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ON SOME NEW SEQUENCES GENERALIZING THE CATALAN AND MOTZKIN NUMBERS

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Some new sequences are introduced which satisfy quadratic recurrence rules similar to those satisfied by the classical Catalan numbers and the less well-known Motzkin numbers. For each sequence the general term is expressed as a sum of products of Catalan numbers and generalized Fibonacci numbers. In addition, first-order asymptotic formulae are given for the most interesting cases.

1

The two-dimensional self-bonding of single-stranded nucleic acids (e.g. RNA) gives rise to what biologists call "secondary structure". Secondary structure largely determines the three-dimensional shape of the molecule and hence its function. Enumeration of the distinct secondary structures which can occur under various reasonable restrictions suggests a new class of recurrence rules whose solutions may be considered natural generalizations of the Catalan and Motzkin numbers. These new sequences are "elementary"; in fact, the general term can be given explicitly as a sum of products of Catalan numbers with suitably generalized Fibonacci numbers. In addition, the recurrences have the pleasant property of allowing a simple first-order analysis.

2

Let $m \geq 1$ be an integer, and consider the recurrence rule

$$S_{m+j} = S_{m+j-1} + S_{m+j-2} + \cdots + S_{j-1} + \sum_{i=0}^{m+j-2} S_i S_{m+j-2-i}, \quad j \geq 1, \tag{1}$$

with the boundary values

$$S_0 = S_1 = \cdots = S_{m-1} = 0, \qquad S_m = 1. \tag{2}$$

Since m plays the role of a parameter, it is appropriate to write $S_n(m)$ for the nth term of the sequence. In the biological application, $S_n(m)$ is the number of distinct secondary structures for a molecule of n "elements" (e.g. bases), where a

bonding loop must contain at least m internal elements. The case $m=1$ is that of greatest general interest, while $m=3$ or $m=4$ is the most realistic biologically; for an extensive discussion with examples, see [1] and [2]. As remarked in [1], an abstract model of secondary structure can be given in terms of points and lines. Let a set of n points be thought of as lying on the x-axis, and let these be labelled $1, 2, \ldots, n-1, n$ from left to right. Consider a subset of these points of cardinality $2j$, $0 \leq 2j < n$. Let these $2j$ points be completely paired by connecting them with j arcs, each point of the subset being connected to exactly one other point of the subset, with no point incident on more than one arc. The following restrictions are imposed on this pairing:

(a) no two adjacent points (i.e. with labels $i, i+1$) can be connected by an arc, and

(b) no two arcs may intersect. This is the abstract model for $m=1$; for general m, any two points connected by an arc must be separated by at least m unpaired points.

It is clear that each allowed configuration can be specified by listing the pairs (ij) of connected points. Thus for $n=6$, $m=1$, the following 17 configurations occur:

$j=0$ (no pairs)	1 configuration	
$j=1$ (1 pair)	(13), (14), (15), (16), (24), (25), (26), (35), (36), (46).	10 configurations
$j=2$ (2 pairs)	(13) (46), (15)(24), (16) (24), (16) (25), (16) (35), (26) (35).	6 configurations

On the other hand, with $m=2$ (and $n=6$) only 8 of the above configurations are allowed: the unpaired configuration, 6 of the single pairs (omit the leftmost pairing in each row), and the one double pairing (16) (25). If we take $m=3$, only 4 of these configurations survive, and so forth. Note that this enumeration distinguishes between mirror images, for example, the configurations (15) (24) and (24) (15) above. The "symmetry reduced" problem, in which mirror images are identified, has not yet been considered, owing to lack of biological interest.

So far as the above combinatorial model is concerned, the parameter value $m=0$ makes perfect sense; it merely does away with the adjacency restrictions on the pairs of points which may be connected (of course the stricture that arcs may not cross remains). Formally, the recurrence rule and the boundary conditions become

$$S_n(0) \equiv S_n = S_{n-1} + \sum_{j=0}^{n-2} S_j S_{n-2-j} \tag{3}$$

with

$$S_0 = 1. \tag{4}$$

This recurrence rule generates the sequence 1, 1, 2, 4, 9, 21, 51, 127, 323, 835, ..., which is #456 is Sloane [3]. A recent comprehensive article [4] calls these integers—with some justification—the Motzkin numbers, and gives several combinatorial settings in which the numbers occur; superficially at least, the present setting is new. As remarked in [4], the Motzkin numbers m_n are given explicitly by

$$m_n = S_n(0) = \sum_{j=0} c_{j+1}\binom{n}{2j}, \tag{5}$$

where

$$c_{j+1} = \frac{1}{j+1}\binom{2j}{j}, \tag{6}$$

the familiar Catalan numbers. We shall give our own derivation of Eq. (5) in Section 3 below.

