverse $(y, B) \mapsto (B \cup \{y\}, y)$, and hence it is a bijection.

d) Let $A \subseteq [n]$ be an r-subset. If $n \in A$, then A can be chosen in $\binom{n-1}{r-1}$ ways and otherwise in $\binom{n-1}{r}$ ways. So, by adding these two possibilities the Pascal formula follows.

e) The left-hand side counts all ordered pairs $(A_1, A_2) \in \binom{[n]}{r} \times \binom{[r]}{k}$, while the right-hand side counts all ordered pairs (B_1, B_2) where B_1 is a k-subset of $[n]$ and B_2 an $(r-k)$-subset of $[n] \setminus B_1$. The map $(A_1, A_2) \mapsto (A_2, A_1 \setminus A_2)$ is a bijection, and the product rule follows.

f) The binomial formula can be considered for a fixed n as an equality of two polynomials in variables x and y. Hence, it is enough to prove this polynomial equality for positive integers x and y. Let X, Y and N be finite sets with $|X| = x$, $|Y| = y$, $|N| = n$, where X and Y are disjoint sets. The left-hand side of the formula counts all maps f from N to the disjoint union $X \cup Y$. But we can count all maps $N \to X \cup Y$ so that we first decide which k elements of N we send to X (and hence the rest of $n-k$ elements to Y). By adding all possibilities we get the formula. The sketch in *Figure 1* visualizes this (bijective) proof.

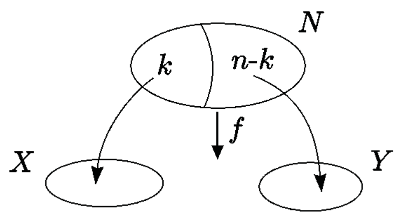

Figure 1. *"Proof without words" of binomial formula*

g) Literally the same proof as f) but considering injections $(X \cup Y)^{\underline{N}}$ instead of all maps $(X \cup Y)^N$ yields the first formula in g), while the second one follows then immediately from the reciprocity formula $a^{\overline{n}} = (-1)^n(-a)^{\underline{n}}$. So, the rule g) says that we can "underline" and "overline" the exponents in the binomial formula.

h) The rule a) is equivalent to $r!\binom{n}{r} = n^{\underline{r}}$ and can be viewed as an equality between two polynomials in variable n. Hence it holds for any $x \in \mathbb{C}$ instead of n. So, $r!\binom{x}{r} = x^{\underline{r}}$. Therefore we have $(x+y)^{\underline{n}} = n!\binom{x+y}{n}$ and $x^{\underline{k}} = k!\binom{x}{k}$ and $y^{\underline{y-k}} = (n-k)!\binom{y}{n-k}$. By plugging in these equalities to the first formula in g) we get h).

i) The following well known bijection (de Moivre, 18-th century) establishes the equality $\#\mathcal{C}_{n,k} = \binom{n-1}{k-1}$ for n, $k \geq 1$ (with $\binom{0}{0} := 1$):

$$\mathcal{C}_{n,k} \to \binom{[n-1]}{k-1}, \quad (a_1, a_2, \ldots, a_k) \mapsto \{a_1, a_1 + a_2, \ldots, a_1 + \cdots + a_{k-1}\}.$$

j) The log-concavity property can be easily obtained algebraically by using the basic formula a) written in the form $\binom{n}{r} = n!/r!(n-r)!$. But we shall later give a combinatorial proof (see *Theorem 4 f)*). Claim about the peak follows easily from $k\binom{n}{k} = (n-k+1)\binom{n}{k-1}$. □

There are, of course, "billions" of consequences, generalizations, and analogues of these basic laws. For example, the multinomial theorem, and in fact, multinomial versions of formulas f) and g) in the above theorem with basically the same proof (just take disjoint sets X_1, X_2, ... , X_k instead of X and Y), is a natural generalization of the binomial formula. A natural q-analogue of the binomial coefficient is called a q-**binomial coefficient**, denoted by $\binom{n}{k}_q$, is the number of k-dimensional subspaces of the n-dimensional vector space $V_n(q)$ over the field $\mathbb{F}_q$ of q (=prime power) elements. Then it is well known (see e.g. [6]) that all fundamental laws of *Theorem 1* hold for $\binom{n}{k}_q$'s. The basic formula being:

$$\binom{n}{k}_q = \frac{(q^n-1)(q^n-q)\ldots(q^n-q^{n-1})}{(q^k-1)(q^k-q)\ldots(q^k-q^{k-1})}.$$

The proof of this formula is essentially the same as our proof of a) in the above theorem, by taking vector spaces and their isomorphisms (and monomorphisms) instead of sets and their permutations (and injections). Note that $\lim_{q\to 1}\binom{n}{k}_q = \binom{n}{k}$.

We mention here only that virtually all asymptotics in this "primary" world relies on the famous **Stirling formula** $n! \sim \sqrt{2\pi n}(n/e)^n$.

The next step in the foundation of combinatorics is to express the (ordinary) powers in terms of falling and rising powers and in terms of binomial coefficients, because $(x^n)_{n\geq 0}$, $(x^{\underline{n}})_{n\geq 0}$ and $(\binom{x}{n})_{n\geq 0}$ form the most important bases of the vector space of polynomials. So, let's do it.

