

CALCULUS PROOFS OF SOME COMBINATORIAL INEQUALITIES

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Abstract. Using calculus we show how to prove some combinatorial inequalities of the type log-concavity or log-convexity. It is shown by this method that binomial coefficients and Stirling numbers of the first and second kinds are log-concave, and that Motzkin numbers and secondary structure numbers of rank 1 are log-convex. In fact, we prove via calculus a much stronger result that a natural continuous “patchwork” (i.e. corresponding dynamical systems) of Motzkin numbers and secondary structures recursions are increasing functions. We indicate how to prove asymptotically the log-convexity for general secondary structures. Our method also applies to show that sequences of values of some orthogonal polynomials, and in particular the sequence of central Delannoy numbers, are log-convex.

1. Introduction

In combinatorics the most prominent question is usually to find explicitly the size of certain finite set defined in an intricate way. It often happens that there is no explicit expression for the size in question, but instead one can find recursion, generating function or other gadgets which enable us to compute concrete sizes or numbers. The next question then usually asks how the sequence of numbers satisfying certain recursion behaves. By behavior of the sequence $(a_n)_{n \geq 0}$ of positive real numbers it is often meant its log-concavity (or log-convexity). Recall that a sequence $(a_n)_{n \geq 0}$ of positive real numbers is *log-concave* if $a_n^2 \geq a_{n-1}a_{n+1}$ for all $n \geq 1$, and *log-convex* if $a_n^2 \leq a_{n-1}a_{n+1}$ for all $n \geq 1$. We say that a sequence $(a_n)_{n \geq 0}$ is *log-straight* or *geometric* if $a_n^2 = a_{n-1}a_{n+1}$ for all $n \geq 1$. A (finite) sequence of positive numbers a_0, a_1, \dots, a_n is said to be *unimodal* if, for some $0 \leq j \leq n$ we have $a_0 \leq a_1 \leq \dots \leq a_j \geq a_{j+1} \geq \dots \geq a_n$. This place j is called a *peak* of the sequence if it is unique. If there are more such maximal values, we speak about a *plateau* of the sequence. It is easy to see that a log-concave positive sequence is unimodal. The literature on log-concavity and unimodality is vast. We refer the interested reader to the book [7]. Combinatorial inequalities, and in particular, the questions concerning log-concavity (or log-convexity) are surveyed in [3], [12] and [10]. Some analytic methods are described in [2].

In combinatorics, a preferable way to prove a combinatorial inequality is to give a *combinatorial proof*. There are two basic ways to do it. Suppose that we are given finite

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sets A and B with $|A| = a$ and $|B| = b$ and we want to prove, say, $a \leq b$. One way to prove it is to construct an injection $A \rightarrow B$ (or a surjection $B \rightarrow A$), and the other is to show that the number $c = b - a$ is nonnegative, by showing that c is cardinality of certain set or that c is the dimension of certain vector space (and hence nonnegative) etc. As an example, let us show that binomial coefficients $\binom{n}{k}$, $k = 0, 1, \dots, n$ are log-concave. It is trivial to check algebraically that $\binom{n}{k}^2 \geq \binom{n}{k-1} \binom{n}{k+1}$ by using the standard formula $\binom{n}{k} = \frac{n!}{k!(n-k)!}$, but combinatorially it goes as follows.

First define the *Narayana numbers* $N(n, k)$ for integers $n, k \geq 1$ as

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

and $N(0, 0) := 1$. Next we note that

$$\binom{n}{k}^2 - \binom{n}{k-1} \binom{n}{k+1} = \left| \begin{matrix} \binom{n}{k} & \binom{n}{k+1} \\ \binom{n}{k-1} & \binom{n}{k} \end{matrix} \right| = N(n+1, k+1).$$

Finally, we need the fact that Narayana numbers have a combinatorial meaning, i.e. they count certain finite sets (see below). Therefore we get $\binom{n}{k}^2 - \binom{n}{k-1} \binom{n}{k+1} \geq 0$. There are also other combinatorial proofs of log-concavity of binomial coefficients, as well as log-concavity of Stirling numbers (of both kinds) etc., but they are all rather involved and/or tricky. In this paper we present a way to prove various combinatorial inequalities by a straightforward method of calculus. Inductive and injective proofs of log-convexity results are described in [9].

2. Calculus proofs of log-concavity and log-convexity properties

Let us first recall briefly calculus proofs of log-concavity of binomial coefficients and Stirling numbers. Let $c(n, k)$ be the number of permutations of the set $[n] := \{1, 2, \dots, n\}$ with exactly k cycles and $S(n, k)$ the number of partitions of $[n]$ into exactly k parts (or blocks). The numbers $c(n, k)$ and $S(n, k)$ are called *Stirling numbers* of the *first* and *second kind*, respectively. The following formulae are well known (see [11]).

$$(x+1)^n = \sum_{k=0}^n \binom{n}{k} x^k, \tag{1}$$

$$x^{\bar{n}} = x(x+1) \dots (x+n-1) = \sum_{k=0}^n c(n, k) x^k, \tag{2}$$

$$x^n = \sum_{k=0}^n S(n, k) x^{\underline{k}}, \tag{3}$$

where $x^{\underline{k}} := x(x-1) \dots (x-k+1)$ is the k -th *falling power* and $x^{\bar{k}} = x(x+1) \dots (x+k-1)$ the k -th *rising power* of x .

