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ON SOME NEW SEQUENCES GENERALIZIN 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.

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.

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

$$S_{m+j} = S_{m+j-1} + S_{m+j-2} + \dots + S_{j-1} + \sum_{i=0}^{m+j-2} S_i S_{m+j-2-i}, \quad j \ge 1,$$
 (1)

with the boundary values

$$S_0 = S_1 = \dots = S_{m-1} = 0, \qquad S_m = 1.$$
 (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

are imposed on this pairing: with j arcs, each point of the subset being connected to exactly one other point of 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 the subset, with no point incident on more than one arc. The following restrictions ity 2j. $0 \le 2j \le n$. Let these 2j points be completely paired by connecting them $1, 2, \ldots, n-1$, n from left to right. Consider a subset of these points of cardinalfor an extensive discussion with examples, see [1] and [2]. As remarked in [1], an greatest general interest, while m = 3 or m = 4 is the most realistic biologically. bonding loop must contain at least m internal elements. The case m = 1 is that of

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

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

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

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

allowed: the unpaired configuration, 6 of the single pairs (omit the leftmost distinguishes between mirror images, for example, the configurations (15) (24) and identified, has not yet been considered, owing to lack of biological interest. (26) (35) above. The "symmetry reduced" problem, in which mirror images are 4 of these configurations survive, and so forth. Note that this enumeration pairing in each row), and the one double pairing (16) (25). If we take m = 3, only On the other hand, with m = 2 (and n = 6) only 8 of the above configurations are

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

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

W11.

$$S_0 = 1.$$

(4)

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

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

where

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

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

 $S_n(m)$ for the range $0 \le m \le 6$, $m \le n \le 20$. The same derivation holds for the special case m = 0, yielding Eqs. (3) and (4). boundary conditions (2), we may write the recurrence in precisely the form (1). giving rise to the nonvanishing quadratic terms in Eq. (1). Introducing the point set is divided into two parts, on each of which nontrivial pairings can occur. until it is paired with a point whose label j satisfies $m+3 \le j \le n-3$; then the point is paired with the leftmost point j = 1, the contribution is $S_{n-1}(m)$, and so on tion to $S_{n+1}(m)$, the new total number of configurations, is $S_n(m)$. If the new the new point (with label n+1) is not paired with any other point, the contribuimmediate. Add a new point—on the right, say—to the previous set of n points. If For the convenience of the reader we give in Table 1 a short list of values of Finally, we note that the derivation of Eq. (1) from the combinatorial model is

The explicit solution

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

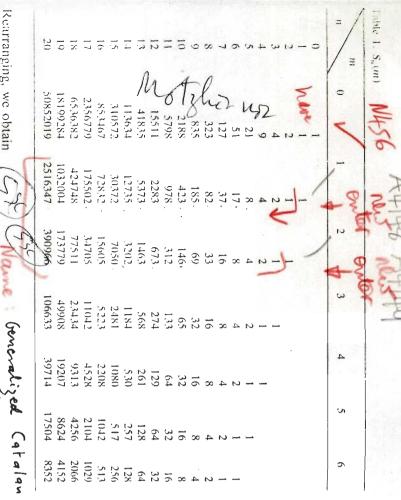
$$y = \sum_{n=0}^{\infty} S_n x^n = x^m + \sum_{j=1}^{\infty} S_{m+j} x^{m+j}, \tag{7}$$

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

$$y^{2} = (S_{m+1} - S_{m} - S_{m-1} - \dots - S_{0})x^{m-1}$$

$$+ (S_{m+2} - S_{m+1} - S_{m} - \dots - S_{1})x^{m}$$

$$+ (S_{m+3} - S_{m+2} - S_{m+1} - \dots - S_{2})x^{m-1} + \dots$$



Rearranging, we obtain

$$y^{2} = (S_{m+1}x^{m-1} + S_{m+2}x^{m} + \cdots)$$
$$-(S_{m}x^{m-1} + S_{m+1}x^{m} + \cdots)$$
$$-(S_{m-1}x^{m-1} + S_{m}x^{m} + \cdots)$$