Theorem 2. *For any integer $n \geq 0$ and any complex number x we have:*

a)

$$x^n = \sum_{k=0}^{n} S(n,k)x^{\underline{k}},$$

*where $S(n,k)$ is the **Stirling partition number**, i.e. the number of partitions of an n-set into k blocks (parts);*

b)

$$x^{\overline{n}} = \sum_{k=0}^{n} c(n,k)x^k,$$

*where $c(n,k)$ is the **Stirling cycle number**, i.e. the number of permutations of $[n]$ with exactly k cycles;*

c)

$$x^n = \sum_{k=0}^{n} E(n,k)\binom{x+k}{n},$$

*where $E(n,k)$ is the **Eulerian number**, i.e. the number of permutations of $[n]$ with exactly k ascents. A permutation $\pi \in S_n$ written as a word $\pi = i_1 i_2 \dots i_n$ (i.e. $\pi(j) = i_j$) has an **ascent** at j if $i_j < i_{j+1}$ (it has a **descent** at j if $i_j > i_{j+1}$). Note the* symmetry law *$E(n,k) = E(n, n-k-1)$, because the mirror permutation $\overline{\pi} = i_n \dots i_2 i_1$ has $n-k-1$ ascents.*

Proof.

a) Again, it is enough to prove this identity for positive integers x. The left-hand side counts all maps $f : N \to X$ (as usual $|N| = n$, $|X| = x$). Suppose the image of f, denoted by $\operatorname{Im} f$, has k elements. Then the so-called kernel of f, $\operatorname{Ker} f := \{f^{-1}(x) | x \in \operatorname{Im} f)\}$, defines a k-partition of N and a natural injection $f' : \operatorname{Ker} f \to X$ defined by $f'(f^{-1}(x)) = x$. For a fixed k we have a natural bijection $f \mapsto (\operatorname{Ker} f, f')$ and there are $S(n,k)x^{\underline{k}}$ ways to choose such a pair. By adding all possible cases for $k = 0, 1, \dots, n$, the formula a) follows.

b) Since $x^{\overline{n}} = (x+n-1)^{\underline{n}}$, it is enough to establish a bijection (for a positive integer x):

$$[x+n-1]^{\underline{[n]}} \to \{(\pi, f) | \pi \in S_n, f : C(\pi) \to [x]\},$$

where $C(\pi)$ is the set of all cycles of the permutation π. An algorithm yielding a bijection is described in [6] and we will not repeat it here.

c) The left-hand side for a positive integer x counts all functions $f : [n] \to [x]$ and the right hand side counts all pairs (π, A) where $\pi \in S_n$ has exactly k ascents and A is an n-subset of $[x+k]$ for some $k \geq 0$. We shall assign $f \mapsto (\pi, A)$ as follows. Let $f : [n] \to [x]$ be given and denote $f(i) = a_i$, $i = 1, \dots, n$. Order $a_1, \dots, a_n$ such that $1 \leq a_1 \leq a_2 \leq \cdots \leq a_n \leq x$ and if for some j we have $i_j < i_{j+1}$ and $a_{i_j} = a_{i_{j+1}}$, then we write $a_{i_j} \leq a_{i_{j+1}}$. In this way we get the permutation $\pi = i_1 i_2 \dots i_n \in S_n$. Clearly π has k descends (i.e. $n-k-1$ ascents) if and only if the sequence $a_{i_1} \leq a_{i_2} \leq \cdots \leq a_{i_n}$ has k strict inequalities. Denote $b_j := a_{i_j}$. Hence $1 \leq b_1 \leq b_2 \leq \cdots \leq b_n \leq x$. Let strict inequalities occur precisely at places $r_1, \dots, r_k$ (in an increasing order). Then we have:

$$1 \leq b_1 \leq \cdots \leq b_{r_1} < b_{r_1+1} \leq \cdots \leq b_{r_2} < b_{r_2+1} \leq \cdots \leq b_{r_k} < b_{r_k+1} \leq \cdots \leq b_n \leq x.$$

Now form the sequence $1 \leq c_1 < c_2 < \cdots < c_n \leq x + k$, where $c_1 = b_1$, $c_2 = b_1 + 1$, … ,$c_{r_1} = b_{r_1} + (r_1 - 1)$, $c_{r_1+1} = b_{r_1+1} + (r_1 - 1)$, … and put $A = \{c_1, c_2, \dots, c_n\}$. Then $A \subseteq [x+k]$ is an n-subset and it is not hard to check that $f \mapsto (\pi, A)$ is a bijection. Hence the equality c) (called Worpitzky's identity) follows. □

This theorem has also numerous consequences, analogues etc. Let us mention only two. From *Theorem 2 a)* and *b)* it follows easily that the transition matrices $[S(n,k)]_{n,k\geq 0}$ and $[s(n,k)]_{n,k\geq 0}$ between bases $\{1, x, x^2, \dots\}$ and $\{1, x^{\underline{1}}, x^{\underline{2}}, \dots\}$

are inverse to each other, where $s(n,k) := (-1)^{n-k}c(n,k)$, establishing thus the relationship between $s(n,k)$ and $S(n,k)$ (called the **Stirling inversion**):

$$\sum_{k\geq 0} S(m,k)s(k,n) = \delta_{m,n}.$$

The basic relation between Stirling and Eulerian numbers is for integers $n, x \geq 0$ given by:

$$x!S(n,x) = \sum_{k\geq 0} E(n,k)\binom{k}{n-x},$$

and this can be proved in the same manner as *Theorem 2 c)*, but only looking at surjections $[n] \to [x]$ instead of all functions.

It is not hard to prove that $S(n,0)$, $S(n,1)$, … ,$S(n,n)$ and $c(n,0)$, $c(n,1)$, … , $c(n,n)$ are log-concave sequences (by using *Theorem 2*), but it is harder to find the peak; for $S(n,k)$'s it is (asymptotically) at $k \approx n/\log n$ (see [8] and references cited there).