The following Newton's lemma is a consequence of the Rolle's theorem from calculus.

LEMMA 1. Let $P(x) = \sum_{k=0}^n a_k x^k$ be a real polynomial whose all roots are real numbers. Then its coefficients are log-concave, i.e. $a_k^2 \geq a_{k-1} a_{k+1}, k = 1, \dots, n - 1$. (Moreover, $\frac{a_k}{\binom{n}{k}}$ are log-concave).

Now, from (1) and (2) we see that $(x + 1)^n$ and x^i have only real roots and by Lemma 1. we conclude that the sequences $\binom{n}{k}$ and $c(n, k)$ are log-concave.

The case of the sequence $S(n, k)$ is a bit more involved. We claim that the polynomial

$$P_n(x) = \sum_{k=0}^n S(n, k) x^k \tag{4}$$

has all real roots (in fact non-positive and different). Namely, $P_0(x) = 1$ and from the basic recursion

$$S(n, k) = S(n - 1, k - 1) + kS(n - 1, k)$$

it follows at once that

$$P_n(x) = x [P'_{n-1}(x) + P_{n-1}(x)].$$

The function $Q_n(x) = P_n(x)e^x$ has the same roots as $P_n(x)$ and it is easy to verify $Q_n(x) = xQ'_n(x)$. By induction on n and by using the Rolle's theorem it follows easily that Q_n and hence P_n have only real and non-positive roots.

So, we have proved by calculus the following.

THEOREM 1. The sequences $\binom{n}{k}_{k \geq 0}, (c(n, k))_{k \geq 0}, (S(n, k))_{k \geq 0}$ are log-concave. Hence they are also unimodal.

It is also well known that the peak of the sequence $\binom{n}{k}$ is at $k = \lfloor n/2 \rfloor$, while the peak for the other two sequences is much harder to determine. It is known that $S(n, k)$'s reach their peak for $k \approx n/\log n$, if n is large enough. (An inductive proof of Theorem 1. is given in [9].)

Now we turn to a different kind of combinatorial entities. Recall that a *Dyck path* is a path in the coordinate (x, y) -plane from $(0, 0)$ to $(2n, 0)$ with steps $(1, 1)$ and $(1, -1)$ never falling below the x -axis. Denote the set of all such paths by \mathcal{D}_n . A *peak* of a path $P \in \mathcal{D}_n$ is a place at which the step $(1, 1)$ is directly followed by the step $(1, -1)$. Denote by $\mathcal{D}_{n,k} \subseteq \mathcal{D}_n$ the set of all Dyck paths of length $2n$ with exactly k peaks. Note that $1 \leq k \leq n$. The following facts are also well known (see [11]).

$$|\mathcal{D}_n| = \frac{1}{n + 1} \binom{2n}{n} = C_n$$

$$|\mathcal{D}_{n,k}| = N(n, k),$$

where C_n is n -th *Catalan number*. The Catalan numbers are log-convex. The Narayana numbers are log-concave in k for fixed n . Both these facts can easily be proved algebraically, but there are also combinatorial proofs, as well as calculus proofs. We omit here these proofs, since we want to emphasize the following more intricate combinatorial quantities, related to the above just introduced.

A *Motzkin path* is a path in the coordinate (x, y) -plane from $(0, 0)$ to $(n, 0)$ with steps $(1, 1)$, $(1, 0)$ and $(1, -1)$ never falling below the x -axis. Let \mathcal{M}_n be the set of all such paths and let $M_n = |\mathcal{M}_n|$. The number M_n is called the n -th *Motzkin number*.

Some basic properties of Motzkin numbers are as follows ([11], [6]).

- THEOREM 2. (a) $M_n = \sum_{k \geq 0} \binom{n}{2k} C_k$, $C_{n+1} = \sum_{k \geq 0} \binom{n}{k} M_k$;
 (b) $M_{n+1} = M_n + \sum_{k=0}^{n-1} M_k M_{n-k-1}$;
 (c) The generating function of $(M_n)_{n \geq 0}$ is given by

$$M(x) = \sum_{n \geq 0} M_n x^n = \frac{1 - x - \sqrt{1 - 2x - 3x^2}}{2x^2};$$

(d) $(n + 2)M_n = (2n + 1)M_{n-1} + 3(n - 1)M_{n-2}$;

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

The log-convexity of the sequence of Motzkin numbers was first established algebraically in [1], and shortly afterwards combinatorial proof appeared in [4]. We shall prove now by calculus that $(M_n)_{n \geq 0}$ is a log-convex sequence and some consequences of this property.

THEOREM 3.

- (a) The sequence $(M_n)_{n \geq 0}$ is log-convex;
 (b) $M_n \leq 3M_{n-1}$, for all $n \geq 1$;
 (c) There exists $x = \lim_{n \rightarrow \infty} \frac{M_n}{M_{n-1}}$, and $x = 3$.