Finally, we note that the derivation of Eq. (1) from the combinatorial model is immediate. Add a new point—on the right, say—to the previous set of n points. If the new point (with label $n+1$) is not paired with any other point, the contribution to $S_{n+1}(m)$, the new total number of configurations, is $S_n(m)$. If the new point is paired with the leftmost point $j=1$, the contribution is $S_{n-1}(m)$, and so on until it is paired with a point whose label j satisfies $m+3 \leqslant j \leqslant n-3$; then the point set is divided into two parts, on each of which nontrivial pairings can occur, giving rise to the nonvanishing quadratic terms in Eq. (1). Introducing the boundary conditions (2), we may write the recurrence in precisely the form (1). The same derivation holds for the special case $m=0$, yielding Eqs. (3) and (4).

For the convenience of the reader we give in Table 1 a short list of values of $S_n(m)$ for the range $0 \leqslant m \leqslant 6$, $m \leqslant n \leqslant 20$.

3. The explicit solution

For given $m \geqslant 1$ we write $S_n = S_n(m)$ and introduce the generating function

$$y = \sum_{n=0} S_n x^n = x^m + \sum_{j=1} S_{m+j} x^{m+j}, \tag{7}$$

the second expression following from the boundary condition (2). Then, using the recurrence rule, we may write

$$\begin{aligned} y^2 = {} & (S_{m+1} - S_m - S_{m-1} - \cdots - S_0)x^{m+1} \\ & + (S_{m+2} - S_{m+1} - S_m - \cdots - S_1)x^{m+2} \\ & + (S_{m+3} - S_{m+2} - S_{m+1} - \cdots - S_2)x^{m+3} + \cdots . \end{aligned}$$

Table 1. $S_n(m)$

n \ m	0	1	2	3	4	5	6
0	1						
1	1	1					
2	2	1	1				
3	4	2	1	1			
4	9	4	2	1	1		
5	21	8	4	2	1	1	
6	51	17	8	4	2	1	1
7	127	37	16	8	4	2	1
8	323	82	33	16	8	4	2
9	835	185	69	32	16	8	4
10	2188	423	146	65	32	16	8
11	5798	978	312	133	64	32	16
12	15511	2283	673	274	129	64	32
13	41835	5373	1463	568	261	128	64
14	113634	12735	3202	1184	530	257	128
15	310572	30372	7050	2481	1080	517	256
16	853467	72832	15605	5223	2208	1042	513
17	2356779	175502	34705	11042	4528	2104	1029
18	6536382	424748	77511	23434	9313	4256	2066
19	18199284	1032004	173779	49908	19207	8624	4152
20	50852019	2516347	390966	106633	39714	17504	8352

Rearranging, we obtain

$$\begin{aligned} y^2 = {} & (S_{m+1}x^{m-1} + S_{m+2}x^m + \cdots) \\ & -(S_m x^{m-1} + S_{m+1}x^m + \cdots) \\ & -(S_{m-1}x^{m-1} + S_m x^m + \cdots) \\ & \cdot \\ & \cdot \\ & \cdot \\ & -(S_0 x^{m-1} + S_1 x^m + \cdots) \\ = {} & \frac{1}{x^2}(y - x^m) - \frac{1}{x}y - y - xy - \cdots - x^{m-1}y. \end{aligned}$$

Defining

$$T(r) \equiv \frac{1}{1 - x - x^2 - \cdots - x^r}, \tag{8}$$

we write this functional equation in the form

$$F(x, y) = x^2y^2 - y/T(m+1) + x^m = 0. \tag{9}$$

This also holds for $m = 0$. The formal solution of Eq. (9) is

$$y = \frac{1}{2x^2T(m+1)}\left(1 - \sqrt{1 - 4x^{m+2}T^2(m+1)}\right). \tag{10}$$