There are many other "primary" combinatorial numbers. For example, the **Fibonacci numbers** F_n, defined by $F_0 = 0$, $F_1 = 1$ and $F_{n+2} = F_n + F_{n+1}$. The number b_n of binary sequences of length n without neighboring zeroes is $b_n = F_{n+2}$, because for $n \geq 3$ such a sequence starts either with 1 or with 0, and hence $b_n = b_{n-1} + b_{n-2}$, while $b_1 = 1$, $b_2 = 3$. The number of such sequences of length $m+n-2$ is equal to F_{m+n} and by considering which digit (0 or 1) sits at the $(m+1)$-th place we get $F_{m+n} = F_{m-1}F_n + F_mF_{n+1}$. Defining $F_{-n} := (-1)^{n-1}F_n$ for $n \geq 0$, we get (by putting $m = -n+1$) the basic **Cassini identity**

$$F_{n+1}F_{n-1} - F_n^2 = (-1)^n.$$

(The other short proof of the Cassini identity is to show inductively $\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^n = \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix}$ and taking determinants.). So F_n's are neither log-concave nor log-convex. Still the sequence $x_n = F_n/F_{n-1}$ converges because the even and the odd subsequences converge and $|x_{2n} - x_{2n-1}|$ becomes arbitrarily small (by using the Cassini identity). The limit is the famous **golden ratio** $\varphi = (1+\sqrt{5})/2$.

Here we end this "mini course" in the basic combinatorics of the "primary" combinatorial structures and turn to secondary structures.

3. Secondary structures and their numbers

Let us first define some basic concepts and numbers. A **Dyck**[1] **path** (or a "mountain path") of length $2n$ is a lattice path in the coordinate plane (x,y) from $(0,0)$ to $(2n,0)$ with steps $(1,1)$ ("up's") and $(1,-1)$ ("down's"), never falling below the x-axis. The set $\mathcal{D}_n$ of all such Dyck paths is in an obvious bijection with all sequences $(\varepsilon_1, \varepsilon_2, \dots, \varepsilon_{2n})$, $\varepsilon_i = \pm 1$, such that all partial sums of ε_i's are ≥ 0, and the total sum is zero. Namely, to any step "up" assign $+1$, and to any step "down" assign

[1] Walther von Dyck (1856 – 1934), a German mathematician

-1. Such sequences are called **ballot sequences**. "Dyck family" $\mathcal{D}_3$ is shown in *Figure 2.*

Figure 2. $\mathcal{D}_3$

Note that projecting to the y axis, a Dyck path of length $2n$ can also be regarded as an n-step closed walk on $\mathbb{N}$ (nonnegative integers) from 0 to 0 with steps 1 and -1.

The n-th **Catalan number** C_n, $n \geq 0$, is defined by

$$C_n = \frac{1}{n+1}\binom{2n}{n} = \frac{1}{2n+1}\binom{2n+1}{n}.$$

There are many combinatorial interpretations of C_n's, e.g. C_n is the number of diagonal triangulations of a convex $(n+2)$-gon, the number of binary trees on n vertices, etc. There are over 70 (seemingly) different interpretations of C_n's and the real "Catalomania" is nicely described in Ex. 6.19-6.35 in the book [7].

A **peak** of a Dyck path $P \in \mathcal{D}_n$ is a place where a step $(1,1)$ is directly followed by a step $(1,-1)$. Denote by $\mathcal{D}_{n,k}$ the set of all Dyck paths $P \in \mathcal{D}_n$ with exactly k peaks (note: $1 \leq k \leq n$).

The **Narayana numbers** $N(n,k)$ are defined for integers $n, k \geq 0$ by

$$N(n,k) = \frac{1}{n}\binom{n}{k}\binom{n}{k-1} = \frac{1}{k}\binom{n}{k-1}\binom{n-1}{k-1},$$

with the initial value $N(0,0) := 1$. The boundary values are $N(n,0) = 0$ and $N(n,1) = 1$, for $n \geq 1$.

The basic properties of the concepts and numbers just introduced are summarized in the following theorem.

Theorem 3. *For integers $n, k \geq 0$ we have:*

a) $\#\mathcal{D}_n = C_n$;

b) $\#\mathcal{D}_{n,k} = N(n,k)$;

c) $\sum_{k\geq 0} N(n,k) = C_n$;

d) $\sum_{r=0}^{n} C_r C_{n-r} = C_{n+1} = \sum_{i,j,k\geq 0} \binom{n}{k}\binom{k}{2j} N(j,i)$;

e) The Catalan sequence $(C_n)_{n\geq 0}$ *is log-concave;*

f) The generating function for a Catalan sequence is equal to $(1-\sqrt{1-4x})/2x$.

Proof.

a) The simplest way to prove a) and b) is to use the next lemma (see [3]).

Raney's lemma. If $(x_1, x_2, \ldots, x_m)$ is an integer sequence whose sum is 1, then exactly one of the cyclic shifts $(x_j, x_{j+1}, \ldots, x_m, x_1, \ldots, x_{j-1})$, $1 \le j \le m$, has all partial sums positive.

Proof of lemma. First extend the sequence periodically to the infinite sequence $(x_1, x_2, \ldots, x_m, x_1, x_2, \ldots, x_m, x_1, x_2, \ldots)$. Then look at the graph of the function of partial sums $n \mapsto s_n = x_1 + \cdots + x_n$ and connect the consecutive points (n, s_n) by a straight segment. The obtained graph is contained between two parallel lines with slopes $1/m$ and the desired place j is (considered $\bmod m$) the first place on the x-axis after which the obtained graph is entirely above the x-axis.