Proof. (a) Let us start from the short recursion in Theorem 2.(d):

$$M_n = \frac{2n + 1}{n + 2} M_{n-1} + \frac{3(n - 1)}{n + 2} M_{n-2}.$$

Divide this recursion by M_{n-1} and denote $x_n := \frac{M_n}{M_{n-1}}$. Then we obtain the following recursion:

$$x_n = \frac{2n + 1}{n + 2} + \frac{3(n - 1)}{n + 2} \frac{1}{x_{n-1}} \quad (5)$$

with initial condition $x_1 = 1$. The log-convexity $M_n^2 \leq M_{n-1}M_{n+1}$ is equivalent to $x_n \leq x_{n+1}$. To prove that $(x_n)_{n \geq 0}$ is an increasing sequence, we shall prove a much stronger claim. To this end, define the following function $f : [2, \infty) \rightarrow \mathbb{R}$. For $x \in [2, 3]$, define $f(x) = 2$. For $x \geq 3$, let (by simulating (5))

$$f(x) = \frac{2x + 1}{x + 2} + \frac{3(x - 1)}{x + 2} \frac{1}{f(x - 1)}. \quad (6)$$

Note that $f(n) = x_n$. We shall prove that f is an increasing function, and consequently that $(x_n)_{n \geq 0}$ is an increasing sequence. Note first that the function f is continuous (f is, in fact, a dynamical system), and on every open interval $(n, n + 1)$, where $n \geq 2$ is an integer, f is a rational function, with no poles on it. Therefore, f is smooth on every open interval $(n, n + 1)$, for $n \geq 2$. Note that, for example, $f(x) = \frac{7x-1}{2(x+2)}$ for

$x \in [3, 4]$, $f(x) = \frac{20x^2 - 9x - 14}{7x^2 + 6x - 16}$ for $x \in [4, 5]$, etc. It is trivial to check that $f(x) \geq 2$, for all $x \geq 2$. Suppose inductively that f is an increasing function on a segment $[3, n]$. For $n = 4$ it is (almost evidently) true. Let $n \geq 4$, and take a point $x \in (n, n + 1)$. By taking the derivative $f'(x)$ of (6), and plugging in once more the term for $f'(x - 1)$, we have:

$$f'(x) = \frac{3}{[(x + 2)f(x - 1)]^2} \left[f^2(x - 1) + 3f(x - 1) - 3 \frac{(x - 1)(x + 2)}{(x + 1)^2 f(x - 2)} [f(x - 2) + 3] + 3 \frac{(x^2 - 1)(x^2 - 4)}{[(x + 1)f(x - 2)]^2} f'(x - 2) \right]$$

By inductive hypothesis, f is an increasing function on $[3, n]$ and hence $f(x - 1) \geq f(x - 2) \geq 2$ and $f'(x - 2) \geq 0$. So, it is enough to prove that $f'(x) \geq 0$. However, this follows from the following.

The last term in square brackets is clearly positive, by the induction hypothesis. We claim that the rest is positive, too. This claim is equivalent with

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

But this inequality is true, since by inductive hypothesis $f(x - 1) \geq f(x - 2) \geq 2$, and hence the left hand side is at least equal to $f^2(x - 2) \geq 4$, while the right hand side has the maximum (for $x \geq 3$) equal to 3. Hence $f'(x) > 0$ for all $x \in (n, n + 1)$. So, the function f is strictly increasing on $(n, n + 1)$, and then, by continuity, also on $[3, n + 1]$. In particular, $f(n + 1) = x_{n+1} \geq x_n = f(n)$. This completes the step of induction.

(b) and (c) follow now simultaneously, because by (a), the sequence $(x_n)_{n \geq 0}$ is increasing and from (5) it follows easily by induction on n that $2 \leq x_n \leq 7/2$, i.e. (x_n) is bounded. \square

Closely related combinatorial structures to Motzkin paths are the so called secondary structures. A *secondary structure* is a simple planar graph on vertex set $[n]$ with two kinds of edges: segments $[i, i + 1]$, for $1 \leq i \leq n - 1$ and arcs in the upper half-plane which connect some i, j , where $i < j$ and $j - i > l$, for some fixed integer $l \geq -1$, such that the arcs are totally disjoint. Such a structure is called a secondary structure of *size* n and *rank* l . The importance for the study of these structures comes from biology. They are crucial in understanding the role of RNA in the cell metabolism and in decoding the hereditary information contained in DNA. Biologists call the vertices of a secondary structure *bases*, the segments they call *p-bonds* (p stands for phosphorus) and arcs they call *h-bonds* (h stands for hydrogen). Let $\mathcal{S}^{(l)}(n)$ be the set of all secondary structures of rank l on n vertices and $S^{(l)}(n) = |\mathcal{S}^{(l)}(n)|$ the *secondary structure numbers* of rank l . In a sense, the Motzkin numbers are secondary structure numbers of rank 0, and the Catalan numbers are secondary structure numbers of the (degenerate) rank -1 . In these cases the corresponding graphs are not simple, but the other requirements on secondary structures remain.