Now for arbitrary p and T,

$$\begin{aligned}
&\tfrac{1}{2}(1-\sqrt{1-2^2x^pT^2})= \\
&=\frac{1}{2}\left(1-\left[1-\frac{\frac{1}{2}}{1!}2^2x^pT^2+\frac{\frac{1}{2}(-\frac{1}{2})}{2!}2^4x^{2p}T^4-\frac{\frac{1}{2}(-\frac{1}{2})(-\frac{3}{2})}{3!}2^6x^{3p}T^6+\cdots\right]\right) \\
&=\frac{1}{2}\left(\frac{\frac{1}{2}}{1!}2^2x^pT^2+\frac{\frac{1}{2}(\frac{1}{2})}{2!}2^4x^{2p}T^4+\frac{\frac{1}{2}(\frac{1}{2})(\frac{3}{2})}{3!}2^6x^{3p}T^6+\cdots\right) \\
&=x^pT^2+\sum_{j=2}^{\infty}\frac{(2j-2)!}{j!(j-1)!}x^{pj}T^{2j} \\
&=\sum_{j=1}^{\infty}c_jx^{pj}T^{2j},
\end{aligned} \tag{11}$$

with c_j the Catalan numbers (6). Eq. (10) then becomes

$$y=\sum_{j=0}^{\infty}c_{j+1}x^{(m+2)j+m}T^{2j+1}(m+1). \tag{12}$$

We now introduce the "convolved generalized Fibonacci numbers" $f_n(r,k)$ by means of the definition

$$T^k(r)=\frac{1}{(1-x-x^2-\cdots-x^r)^k}=\sum_{n=0}f_n(r,k)x^n; \tag{13}$$

note that for $r=2$, $k=1$ these are the usual Fibonacci numbers.

On comparing Eqs. (12) and (7) we see that, in terms of the $f_n(r,k)$, the solution of the recurrence (1) is

$$S_n(m)=\sum_{j=0}c_{j+1}f_q(m+1,2j+1), \qquad q\equiv n-m-mj-2j. \tag{14}$$

From the definition (13) it is clear that

$$f_n(1,k)=\binom{k+n-1}{n}, \tag{15}$$

whence

$$f_{n-2j}(1,2j+1)=\binom{n}{2j},$$

so that for $m=0$ Eq. (14) reduces to Eq. (5), the explicit expression for the Motzkin numbers given in [4].

4

The numbers $f_n(r,k)$ are not extensively tabulated. There are short tables in [3] for $r=2$, $k\leq 6$, but these contain some errors; one may also find there values of

$f_n(r, 1)$, $2 \leq r \leq 5$, for a small range of n. For $r = 1$, of course, the $f_n(r, k)$ reduce to binomial coefficients, as given in Eq. (15) above.

To get an explicit formula for $f_n(r, k)$, we start from the definition (13) and use the binomial theorem, obtaining

$$T^k(r) = \sum_{j=0} \binom{k+j-1}{j} x^j (1 + x + \cdots + x^{r-1})^j.$$

To simplify the notation, we introduce the three-index constants $C_{r,j,i}$ by means of

$$(1 + x + \cdots + x^{r-1})^j = \sum_{i=0}^{(r-1)j} C_{r,j,i} x^i, \qquad (j, r \geq 1). \tag{16}$$

It can be shown that

$$C_{r,j,i} = \sum_{s=0}^{[i/r]} (-1)^s \binom{j}{s} \binom{j+i-1-rs}{j-1}, \qquad (0 \leq i \leq (r-1)j). \tag{17}$$

Setting $i = n - j$, we have

$$f_n(r, j) = \sum_{j=0} \binom{k+j-1}{j} C_{r,j,n-j}. \tag{18}$$

This formula is useful for obtaining selected values of $f_n(r, k)$; to prepare a table, however, it is better to use the following recurrence rules.