To prove a), we count all ballot sequences $(\varepsilon_1, \ldots, \varepsilon_{2n})$, or what is the same, all sequences $(\varepsilon_0, \varepsilon_1, \ldots, \varepsilon_{2n})$ with $\varepsilon_0 = +1$ put in front. Its sum is 1 and all its partial sums are positive. It has n places with -1 and $n+1$ places with $+1$, so alltogether there are $\binom{2n+1}{n}$ such sequences. But, by Raney's lemma only $1/(2n+1)$ of them have all positive partial sums and the claim follows.

b) Any Dyck path $P \in \mathcal{D}_{n,k}$ can be identified with the sequence $(u_1, d_1, u_2, d_2, \ldots, u_k, d_k)$, where u_1 is the number of steps $(1,1)$ ("up's") of the first ascent of P, d_1 the number of steps $(1,-1)$ ("down's") of the first descent of P, etc. So, we can write $P = (u, d)$, where $u = (u_1, \ldots, u_k)$, $d = (d_1, \ldots, d_k)$ and u_i, d_i are positive integers such that $\sum_{i=1}^{j} u_i \ge \sum_{i=1}^{j} d_i$, for all $1 \le j \le k-1$ and $\sum_{i=1}^{k} u_i = \sum_{i=1}^{k} d_i = n$ (as any mountain climber knows). We write this as $u \succcurlyeq_n d$ and say that u n-**dominates** d. For example, for $n = 7$, $k = 3$ a Dyck path $P \in \mathcal{D}_{7,3}$, $P = ((2,2,3),(1,3,3))$ is shown in *Figure 3*.

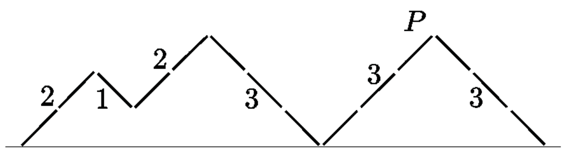

Figure 3.

Now recall the set $\mathcal{C}_{n,k}$ of all compositions of n with k parts from *Theorem 1 i)* and define a map $\psi = \psi_{n,k} : \mathcal{C}_{n+1,k} \times \mathcal{C}_{n,k} \to [k] \times \mathcal{D}_{n,k}$ as follows. Let $(A, B) \in \mathcal{C}_{n+1,k} \times \mathcal{C}_{n,k}$, $A = (a_1, \ldots, a_k)$, $B = (b_1, \ldots, b_k)$ and apply the above Raney's lemma to the sequence $(a_1, -b_1, \ldots, a_k, -b_k)$ to find the unique $j \in [k]$ such that all partial sums of $(a_j, -b_j, a_{j+1}, -b_{j+1}, \ldots, a_{j-1}, -b_{j-1})$ are positive (note that $a_j \ge 2$). Hence, all partial sums of $(a_j - 1, -b_j, a_{j+1}, -b_{j+1}, \ldots, a_{j-1}, -b_{j-1})$ are ≥ 0. Let $u_1 = a_j - 1$, $u_2 = a_{j+1}$, $\ldots$, $u_k = a_{j-1}$ and $d_1 = b_j$, $d_2 = b_{j+1}$, $\ldots$, $d_k = b_{j-1}$. Then clearly $u = (u_1, \ldots, u_k) \succcurlyeq_n d = (d_1, \ldots, d_k)$ and hence the pair (u, d) defines the unique Dyck path $P = (u, d) \in \mathcal{D}_{n,k}$. Put $\psi(A, B) := (j, P)$.

Define now the map $\varphi = \varphi_{n,k}$ in the opposite direction $\varphi(j,P) := (A,B)$, $A = (a_1,\dots,a_k)$, $B = (b_1,\dots,b_k)$ as follows. For given $j \in [k]$ and $P = (u,d) \in \mathcal{D}_{n,k}$ read off cyclically $a_j = u_1 + 1$, $a_{j+1} = u_2$, $\dots$, $a_{j-1} = u_k$ and $b_j = d_1$, $b_{j+1} = d_2$, $\dots$, $b_{j-1} = d_k$. It is easy to check that $\varphi\psi = \mathrm{id}$ and $\psi\varphi = \mathrm{id}$, and hence we have established a bijection $[k] \times \mathcal{D}_{n,k} \to \mathcal{C}_{n+1,k} \times \mathcal{C}_{n,k}$. Therefore, $k(\#\mathcal{D}_{n,k}) = \binom{n}{k-1}\binom{n-1}{k-1}$ and the claim follows.

c) This is an immediate consequence of a), b) and decomposition $\bigcup_{k=1}^{n} \mathcal{D}_{n,k} = \mathcal{D}_n$.

d) The left-hand equality is the basic convolutive recursion for Catalan's numbers. We argue this time by using binary trees. The set $\mathcal{D}_{n+1}$ is (almost evidently) in bijection with all binary trees with $n{+}1$ vertices. Any such tree is an ordered pair (B, B') consisting of the left and right binary subtree having totally n vertices (away of the root). If B has, say, r vertices and B' the rest of $n-r$ vertices then there are $C_r C_{n-r}$ of such pairs. By adding all the cases $r = 1,\dots,n$ we get the convolutive recursion. The right-hand equality follows from the left-hand one and c).

e) It is trivial to check that $C_n^2 \le C_{n-1}C_{n+1}$ from the definition.

f) It is a standard trick to consider the square of the generating function and use the convolutive recursion d) to get this result. □

Let us list now some basic properties of the Narayana numbers (partially in the spirit of *Theorem 1*).