Now we shall apply our method of calculus to prove that in the case $l = 1$ the behavior of the numbers $S^{(1)}(n)$ is also log-convex. So, we have:

THEOREM 4. *The sequence $(S^{(1)}(n))_{n \geq 0}$ is log-convex.*

Proof. As for the Motzkin numbers, it turns out that for $S^{(1)}(n)$ the following short recursion holds (see [6] and [5]):

$$(n+2)S^{(1)}(n) = (2n+1)S^{(1)}(n-1) + (n-1)S^{(1)}(n-2) \\ + (2n-5)S^{(1)}(n-3) - (n-4)S^{(1)}(n-4) \quad (7)$$

with initial conditions $S^{(1)}(0) = S^{(1)}(1) = S^{(1)}(2) = 1, S^{(1)}(3) = 2$. By dividing this recursion with $S^{(1)}(n-1)$ and denoting

$$x_n = \frac{S^{(1)}(n)}{S^{(1)}(n-1)},$$

we get

$$x_n = \frac{1}{n+2} \left[2n+1 + \frac{n-1}{x_{n-1}} + \frac{2n-5}{x_{n-1}x_{n-2}} - \frac{n-4}{x_{n-1}x_{n-2}x_{n-3}} \right], \quad (8)$$

with initial conditions $x_3 = x_4 = x_5 = 2$ (note that $x_1 = x_2 = 1$).

The log-convexity of $S^{(1)}(n)$'s is equivalent with the fact that (x_n) is an increasing sequence.

Now define the function $f : [2, \infty) \rightarrow \mathbb{R}$ by simulating (8) as:

$$f(x) = \begin{cases} 2, & \text{if } x \in [2, 5], \\ \frac{1}{x+2} \left[2x+1 + \frac{x-1}{f(x-1)} + \frac{2x-5}{f(x-1)f(x-2)} - \frac{x-4}{f(x-1)f(x-2)f(x-3)} \right], & \text{if } x \geq 5. \end{cases} \quad (9)$$

Clearly, for any integer $n \geq 3$, $f(n) = x_n$, and f is continuous, and, in fact, piecewise rational and smooth on any open interval $(n, n+1)$ for $n \geq 2$. The basic idea is, as in the proof of Theorem 3.(a), to show that f is an increasing and bounded function, and hence (x_n) is an increasing sequence. In next few lemmas we proceed with details.

LEMMA 2. *For all $x \geq 2$, we have $2 \leq f(x) \leq 3$, while for $x \geq 53$ we have even stronger bounds:*

$$2.5 \leq f(x) \leq 2.67.$$

Proof. We prove inductively that $2 \leq f(x) \leq 3$ for $x \in [2, n]$. For $n \leq 11$ it can be checked directly. Let $n \geq 11$ and $x \in (n, n+1]$. Then

$$f(x) \leq \frac{1}{x+2} \left[2x+1 + \frac{x-1}{f(x-1)} + \frac{2x-5}{f(x-1)f(x-2)} \right] \\ \leq \frac{1}{x+2} \left[2x+1 + \frac{x-1}{2} + \frac{2x-5}{4} \right] = \frac{12x-3}{4x+8} \leq 3.$$

On the other hand,

$$f(x) \geq \frac{1}{x+2} \left[2x+1 + \frac{x-1}{3} + \frac{2x-5}{9} - \frac{x-4}{8} \right] = \frac{175x+44}{72x+144} \geq 2,$$

for all $x \geq 8$. So, $2 \leq f(x) \leq 3$ on $(n, n + 1]$ and the first claim is proved.

The stronger bounds also follow by induction. By direct computation, (using *Mathematica*) one can check that they hold on the interval $[53, 56]$. Suppose $2.5 \leq f(x) \leq 2.67$ on some interval $[53, n]$, where $n \geq 56$ and take $x \in [n, n + 1]$. From (8) we get

$$f(x) \leq \frac{1}{x+2} \left[2x + 1 + \frac{x-1}{2.5} + \frac{2x-5}{2.5^2} - \frac{x-4}{2.67^3} \right] = \frac{2.6675x + 0.010148}{x+2} \leq 2.67,$$

for all $x \geq 0$. On the other hand,

$$f(x) \geq \frac{1}{x+2} \left[2x + 1 + \frac{x-1}{2.67} + \frac{2x-5}{2.67^2} - \frac{x-4}{2.5^3} \right] = \frac{2.59108x + 0.0181}{x+2},$$

and this is greater than 2.5 for $x \geq 53$ (since the right hand side is equal to 2.5 for $x = 52.918$). So, Lemma 2. is proved. \square

LEMMA 3. *The function f is increasing.*

Proof. Suppose again inductively on $n \in \mathbb{N}$ that f increases on $(5, n]$. We shall prove that f increases on $(n, n + 1)$. One can check directly (using, e.g. *Mathematica*) that f increases on $(5, n_0]$, as far as $n_0 = 61$. Namely, the function f on interval $(n, n + 1)$ is a rational function whose both numerator and denominator are polynomials with integer coefficients of degree $n - 4$. The derivative of f is also a rational function, and its denominator is always positive. So, we need to show that the numerators of the derivative of f are positive on every interval $(n, n + 1)$, for $n \leq n_0 - 1$. An advanced computer algebra system, such as *Mathematica*, gives us readily explicit expressions for $f(x)$ and $f'(x)$ on any given interval $(n, n + 1)$. Let us denote $f'(x) = \frac{N_n(x)}{D_n(x)}$ on interval $(n, n + 1)$. If we can find some $k \in \mathbb{N}$, $k \leq n$, such that all coefficients of $N_n(x + k)$ are nonnegative, we are done, since then $f'(x)$ can not change its sign on the considered interval. It turns out that $k = 2$ works for all intervals $(n, n + 1)$ with $n \leq 60$. Hence, $f'(x) \geq 0$ for $x \in (n, n + 1)$, $n \leq 60$ and $f(x)$ is increasing on $[5, 61]$. It is important to note here that all performed computations include only integer quantities, and no round-off errors occur.