$$\left.\begin{array}{l} f_0(r, 1) = 1 \\ f_1(r, 1) = 1 \\ f_2(r, 1) = 2 \\ \cdot \\ \cdot \\ \cdot \\ f_r(r, 1) = 2^{r-1} \\ \text{and for } j > r \\ f_j(r, 1) = f_{j-1}(r, 1) + f_{j-2}(r, 1) + \cdots + f_{j-r}(r, 1). \end{array}\right\} \quad k = 1 \tag{19}$$

$$\left.\begin{array}{l} f_0(r, k) = f_0(r, k-1) = 1 \\ f_1(r, k) = f_1(r, k-1) + f_0(r, k) \\ f_2(r, k) = f_2(r, k-1) + f_1(r, k) + f_0(r, k) \\ \cdot \\ \cdot \\ \cdot \\ f_r(r, k) = f_r(r, k-1) + f_{r-1}(r, k) + \cdots + f_0(r, k) \\ \text{and for } j > r \\ f_j(r, k) = f_j(r, k-1) + f_{j-1}(r, k) + \cdots + f_{j-r}(r, k). \end{array}\right\} \quad k > 1 \tag{20}$$

These rules follow trivially from Eq. (13) on setting $T^k(r) = T(r)T^{k-1}(r)$. In Table 2 we list values of $f_n(2, 2j+1)$ over a range just sufficient to check the values of

Table 2. $f_n(2, 2j+1)$

n	$f_n(2,1)$	$f_n(2,3)$	$f_n(2,5)$	$f_n(2,7)$	$f_n(2,9)$	$f_n(2,11)$	$f_n(2,13)$
0	1	1	1	1	1	1	1
1	1	3	5	7	9	11	13
2	2	9	20	35	54	77	
3	3	22	65	140	255	418	
4	5	51	190	490	1035	1925	
5	8	111	511	1554	3762		
6	13	235	1295	4578	12573		
7	21	474	3130	12720	39303		
8	34	942	7285	33705			
9	55	1836	16435	85855			
10	89	3522	36122	211519			
11	144	6666	77645				
12	233	12473	163730				
13	377	23109	339535				
14	610	42447					
15	987	77378					
16	1597	140109					
17	2584						
18	4181						
19	6765						

$S_n(1)$ given in Table 1, using Eq. (14). Note that the $f_n(2, k)$ that occur here are the "ordinary" convolved Fibonacci numbers studied by Riordan [5].

5. Asymptotics

We now give a first-order asympotic formula for $S_n(m)$. The only tool required is a theorem given by Bender in his review paper [6] (his Theorem 5). Bender apparently considers this theorem part of the mathematical folklore; for this reason we refer to it in the sequel as the "folklore theorem". Under certain analyticity conditions, which we omit (see [6]), this theorem asserts the following. Let $y(x)=\sum_{n=0} a_n x^n$ be the ordinary generating function of the sequence a_n which is known to have the property $a_n>0$ from some point on. Let y satisfy the functional equation $F(x, y)=0$. Finally, let $r>0, s>a_0$ be the unique real solutions of the system

$$F(r, s)=0, \qquad F_y(r, s)=0. \tag{21}$$

Then

$$a_n \sim \sqrt{\frac{rF_x(r, s)}{2\pi F_{yy}(r, s)}}\, n^{-\frac{3}{2}} r^{-n}. \tag{22}$$

In the present case the functional equation is (9), and the system (21) becomes

$$r^2s^2-(1-r-r^2-\cdots-r^{m+1})s+r^m=0,$$

$$2r^2s-(1-r-r^2-\cdots-r^{m+1})=0 \quad (r\neq 0).$$

Multiplying the second equation by s and subtracting the first equation from it, we obtain

$$s^2 = r^{m-2}, \qquad 2r^{(m+2)/2} + r + \cdots + r^{m+1} = 1. \tag{23}$$

We now consider some special cases.

(a) $m = 0$. As remarked in Section 2, these are the Motzkin numbers, given explicitly by formula (5). The solution of (23) is $r = \frac{1}{3}$, and the folklore theorem gives

$$S_n(0) \sim \sqrt{\frac{3}{4\pi}}\, n^{-\frac{3}{2}} 3^n. \tag{24}$$

At $n = 149$, formula (24) yields $S_{149}(0) \sim 9.9395 \times 10^{67}$; the correct value, to this accuracy, is 9.7792×10^{67}.