Theorem 4. *For integers $n,k \ge 0$, we have the following properties of Narayana numbers.*

a) $N(n,k) = N(n, n-k+1)$ (symmetry);

b) $\binom{k+1}{2} N(n+1,k+1) = \binom{n+1}{2} N(n,k)$ (absorption law);

c) $\binom{n}{k-1} N(n,k+1) = \binom{n}{k+1} N(n,k)$;

d) $\binom{n-k+2}{2} N(n+1,k) = \binom{n+1}{2} N(n,k)$;

e) $(n+1)N(n,k) = (n-1)\,[N(n-1,k-1) + N(n-1,k)] + 2\binom{n-1}{k-1}^2$;

f) $N(n+1,k+1) = \binom{n}{k}^2 - \binom{n}{k-1}\binom{n}{k+1} = \det \begin{bmatrix} \binom{n}{k} & \binom{n}{k+1} \\ \binom{n}{k-1} & \binom{n}{k} \end{bmatrix}$ *(hence, binomial coefficients are log-concave, because $N(n+1,k+1)$ has a combinatorial meaning by* Theorem 3 b)*);*

g) The sequence $N(n,0), N(n,1), \dots, N(n,n)$ is log-concave, and hence unimodal; it has one peak for n odd and a plateau of two peaks for n even;

h) The bivariate generating function $F = F(x,y) = \sum_{n,k\ge 1} N(n,k)x^n y^k$ is given by $xF^2 + (xy + x - y)F + xy = 0$.

Proof. By using the explicit formula for $N(n,k)$ it is rather simple to check all these properties algebraically. For example, to prove e) apply Pascal formula to both factors in $N(n,k) = \frac{1}{n}\binom{n}{k}\binom{n}{k-1}$ etc. But, let us prove combinatorially only the symmetry property a) by finding a "natural" bijection $f : \mathcal{D}_{n,k} \xrightarrow{\approx} \mathcal{D}_{n,n-k+1}$. Let $\rho_{n,k} : \mathcal{C}_{n+1,k+1} \xrightarrow{\approx} \binom{[n]}{k}$ be the de Moivre bijection from the proof of *Theorem 1 i)*, $c_{n,k} : \binom{[n]}{k} \xrightarrow{\approx} \binom{[n]}{n-k}$, $c_{n,k}(A) = [n] \setminus A = \overline{A}$ the complementation, $\sigma_{n,k} = \rho^{-1}_{n,n-k} \circ c_{n,k} \circ \rho_{n,k} : \mathcal{C}_{n+1,k+1} \xrightarrow{\approx} \mathcal{C}_{n+1,n-k+1}$ and $\varphi_{n,k} : [k] \times \mathcal{D}_{n,k} \xrightarrow{\approx} \mathcal{C}_{n+1,k} \times \mathcal{C}_{n,k}$ the bijection from the proof of *Theorem 3 b)*. Finally, let $\chi_{n,k} : [n-k+1] \times \binom{[n]}{k-1} \xrightarrow{\approx} [k] \times \binom{[n]}{n-k}$ be the natural bijection representing the equality $(n-k+1)\binom{n}{k-1} = k\binom{n}{n-k}$. The left-hand side of this equality counts all pairs (x, A), where $A \in \binom{[n]}{k-1}$ and $x \in \overline{A}$, while the right-hand side counts all pairs (y, B), $B \in \binom{[n]}{n-k}$ and $y \in \overline{B}$. Then $\chi_{n,k} : (x, A) \mapsto (y, B)$, where $B = \overline{A} \setminus \{x\}$ and $y = x$. The desired bijection f is then given by the following commutative diagram:

$$
\begin{array}{ccccc}
\begin{array}{c}[n-k+1]\\ \times\\ ([k]\times\mathcal{D}_{n,k})\end{array} & \xrightarrow[\approx]{\mathrm{id}\times\varphi_{n,k}} & \begin{array}{c}[n-k+1]\\ \times\\ \mathcal{C}_{n+1,k}\times\mathcal{C}_{n,k}\end{array} & \xrightarrow[\approx]{\mathrm{id}\times\rho_{n,k-1}\times\mathrm{id}} & \begin{array}{c}[n-k+1]\\ \times\\ \binom{[n]}{k-1}\times\mathcal{C}_{n,k}\end{array}\\
\Big\downarrow f & & & & \approx\Big\downarrow \begin{smallmatrix}\chi_{n,k}\\ \times\\ \sigma_{n-1,k-1}\end{smallmatrix}\\
\begin{array}{c}[k]\times([n-k+1]\\ \times\\ \mathcal{D}_{n,n-k+1})\end{array} & \xrightarrow[\mathrm{id}\times\varphi_{n,n-k+1}]{\approx} & \begin{array}{c}[k]\times\mathcal{C}_{n+1,n-k+1}\\ \times\\ \mathcal{C}_{n,n-k+1}\end{array} & \xrightarrow[\mathrm{id}\times\rho_{n,n-k}\times\mathrm{id}]{\approx} & \begin{array}{c}[k]\times\binom{[n]}{n-k}\\ \times\\ \mathcal{C}_{n,n-k+1}\end{array}
\end{array}
$$

We show by two examples how this symmetry f acts. First, for $n = 3$, $k = 2$ (*Figure 4*), and for $n = 4$, $k = 3$, let $P = ((2,2,3),(1,3,3)) \in \mathcal{D}_{7,3}$ we have $f(P) \in \mathcal{D}_{7,5}$ (*Figure 5*).

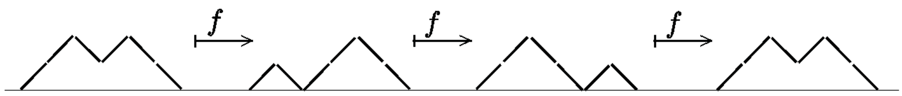

Figure 4.

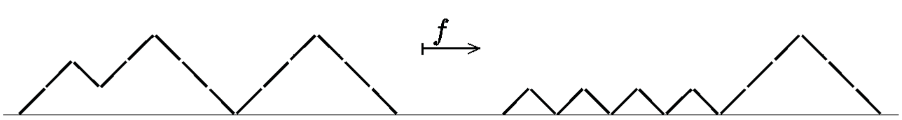

Figure 5.