Take $x \in (n, n + 1)$ for $n \geq n_0$. Then $f'(x) > 0$ for $x \in (i, i + 1)$, $i = 5, \dots, n - 1$, and also $f(x) \geq f(x - 1)$, for $4 \leq x \leq n$.

Denote for short $f_i = f(x - i)$, $i \geq 1$. Then (9) can be written as

$$(x + 2)f_1 f_2 f_3 f(x) = (2x + 1)f_1 f_2 f_3 + (x - 1)f_2 f_3 + (2x - 5)f_3 - (x - 4).$$

By taking derivative, we get

$$f'(x) = \frac{1}{D(x)} [F(x) + F_3(x)f_3'(x) - F_1(x)f_1'(x) - F_2(x)f_2'(x)],$$

where

$$D(x) = (x + 2)f_1f_2f_3,$$

$$F(x) = 2f_1f_2f_3 + f_2f_3 + 2f_3 - 1 - f_1f_2f_3f'(x),$$

$$F_1(x) = [(x + 2)f(x) - (2x + 1)]f_2f_3,$$

$$F_2(x) = [(x + 2)f_1f'(x) - (2x + 1)f_1 - (x - 1)]f_3,$$

$$F_3(x) = 2x - 5 + (2x + 1)f_1f_2 + (x - 1)f_2 - (x + 2)f_1f_2f'(x).$$

Using (9), let us express $D(x), F(x), F_i(x), i = 1, 2, 3$ only in terms of f_i 's and x :

$$D(x) = (x + 2)f_1f_2f_3,$$

$$F(x) = \frac{3}{x + 2}(f_1f_2f_3 + f_2f_3 + 3f_2 - 2),$$

$$F_1(x) = \frac{1}{f_1}[(f_2f_3 + 2f_3 - 1)x - (f_2f_3 + 5f_3 - 4)],$$

$$F_2(x) = \frac{1}{f_2}[(2f_3 - 1)x - (5f_3 - 4)],$$

$$F_3(x) = \frac{1}{f_3}(x - 4).$$

Now plug in derivatives f_1' and f_2' by the same rule, to obtain

$$\begin{aligned} f'(x) &= \frac{1}{D(x)} \left\{ F(x) - \frac{F_1(x)F(x-1)}{D(x-1)} - \frac{F_2(x)F(x-2)}{D(x-2)} + \frac{F_1(x)F_1(x-1)}{D(x-1)} f_2' \right. \\ &+ \left[\frac{F_1(x)F_2(x-1)}{D(x-1)} + \frac{F_2(x)F_1(x-2)}{D(x-2)} + F_3(x) \right] f_3' \\ &+ \left. \left[\frac{F_2(x)F_2(x-2)}{D(x-2)} - \frac{F_1(x)F_3(x-1)}{D(x-1)} \right] f_4' - \frac{F_2(x)F_3(x-2)}{D(x-2)} f_5' \right\}. \quad (10) \end{aligned}$$

The “coefficients” by f_2' and f_3' are positive. By further pumping in f_5' , the terms f_6' and f_7' will appear with positive “coefficients”, while f_8' will appear with negative “coefficient” and a “free” negative term

$$- \frac{F_2(x)F_3(x-2)F(x-5)}{D(x-2)D(x-5)}$$

also appears. Every further pumping in for f_{3k+2}' contributes positive terms by f_{3k+3}' and f_{3k+4}' , a negative term by f_{3k+5}' and a negative “free” term. If we continue to pump in long enough, the argument of the negative term will be eventually “trapped” in the interval $(2, 5)$, and there $f' = 0$. So, to prove that $f'(x) > 0$ we only have to show that the “coefficient” of f_4' is positive and that “free” term (i.e. the term without any f_i') is also positive. These two facts we prove in the next lemma.

LEMMA 4. The “coefficient” of f'_4 and the “free” term, obtained by pumping in f'_5, f'_8, \dots in (10) are both positive. More precisely, with previous notations we have:

$$(a) \quad L_4(x) := \frac{F_2(x)F_2(x-2)}{D(x-2)} - \frac{F_1(x)F_3(x-1)}{D(x-1)} \geq 0,$$

for $x \geq n_0$;

$$(b) \quad L(x) := F(x) - \frac{F_1(x)F(x-1)}{D(x-1)} - \frac{F_2(x)F(x-2)}{D(x-2)} - \frac{F_2(x)F_3(x-2)}{D(x-2)} \frac{F(x-5)}{D(x-5)} \left[1 + \frac{F(x-8)}{D(x-8)} + \frac{F(x-8)}{D(x-8)} \frac{F(x-11)}{D(x-11)} + \dots \right] \geq 0,$$

for $x \geq n_0$, where n_0 can be taken in the worst case to be $n_0 = 61$.