(b) $m = 1$. This is the case of greatest general interest (cf. [1, 2]). From formula (14) we obtain

$$S_n(1) = \sum_{j=0} c_{j+1} f_{n-3j-1}^{(2,2j+1)}. \tag{25}$$

To get the asymptotic formula, we first observe that the system (23) reduces to

$$s^2 = 1/r, \qquad 2r^{\frac{3}{2}} + r + r^2 = 1,$$

whence $s^4 - s^2 - 2s - 1 = 0 = (s^2 - s - 1)(s^2 + s + 1)$. The appropriate root is $s = \frac{1}{2}(1 + \sqrt{5})$, so that $1/r = \frac{1}{2}(3 + \sqrt{5})$. Further,

$$F_x(r, s) = 2rs^2 + (1 + 2r)s + 1 = 3 + s + 2rs = \frac{5 + 3\sqrt{5}}{2},$$

$$F_{yy}(r, s) = 2r^2 = 7 - 3\sqrt{5}.$$

Substitution of these values into (22) gives

$$S_n(1) \sim \sqrt{\frac{15 + 7\sqrt{5}}{8\pi}}\, n^{-\frac{3}{2}} \left(\frac{3 + \sqrt{5}}{2}\right)^n. \tag{26}$$

It seems quite laborious to derive (26) directly from (25), that is, without using the folklore theorem. At $n = 150$ this expression gives $S_n(1) \sim 2.9872 \times 10^{59}$; the correct value, to this accuracy, is 2.9397×10^{59}.

(c) $m = 2$. From Eq. (14),

$$S_n(2) = \sum_{j=0} c_{j+1} f_{n-4j-2}^{(3,2j+1)}. \tag{27}$$

The system (23) becomes

$$s = 1, \qquad r^3 + 3r^2 + r - 1 = 0 = (r + 1)(r^2 + 2r - 1),$$

so that $r=\sqrt{2}-1$, $1/r=1+\sqrt{2}$, and

$$F_x(r,s)=1+6r+3r^2=4, \qquad F_{yy}(r,s)=6-4\sqrt{2}.$$

This leads to

$$S_n(2)\sim\sqrt{\frac{1+\sqrt{2}}{\pi}}\,n^{-\frac{3}{2}}(1+\sqrt{2})^n. \tag{28}$$

Evaluating at $n=150$, $S_n(2)\sim 1.2446\times 10^{54}$; the correct value, to this accuracy is 1.2233×10^{54}.

For $m\geqslant 3$, the system (23) must be solved numerically. More, however, can be said about the behaviour of the root $r=r(m)$ as m increases. The following three theorems, which we state without proof, are due to C.J. Everett (private communication).

Theorem 1. *For finite m, $r(m)<\frac{1}{2}$.*

Theorem 2. *$r(m)$ is monotone increasing with m.*

Theorem 3. *$r(m)\to\frac{1}{2}$ from below as $m\to\infty$.*

The behavior implied by these theorems is illustrated in Table 3.

Table 3

m	$r(m)$	m	$r(m)$
0	0.333333333	13	0.497345948
1	0.381966011	14	0.498105305
2	0.414213562	15	0.498650302
3	0.436911127	16	0.499040180
4	0.453397652	17	0.499318358
5	0.465571232	18	0.499516421
6	0.474626618	19	0.499657210
7	0.481373188	20	0.499757161
8	0.486389036	21	0.499828048
9	0.490102038	22	0.499878286
10	0.492835560	23	0.499913869
11	0.494836199	24	0.499939061
12	0.496292071	25	0.499956892

6. Generalizations

The Catalan numbers themselves satisfy the recurrence rule

$$S_n=\sum_{j=0}^{n-1} S_jS_{n-1-j}, \qquad S_0=1; \tag{29}$$

explicitly,

$$S_n = c_{n+1} = \frac{1}{n+1}\binom{2n}{n}. \tag{30}$$

The enumerative interpretations of c_n (bracketing, trees, etc.) are too well known to require restatement here. With $y = \sum_{j=0} S_j x^j$, the functional equation resulting from (29) is $xy^2 - y + 1 = 0$, so that

$$y = \frac{1}{2x}(1 - \sqrt{1-4x}),$$

and formula (30) follows on expanding the radical (cf eq. (11)). The folklore theorem gives

$$S_n \sim \frac{1}{\sqrt{\pi}} n^{-\frac{3}{2}} 4^n,$$

and this agrees with the result of applying Stirling's approximation to (30).