There is no evident geometric interpretation of this symmetry. The other properties can also be proved combinatorially. □

Now define a **Motzkin**[2] **path** of length n as a lattice path in the (x, y)-plane from $(0, 0)$ to $(n, 0)$ with steps $(1, 0)$, $(1, 1)$ and $(1, -1)$, never falling below the x-axis. Let $\mathcal{M}(n)$ be the set of all Motzkin paths of length n and let $M_n := \#\mathcal{M}(n)$ be the n-th **Motzkin number** with $M_0 := 1$. By projecting to the y-axis, M_n is also the number of closed walks on $\mathbb{N}$ with n steps 1, -1 and 0 starting (and ending) at the origin. A handful of other combinatorial interpretations of M_n are presented in Ex. 6.38 in [7]. A member of the Motzkin family $\mathcal{M}(14)$ is in *Figure 6*.

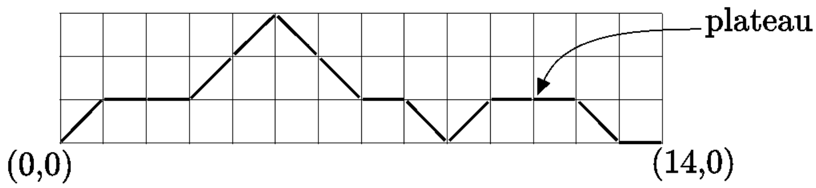

Figure 6.

According to the number of 0-steps, it follows easily that Catalan's and Motzkin's numbers are related as:

$$M_n = \sum_{k \geq 0} \binom{n}{2k} C_k, \qquad C_{n+1} = \sum_{k \geq 0} \binom{n}{k} M_k.$$

Let us summarize some important properties of the Motzkin numbers.

Theorem 5. *We have*

a) $M_{n+1} = M_n + \sum_{k=0}^{n-1} M_k M_{n-k-1}$;

b) The generating function (GF) of the sequence $(M_n)_{n \geq 0}$ *is given by*

$$\begin{aligned} M &= M(x) = \sum_{n \geq 0} M_n x^n = \frac{1 - x - \sqrt{1 - 2x - 3x^2}}{2x^2} = \\ &= 1 + x + 2x^2 + 4x^3 + 9x^4 + 21x^5 + 51x^6 + 127x^7 + 323x^8 + \ldots; \end{aligned}$$

c) $(n + 2)M_n = (2n + 1)M_{n-1} + 3(n - 1)M_{n-2}$ *(short recursion);*

d) The sequence $(M_n)_{n \geq 0}$ *is log-convex, i.e.* $M_n^2 \leq M_{n-1} M_{n+1}$ *for all* $n \geq 1$*;*

e) There exists $\lim_{n \to \infty} M_n / M_{n-1}$ *and it is equal to* 3*;*

f) Asymptotically, $M_n \sim \sqrt{\frac{3}{4\pi}} 3^{n+1} n^{-3/2}$.

[2]Theodore S. Motzkin, (1908 – 1970), Israeli mathematician

Proof.

a) For $n = 0$ and $n = 1$, $M_0 = M_1 = 1$. Let $n \geq 1$. A Motzkin path with $n + 1$ steps starts either with step $(1, 0)$ and then it can continue in M_n ways, or it starts with step $(1, 1)$ and returns for the first time to the x-axis after $k+1$ steps (i.e. arrives to $(k + 2, 0)$). The number of such paths is equal to the number of ordered pairs (P_1, P_2), where P_1 is a Motzkin path from $(1, 1)$ to $(k+1, 1)$ never falling below the line $y = 1$, and P_2 a Motzkin path from $(k+2, 0)$ to $(n+1, 0)$. There are M_k Motzkin paths P_1 and M_{n-k-1} Motzkin paths P_2 (since it has $n + 1 - (k + 2) = n - k - 1$ steps). So, a) follows.

b) By multiplying the recursion in a) with x^{n+1} and summing on $n \geq 0$ we get (since $M_0 = 1$) that $x^2M^2 + (x-1)M + 1 = 0$. Since $M(0) = M_0 = 1$, the claim b) follows.

c) From b) we see that $M(x)$ is an algebraic GF (so, D-finite), and hence (M_n) is a **polynomially recursive** (or P-**recursive**) sequence. Then from Eq. 6.38. in [7] and from $2x^2M(x) + x - 1 = \sqrt{1 - 2x - 3x^2}$ we get c).

d) Now we divide the short recursion in c) by M_{n-1} and denote $x_n = M_n/M_{n-1}$. We get the recursion

$$x_n = \frac{1}{n+2}\left[2n + 1 + \frac{3(n-1)}{x_{n-1}}\right], \qquad n \geq 2 \tag{$*$}$$

with initial condition $x_1 = 1$. The log-convexity $M_n^2 \leq M_{n-1}M_{n+1}$ is equivalent to $x_n \leq x_{n+1}$. So we want to prove that the sequence $(x_n)_{n\geq 1}$ is increasing.