Proof. (a) The condition $L_4(x) \geq 0$ is easily seen to be equivalent to

$$(x+1)f_1 [(2f_3 - 1)x - (5f_3 - 4)] [(2f_5 - 1)(x-2) - (5f_5 - 4)] - xf_5 [(f_2f_3 + 2f_3 - 1)x - (f_2f_3 + 5f_3 - 4)] (x-5) \geq 0.$$

If we leave out the factor $(x+1)f_1$ from the first term and the factor xf_5 from the second term, we obtain even stronger inequality (recall, we are still under inductive hypothesis, and this implies that $f_1 \geq f_5$). By grouping terms by powers of x , this stronger inequality can be written in the form

$$c_{24}(x)x^2 + c_{14}(x)x + c_{04}(x) = [c_{24}(x)x + c_{14}(x)]x + c_{04}(x) \geq 0,$$

where

$$\begin{aligned} c_{24}(x) &= 4f_3f_5 - f_2f_3 - 4f_3 - 2f_5 + 2, \\ c_{14}(x) &= 6f_2f_3 + 17f_5 + 32f_3 - 28f_3f_5 - 19, \\ c_{04}(x) &= 45f_3f_5 - 5f_2f_3 - 36f_5 - 55f_3 + 44. \end{aligned}$$

Now estimate $c_{24}(x)$, $c_{14}(x)$ and $c_{04}(x)$ using the bounds from Lemma 2. We easily obtain $c_{24}(x) \geq 3.8516$, $c_{14}(x) \geq -58.6042$, $c_{04}(x) \geq 46.6355$ for $x \geq n_0$. For example, since $f_{\min} = 2.5$, $f_{\max} = 2.67$ for $x \geq n_0$, we have then

$$c_{24}(x) \geq 4f_{\min}^2 - f_{\max}^2 - 6f_{\max} + 2 = 3.8516.$$

These bounds then imply $c_{24}(x)x + c_{14}(x) \geq 0$, and hence $[c_{24}(x)x + c_{14}(x)]x + c_{04}(x) \geq 0$, for $x \geq n_0$. So, $L_4(x) \geq 0$ for $x \geq n_0$ and the claim (a) is proved.

(b) First of all, the function $\frac{F(x)}{D(x)}$ is easily seen to be less than $\frac{129}{8(x+2)^2}$ (by using $2 \leq f_1, f_2, f_3 \leq 3$). For $x \geq 10$, it follows then that

$$\frac{F(x)}{D(x)} \leq q,$$

where $q = \frac{129}{1152}$. By using $\frac{F(x-i)}{D(x-i)} \leq q$ in the brackets of (b), we see that this sum is less than the sum of the geometric series $1 + q + q^2 + \dots = \frac{1}{1-q} < 2$. Hence $L(x) \geq 0$ will be a consequence of the stronger inequality:

$$F(x) - \frac{F_1(x)F(x-1)}{D(x-1)} - \frac{F_2(x)F(x-2)}{D(x-2)} - 2 \frac{F_2(x)F_3(x-2)}{D(x-2)} \frac{F(x-5)}{D(x-5)} \geq 0.$$

But, since we do not know which one of the quotients $\frac{F(x-1)}{D(x-1)}$, $\frac{F(x-2)}{D(x-2)}$ and $\frac{F(x-5)}{D(x-5)}$ is the largest, the last inequality will be a consequence of the three inequalities in the next Lemma.

LEMMA 5. *Keeping the same notations as above, we have*

- (a) $F(x) \geq \left[F_1(x) + F_2(x) + 2\frac{F_2(x)F_3(x-2)}{D(x-2)} \right] \frac{F(x-5)}{D(x-5)}, \quad x \geq n_0,$
- (b) $F(x) \geq \left[F_1(x) + F_2(x) + 2\frac{F_2(x)F_3(x-2)}{D(x-2)} \right] \frac{F(x-2)}{D(x-2)}, \quad x \geq n_0,$
- (c) $F(x) \geq \left[F_1(x) + F_2(x) + 2\frac{F_2(x)F_3(x-2)}{D(x-2)} \right] \frac{F(x-1)}{D(x-1)}, \quad x \geq n_0.$

Proof. We shall prove only (a) with substantial details. The other two inequalities can be proved essentially in the same manner. The inequality (a) is equivalent to

$$x(x-3)^2 f_1 f_2 f_3 f_4 f_5^2 f_6 f_7 f_8 A \geq [x f_3 f_4 f_5^2 (ax-b) + 2f_1 (cx-d)(x-6)](x+2)B,$$

where

$$\begin{aligned} A &= f_1 f_2 f_3 + f_2 f_3 + 3f_3 - 2, \\ B &= f_6 f_7 f_8 + f_7 f_8 + 3f_8 - 2, \\ a &= f_2^2 f_3 + 2f_1 f_3 + 2f_2 f_3 - f_1 - f_2, \\ b &= f_2^2 f_3 + 5f_1 f_3 + 5f_2 f_3 - 4f_1 - 4f_2, \\ c &= 2f_3 - 1, \\ d &= 5f_3 - 4. \end{aligned}$$