The sequences (14) considered in this paper can clearly be thought of as generalizations of the Catalan numbers despite the fact that there is no value of the parameter m for which the recurrence rule (1) takes the form (29). These "generalized Catalan numbers" preserve the "elementary" character of the original c_n. Other, quite natural, generalizations need not have this property, for example

$$S_{n+1}(b) = (n+b)\sum_{j=1}^{n} S_j(b) S_{n+1-j}(b), \qquad S_1(b) = 1 \quad (b \geq 0).$$

(See [7] for a discussion of these nonelementary sequences).

Further elementary generalizations of c_n are obtained by introducing a second parameter t into the recurrence (1):

$$S_{m+j}^{(m,t)} \equiv S_{m+j} = S_{m+j-1} + \cdots + S_{j-1} + \sum_{i=0}^{t+j-1} S_i S_{t+j-1-i}, \quad 0 \leq t \leq m, \tag{31}$$

with the same boundary conditions (2). The sequences $S_n(m)$ studied above correspond to taking $t = m-1$. Proceeding as in Section 3, we find the functional equation

$$F(x, y) = x^{m+1-t} y^2 - \frac{1}{T(m+1)} y + x^m = 0. \tag{32}$$

It is evident from both (31) and (32) that this generalization includes all the cases studied earlier except the Motzkin numbers and, of course, the Catalan numbers themselves.

Solving Eq. (32) we obtain

$$y = \frac{1}{x^{p-m}T} \cdot \tfrac{1}{2}(1 - \sqrt{1 - 4x^p T^2}), \qquad T = T(m+1), \qquad p = 2m+1-t. \tag{33}$$

Eq. (11) gives the general solution

$$S_n(m,t)=\sum_{j=0} c_{j+1}f_q(m+1,2j+1), \qquad q=n-m-(2m+1-t)j, \quad n\geqslant m. \tag{34}$$

The parameters r, s of the folklore theorem are determined by

$$s^2=r^{t-1}, \qquad 2r^{m+1-t}s-(1-r-\cdots-r^{m+1})=0. \tag{35}$$

Examples. (a) $m=0, t=0$. The recurrence rule is

$$S_j=S_{j-1}+\sum_{i=0}^{j-1} S_iS_{j-1-i}, \qquad S_0=1, \tag{36}$$

and the functional equation is

$$xy^2-\frac{y}{T(1)}+1=0.$$

From (34) we get the explicit solution

$$S_n(0,0)=\sum_{j=0} c_{j+1}\binom{n+j}{2j}. \tag{37}$$

This sequence 1, 2, 6, 22, 90, 394, ... is probably new; at least it cannot be found in [3] or its supplement. The appropriate solutions of the system (35) for this case are $s=1+\sqrt{2}$, $1/r=s^2=3+2\sqrt{2}$, and these lead to

$$S_n(0,0)\sim\sqrt{\frac{4+3\sqrt{2}}{4\pi}}\,n^{-\frac{3}{2}}(3+2\sqrt{2})^n. \tag{38}$$

(b) $m=2, t=0$ (N.B. $m=1, t=0$ is $S_n(1)$, previously studied). The recurrence is

$$\begin{aligned} &S_{n+2}(2,0)\equiv S_{n+2}=S_{n+1}+S_n+S_{n-1}+\sum_{i=0}^{n-1} S_iS_{n-1-i},\\ &S_0=S_1=0, \qquad S_2=1. \end{aligned} \tag{39}$$

From (32) and (34) we have

$$F(x,y)=x^3y^2-\frac{y}{T(3)}+x^2=0, \tag{40}$$

$$S_n(2,0)=\sum_{j=0} c_{j+1}f_{n-5j-2}^{(3,2j+1)}. \tag{41}$$

After simplification, the system determining the folklore theorem parameters reduces to

$$r=1/s^2, \qquad s^5-s^4-s-1=0. \tag{42}$$

Numerical solution yields $s = 1.49709405$, so that $1/r = 2.2412906$; this is, of course, the limit of the ratio S_{n+1}/S_n for this case.

We do not take space for further examples. It is worth remarking, however, that the sequences (34) appear to be new (i.e. not in [3]). Unfortunately, we do not at present have a combinatorial interpretation for any of these numbers, with the exception of the subset given by Eq. (14).

Acknowledgement

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