We define the function $f : [2, \infty) \to \mathbb{R}$ (in fact a dynamical system) as follows. $f(x) = 2$ for $x \in [2, 3]$ and (as the rule $(*)$) $(x+2)f(x-1)f(x) = (2x+1)f(x-1) + 3(x-1)$, $x \geq 3$, so that $f(n) = x_n$, for any integer $n \geq 2$. The function f is continuous and on any open interval $(n, n+1)$, $n \geq 2$, f is a rational function with no poles on the interval, so f is smooth on each $(n, n + 1)$. For example, $f(x) = (7x - 1)/(2x + 4)$ for $x \in [3, 4]$, $f(x) = (20x^2 - 9x - 14)/(7x^2 + 6x - 16)$ for $x \in [4, 5]$ and so on. We shall prove that f is increasing by showing that f increases on any segment $[3, n]$. It is true for $n = 4$, and for $x \in (n, n + 1)$ by computing the derivative $f'(x)$ (and pumping in once more for $f'(x-1)$) we get:

$$\begin{aligned} f'(x) &= \frac{3}{((x+2)f(x-1))^2}\Bigg[f^2(x-1) + 3f(x-1) + \\ &+ \frac{3(x^2-1)(x^2-4)f'(x-2)}{(x+1)^2 f(x-2)} - \frac{3(x-1)(x+2)}{(x+1)^2 f(x-2)}(f(x-2)+3)\Bigg]. \end{aligned}$$

By an inductive hypothesis, f increases on $[3, n]$, hence $f(x-1) \geq f(x-2) \geq 2$ and $f'(x-2) \geq 0$. We claim that $f'(x) \geq 0$. This follows from the following:

$$f^2(x-1)+3f(x-1) \geq \frac{3(x-1)(x+2)}{(x+1)^2} \cdot \frac{f(x-2)+3}{f(x-2)} \Leftrightarrow$$
$$\frac{[f^2(x-1)+3f(x-1)]f(x-2)}{f(x-2)+3} \geq \frac{3(x-1)(x+2)}{(x+1)^2}. \qquad (**)$$

But this last inequality is true since by the inductive hypothesis $f(x-1) \geq f(x-2) \geq 2$, and hence the left-hand side of $(**)$ is at least equal to $f^2(x-2) \geq 4$, while the right-hand side in $(**)$ has the maximum (for $x \geq 3$) equal to 3. So we proved that $f'(x) \geq 0$ for all $x \in (n, n+1)$ and therefore f increases on $(n, n+1)$. By continuity it follows that f increases on $[3, n+1]$. By induction it follows that f is an increasing function. In particular, $x_{n+1} \geq x_n$, completing our calculus proof.

Yet another proof is to interlace (x_n) with the increasing sequence (a_n), where $a_n = 6n/(2n+3)$. Namely, it is easy to check by induction on $n \geq 3$ that $a_n \leq x_n \leq a_{n+1}$. Hence (x_n) is increasing. (A proof of d) is also given in [1].)

We note also that $(*)$ and log-convexity of (M_n) imply easily that the sequence $(M_n/n!)$ is log-concave.

e) Both above proofs of d) show that (x_n) is bounded: $2 \leq f(x) \leq 7/2$, and (a_n) is bounded. Hence (x_n) is convergent. By passing to limit in $(*)$ or in $a_n \leq x_n \leq a_{n+1}$, we get $\lim_{n\to\infty} x_n = 3$.

f) This follows from a well known theorem of Darboux (see e.g. [8]) which in our situation reads
$$M_n \sim \frac{1}{4\sqrt{\pi n^3}}[-r\Delta'(r)]^{1/2} r^{-n-2},$$
where r is the least positive root of the discriminant Δ of the equation $x^2M^2 + (x-1)M + 1 = 0$. □

There is a great deal of other interesting relations between Catalan and Motzkin numbers. For example, writing $2x^2M = 1 - x - \sqrt{1-2x-3x^2}$, by expanding the root here via binomial series, and by equating the coefficient of x^{n+2} on both sides, we get
$$M_n = \left(\frac{3}{2}\right)^{n+2} \sum_{k\geq 0} \frac{1}{3^k} C_{k-1} \binom{k}{n+2-k}.$$

We end with a brief and informal description of secondary structures and their relations to the previous material (the details will appear in [2]). A **secondary structure** is a simple graph whose set of vertices is $[n]$ and having two kinds of edges: the segments $[i, i+1]$, for $1 \leq i \leq n-1$ and arcs in the upper halfplane connecting some i, j such that $j - i > l$, where l is fixed. Any two arcs are (totally) disjoint. Such a structure is said to have **rank** l. Let $\mathcal{S}^{(l)}(n)$ be the set of all secondary structures (up to isomorphism) of rank l on n vertices and $S^{(l)}(n) := \#\mathcal{S}^{(l)}(n)$ the number of secondary structures of rank l on n vertices. For example, for $l = 1$, $n = 5$, there are $S^{(1)}(5) = 8$ secondary structures of rank 1 on $[5]$ (note that here arcs “jump” over at least $l = 1$ vertices) in *Figure 7*:

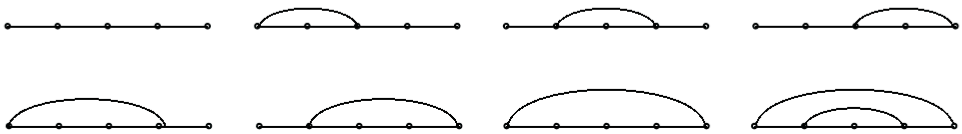

Figure 7.

Let $\mathcal{M}^{(l)}(n)$ denote the family of Motzkin paths of length n whose every plateau (see *Figure 6*) is of length $\geq l$. Then there is a natural bijection $\mathcal{S}^{(l)}(n) \to \mathcal{M}^{(l)}(n)$ as follows. To any vertex in which an arc starts assign step $(1,1)$, to any vertex in which an already encountered arc terminates assign the step $(1,-1)$, and to any “free” vertex assign the step $(1,0)$. By allowing arcs to connect the neighboring vertices, it follows also that $\mathcal{M}^{(0)}(n) = \mathcal{M}(n) \overset{1-1}{\longleftrightarrow} \mathcal{S}^{(0)}(n)$. So, the Motzkin family can be regarded as the border case of the secondary structures (when $l = 0$). If we take $l = -1$, by allowing arcs to be loops, we get the Dyck family. Hence, the Dyck family can be regarded as the degenerate case of secondary structures; more precisely, there is a bijection $\mathcal{S}^{(-1)}(n) \longleftrightarrow \mathcal{D}_{n+1}$. So, we have $S^{(-1)}(n) = C_{n+1}$ and $S^{(0)}(n) = M_n$. Let us mention only that the secondary structures can also be interpreted as sets of certain matchings in graphs.