By inductive hypothesis it follows that $A \geq B$, and so if we prove the stronger inequality by leaving out A and B in the above inequality, we are done. But this stronger inequality turns out to be (after grouping terms by powers of x and some manipulations):

$$c_{35}(x)x^3 + c_{25}(x)x^2 + c_{15}(x)x + c_{05}(x) \geq 0,$$

or, what is the same,

$$[c_{35}(x)x + c_{25}(x)]x^2 + c_{15}(x)x + c_{05}(x) \geq 0, \tag{11}$$

where

$$\begin{aligned} c_{35}(x) &= f_1 f_2 f_3 f_4 f_5^2 f_6 f_7 f_8 - f_2^2 f_3 f_4 f_5^2 - 2f_2 f_3^2 f_4 f_5^2 - 2f_1 f_3^2 f_4 f_5^2 + f_2 f_3 f_4 f_5^2 + f_1 f_3 f_4 f_5^2 - 4f_1 f_3 + 2f_1, \\ c_{25}(x) &= -6f_1 f_2 f_3 f_4 f_5^2 f_6 f_7 f_8 - f_2^2 f_3^2 f_4 f_5^2 + f_2 f_3^2 f_4 f_5^2 + f_1 f_3^2 f_4 f_5^2 - 2f_2 f_3 f_4 f_5^2 - 2f_1 f_3 f_4 f_5^2 + 26f_1 f_3 - 1, \\ c_{15}(x) &= 9f_1 f_2 f_3 f_4 f_5^2 f_6 f_7 f_8 + 2f_2^2 f_3^2 f_4 f_5^2 + 10f_2 f_3^2 f_4 f_5^2 + 10f_1 f_3^2 f_4 f_5^2 - 8f_2 f_3 f_4 f_5^2 - 8f_1 f_3 f_4 f_5^2 + 8f_1 f_3, \\ c_{05}(x) &= 96f_1 - 120f_1 f_3. \end{aligned}$$

Now we estimate the above functions $c_{i5}(x)$ by the bounds from Lemma 2., $f_{min} = 2.5$ and $f_{max} = 2.67$ for $x \geq n_0$. We have

$$c_{35}(x) \geq f_{min}^9 - f_{max}^7 - 4f_{max}^6 + 2f_{min}^5 - 4f_{max}^2 + 2f_{min} = 1569.9574,$$

and similarly $c_{25}(x) \geq -42278.4392$, $c_{15}(x) \geq 38334.7087$ and $c_{05}(x) \geq -615.468$. This altogether then yields $[c_{35}(x)x + c_{25}(x)] \geq 0$ for $x \geq n_0$, and this in turn implies (11) for $x \geq n_0$. Thus we have proved (a).

As we said earlier, the inequalities (b) and (c) can be proved in the same way, and we omit their proofs. \square

To conclude, by lemmas 4. and 5. and induction hypothesis $f'_i \geq 0$ we have shown that $f'(x) \geq 0$ for $x \in (n, n + 1)$. By continuity of f it follows that f is increasing on $(5, n + 1)$, hence on $(5, n + 1]$ and by induction f is increasing on the whole interval $(2, \infty)$. This finally proves Theorem 4. \square

This proof of Theorem 4., although rather involved (mostly computationally), is conceptually quite simple, and can be considered as a calculus proof. Once again, our proofs of Theorems 1., 3. and 4. show the strong interference between “discrete” and “continuous” mathematics.

We note finally that the proofs of Theorems 3 and 4 we have presented here prove much stronger claims than actually stated in these theorems. Namely, they show not only that sequences (x_n) given by recursions (5) and (8) are increasing, but also that their natural continuous “patch-works” are increasing functions, too. Theorems 3 and 4 itself can be proved much simpler in such a way that we interlace the sequences (x_n) given by recursions (5) and (8) with an increasing sequence a_n , i.e. $a_n \leq x_n \leq a_{n+1}$. In the case (5), $a_n = \frac{6n}{2n+3}$ for $n \geq 3$, and in the case (8) $a_n = \frac{2n\phi^2}{2n+3}$, for $n \geq 6$, where $\phi = \frac{1+\sqrt{5}}{2}$ is the golden ratio.

This “interlacing” or “sandwiching” method can also be applied to prove the log-convexity of sequences $S^{(l)}(n)$ for $l = 2, 3$ and 4. The details are rather involved and will appear elsewhere.

We are not aware of any combinatorial proofs of the log-convexity property of the sequences $S^{(l)}(n)$.

It can be proved by geometric reasoning that the numbers $S^{(l)}(n)$ of rank l secondary structures asymptotically behave as

$$S^{(l)}(n) \sim K_l \alpha_l^n n^{-3/2},$$

where K_l and α_l are constants depending only on l , and $\alpha_l \in [2, 3]$ and $\alpha_l \searrow 2$ as $l \rightarrow \infty$. The constant α_l is the largest real solution of $x^l(x - 2)^2 = 1$. For instance, $\alpha_0 = 3$, $\alpha_1 = (3 + \sqrt{5})/2$, $\alpha_2 = 1 + \sqrt{2}$, and $\alpha_3, \alpha_4, \alpha_5$ and α_6 can be also explicitly computed (see [6]).