For any fixed l, the sequence $(S^{(l)}(n))_{n\geq 1}$ of numbers of secondary structures has properties like those in *Theorem 5*. First, for any fixed integer $l(\geq -1)$, the numbers $S^{(l)}(n)$ satisfy the long convolution recurrence

$$S^{(l)}(n+1) = S^{(l)}(n) + \sum_{k=l}^{n-1} S^{(l)}(k)S^{(l)}(n-k-1), \qquad n \geq l+1,$$

with initial conditions $S^{(l)}(0) = S^{(l)}(1) = \cdots = S^{(l)}(l+1) = 1$. Namely, a secondary structure on $[n+1]$ either does not have an arc starting in 1, or else such an arc terminates at some vertex $k+2$. The generating function $S_l(x) = \sum_{n\geq 0} S^{(l)}x^n$ is given by $x^2S_l^2(x) + \omega_l(x)S_l(x) + 1 = 0$, i.e.

$$S_l(x) = \frac{-\omega_l(x) - \sqrt{\omega_l^2(x) - 4x^2}}{2x^2},$$

where $\omega_l(x) = 2x - (1+x+\cdots+x^{l+1})$. But, $S^{(l)}(n)$'s also satisfy a short recurrence. For example, if $l = 1$, then it turns out that the numbers $S^{(1)}(n)$ (written simply as $S(n)$) satisfy

$$(n+2)S(n) = (2n+1)S(n-1) + (n-1)S(n-2) + (2n-5)S(n-3) - (n-4)S(n-4),$$

$n \geq 4$, with initial conditions $S(0) = S(1) = S(2) = 1$, $S(3) = 2$. From this short recursion it can also be proved that $S(n)$'s are log-convex. This follows inductively from the fact $a_n \leq x_n \leq a_{n+1}$, for $n \geq 6$, where $x_n = S(n)/S(n-1)$ and $a_n =$

$2n\varphi^2/(2n+3)$. So, (x_n) is an increasing sequence. Since $2 \le x_n \le 3$, it follows that (x_n) converges and $\lim_{n\to\infty} x_n = \varphi^2 = (3+\sqrt{5})/2$. The asymptotics for $l = 1$ and $l = 2$ are given by:

$$S^{(1)}(n) \sim \sqrt{\frac{15+7\sqrt{5}}{8\pi}} \left(\frac{3+\sqrt{5}}{2}\right)^n n^{-3/2}, \qquad S^{(2)}(n) \sim \sqrt{\frac{1+\sqrt{2}}{\pi}}(1+\sqrt{2})^n n^{-3/2}.$$

In general, $S^{(l)}(n) \sim K_l \alpha_l^n n^{-3/2}$, where K_l and α_l are constants depending only on l and $\alpha_l \searrow 2$ as $l \to \infty$. The precise values of α_l (and K_l) can also be computed for $l \le 6$. Most of the mentioned results are new and proved in [2].

On the other hand, the Narayana numbers are related to secondary structures as follows. By counting the numbers $S_k^{(l)}(n)$ of rank l secondary structures with k arcs (note that $S^{(l)}(n) = \sum_{k\ge 0} S_k^{(l)}(n)$), we get:

$$S_k^{(l)}(n) = \sum_{j=1}^{k} N(k,j)\binom{n-lj}{2k}.$$

In particular, when $l = 1$, then $S_k^{(1)}(n) = N(n-k, k+1)$, and we get (combinatorially proved) recursion

$$N(n-k,k+1) = \sum_{j=1}^{k} N(k,j)\binom{n-j}{2k},$$

or equivalently,

$$N(n,k) = \sum_{j=1}^{k-1} N(k-1,j)\binom{n+k-j-1}{2k-2}.$$

So, to compute $N(n,k)$ when n is big, one has to know only small values $N(k-1,j)$ (and database of binomial coefficients).

A whole story of various interrelations between Catalan, Motzkin and Narayana numbers and their relationship to secondary structures only starts here, not to mention their possible q-analogues, applications, etc. For example, one of the applications of secondary structures in mathematics itself is: $D_k(n) = S_k^{(1)}(n) - S_{k-1}^{(1)}(n-2) = \frac{n}{k(k+1)}\binom{n-k-2}{k}\binom{n-k-1}{k-1}$, where $D_k(n)$ stands for the number of dissections of a convex n-gon by k totally disjoint diagonals. In a sentence we see how this "secondary" combinatorics is much more subtle and intricate than the "primary" combinatorics. Yet, the proofs of the basic "secondary" facts we have given here are rather elementary, and could safely be included in the undergraduate combinatorics curriculum. The importance and simple combinatorial appeal of this material simply call for such an inclusion.

A final word about the origin of secondary structures (see [4], [5] and [9]). They come from biology and are very important in understanding the role which RNA's have in cell metabolism and in decoding genetic informations contained in DNA's. Biologists call the vertices of secondary structures *bases*, the segments *p-bonds* (p

stands for phosphorous), and arcs *h-bonds* (h stands for hydrogene). Note that secondary structures are planar graphs, but of great interest in biology are the also so-called "tertiary structures", huge non-planar molecules, entangled in space in forms of knots and links. One could only speculate how hard, complex and subtle the "tertiary" combinatorics would be. Hopefully, the new millenium will resolve problems there.

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