By taking the quotient $x_n^{(l)} = \frac{S^{(l)}(n)}{S^{(l)}(n-1)}$, we see that

$$x_n^{(l)} = \frac{S^{(l)}(n)}{S^{(l)}(n-1)} \sim \alpha_l \left(1 - \frac{1}{n}\right)^{3/2} := a_n^{(l)}.$$

Clearly, the sequence $\left(a_n^{(l)}\right)_{n \geq 1}$ increasingly tends to α_l as $n \rightarrow \infty$. This suggests that $\left(x_n^{(l)}\right)_{n \geq 1}$ should be interlaced with $\left(a_n^{(l)}\right)_{n \geq 1}$, at least asymptotically.

These and many other properties of general secondary structures will appear elsewhere [6]. More on the biological background of secondary structures the reader can find in [14] and [8].

Our “calculus method” can be applied to many other combinatorial quantities as well. For example, it can be proved in this way (see [6]) that *big Schröder numbers* r_n are log-convex. Recall that r_n is the number of lattice paths from $(0, 0)$ to (n, n) with steps $(1, 0)$, $(0, 1)$ and $(1, 1)$ that never rise above the line $y = x$.

As our final example, let us consider the sequence $P_n(t)$ of the values of Legendre polynomials in some fixed real $t \geq 1$. We start from Bonnet’s recurrence (see [13]):

$$P_n(t) = \frac{2n-1}{n}tP_{n-1}(t) - \frac{n-1}{n}P_{n-2}(t), \quad n \geq 2, \quad (12)$$

with $P_0(t) = 1$, $P_1(t) = t$. Dividing this by $P_{n-1}(t)$ and denoting the quotient $\frac{P_n(t)}{P_{n-1}(t)}$ by $x_n(t)$, we get the following recursion for $x_n(t)$:

$$x_n(t) = t \frac{2n-1}{n} - \frac{n-1}{n} \frac{1}{x_{n-1}(t)} \quad (13)$$

with initial condition $x_1(t) = t$. The log-convexity of the sequence $P_n(t)$ will follow if we show that the sequence $x_n(t)$ is increasing.

To this end we define the function $f_t(x) : [0, \infty) \rightarrow \mathbb{R}$ by

$$f_t(x) = \begin{cases} t, & \text{if } x \in [0, 1], \\ t \frac{2x-1}{x} - \frac{x-1}{x} \frac{1}{f_t(x-1)}, & \text{if } x \geq 1 \end{cases} \quad (14)$$

It is easy to show by induction on n that f_t is continuous and piecewise rational function on any interval $[1, n]$. By the same method it easily follows that f_t is bounded, i.e. $1 \leq f_t(x) \leq 2t$ for all $x \geq 1$. It is clear that $f_t(n) = x_n(t)$, for any integer $n \geq 1$.

THEOREM 5. *The sequence $P_n(t)$ of the values of Legendre polynomials is log-convex for any fixed real $t \geq 1$.*

Proof. The claim will follow if we show that $f_t(x)$ is an increasing function on $[1, \infty)$. From piecewise rationality and boundedness of f_t it follows that f_t is differentiable on every open interval $(n, n+1)$. Suppose that f_t is increasing on $[1, n]$ and take $x \in (n, n+1)$. From (14) we have

$$\begin{aligned} f_t'(x) &= t \frac{1}{x^2} - \frac{1}{x^2} \frac{1}{f_t(x-1)} + \left(1 - \frac{1}{x}\right) \frac{f_t'(x-1)}{f_t^2(x-1)} \\ &= \frac{1}{x^2 f_t(x-1)} [t f_t(x-1) - 1] + \left(1 - \frac{1}{x}\right) \frac{f_t'(x-1)}{f_t^2(x-1)} \end{aligned}$$

The second term is positive by the induction hypothesis, and the first term is positive because $t f_t(x-1) - 1 \geq f_t(x-1) - 1 \geq 0$, for all $x \geq 1$. So, the function $f_t(x)$ is increasing on the interval $(n, n+1)$, and then, by continuity, also on $[1, n+1]$. This completes the step of induction. \square

As a consequence, we get the log-convexity for the sequence of *central Delannoy numbers*. Recall that the n -th central Delannoy number counts the number of lattice paths in (x, y) coordinate plane from $(0, 0)$ to (n, n) with steps $(1, 0)$, $(0, 1)$ and $(1, 1)$. (Such paths are also known as *king's paths*.)

THEOREM 6.

(a) The sequence $D(n)$ of Delannoy numbers is log-convex.

(b) There exists $x = \lim_{n \rightarrow \infty} \frac{D(n)}{D(n-1)}$, and $x = 3 + 2\sqrt{2}$.

Proof. (a) First note that the n -th central Delannoy number is the value of the n -th Legendre polynomial at $t = 3$, $D(n) = P_n(3)$. This follows easily from the explicit expression for the generating function of the sequence $D(n)$, $D(x) = \frac{1}{\sqrt{1-6x+x^2}}$. Now apply Theorem 5.

(b) By (a) we know that $x_n(3)$ is increasing (and clearly bounded), and then by passing to limit in (13) for $t = 3$, the claim follows. \square

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