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$$-(S_0 x^{m-1} + S_1 x^m + \cdots)$$

$$= \frac{1}{x^2} (y - x^m) - \frac{1}{x} y - y - xy - \cdots - x^{m-1} y.$$

Defining

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

we write this functional equation in the form

$$F(x, y) = x^2y^2 - y/T(m+1) + x^m = 0.$$

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

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

Now for arbitrary p and T,

$$\frac{1}{2}(1 - \sqrt{1 - 2^{2}x^{p}T^{2}}) = \frac{1}{2}\left(1 - \left[1 - \frac{1}{2} 2^{2}x^{p}T^{2} + \frac{1}{2}(-\frac{1}{2}) 2^{4}x^{2p}T^{4} - \frac{1}{2}(-\frac{1}{2})(-\frac{3}{2}) 2^{6}x^{3p}T^{6} + \cdots\right]\right) \\
= \frac{1}{2}\left(\frac{1}{2} 2^{2}x^{p}T^{2} + \frac{1}{2}(\frac{1}{2})}{2!} 2^{4}x^{2p}T^{4} + \frac{1}{2}(\frac{1}{2})(\frac{3}{2})}{3!} 2^{6}x^{3p}T^{6} + \cdots\right) \\
= x^{p}T^{2} + \sum_{i=2}^{\infty} \frac{(2j-2)!}{j!(j-1)!} x^{pi}T^{2i} \\
= \sum_{i=1}^{\infty} c_{i}x^{pi}T^{2i}, \tag{11}$$

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

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

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

$$T^{k}(r) = \frac{1}{(1 - x - x^{2} - \dots - x^{r})^{k}} = \sum_{n \ge 0} f_{n}(r, k) x^{n};$$
 (13)

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

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

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

From the definition (13) it is clear that

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

whence

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

<u>S</u>

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

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

(10)

(r, 1), $2 \le r \le 5$, for a small range of n. For r = 1, of course, the $\int_{n} (r, k)$ reduce to

monial coefficients, as given in Eq. (15) above. Fo get an explicit formula for $f_n(r, k)$, we start from the definition (13) and use no binomial theorem, obtaining

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

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

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

t can be shown that

$$C_{r,i,i} = \sum_{s=0}^{\lfloor i/r \rfloor} (-1)^s \binom{j}{s} \binom{j+i-1-rs}{j-1}, \qquad (0 \le i \le (r-1)j).$$
 (17)

etting i = n - j, we have

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

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

$$f_{0}(r, 1) = 1$$

$$f_{1}(r, 1) = 1$$

$$f_{2}(r, 1) = 2$$

$$f_{2}(r, 1) = 2^{r-1}$$

$$f_{1}(r, 1) = f_{1-1}(r, 1) + f_{1-2}(r, 1) + \dots + f_{1-r}(r, 1).$$

$$f_{0}(r, k) = f_{0}(r, k - 1) = 1$$

$$f_{1}(r, k) = f_{1}(r, k - 1) + f_{0}(r, k)$$

$$f_{2}(r, k) = f_{2}(r, k - 1) + f_{1}(r, k) + \dots + f_{0}(r, k)$$

$$f_{1}(r, k) = f_{1}(r, k - 1) + f_{r-1}(r, k) + \dots + f_{0}(r, k)$$
and for $j > r$

$$f_{1}(r, k) = f_{1}(r, k - 1) + f_{1-1}(r, k) + \dots + f_{1-r}(r, k).$$

$$(20)$$

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

Table 2. $f_n(2,2j+1)$ 2584 1597 610 987 377 144 $f_{\rm m}(2,1)$ 55 89 21 $f_n(2,3)$ 140109 42447 77378 23109 12473 3522 6666 1836 474 942 233 A1873, Please enter 339535 11 N1600 163730 $\frac{1}{n}(2,5)$ 77645 36122 16435 7285 3130 1295 511 190 f, (2, 7) 211519 85855 33705 12720 N1865 4578 1554 490 0110 3 Ref: RC1 101. DM 26 267 78. Name: unchanged $f_{n}(2,9)$ 12573 N1600 - corrected & extended 3762 255 1035 N1865 $f_n(2, 11)$ $f_n(2, 13)$

 $S_n(1)$ 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 $y(x) = \sum_{n=0}^{\infty} a_n x^n$ 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

$$F(r, s) = 0,$$
 $F_{\nu}(r, s) = 0.$ (21)

Then

$$a_{\rm n} \sim \sqrt{\frac{rF_{\rm x}(r,s)}{2\pi F_{\rm vy}(r,s)}} \, n^{-\frac{3}{2}r^{-n}}.$$
 (22)

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

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

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

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

$$s^2 = r^{m-2}, \quad 2r^{(m+2)/2} + r + \dots + r^{m+1} = 1.$$
 (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

$$S_n(0) \sim \sqrt{\frac{3}{4\pi}} \, n^{-\frac{1}{2}} 3^n.$$
 (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

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

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

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

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,

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

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

Substitution of these values into (22) gives

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

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

The system (23) becomes

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

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

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

This leads to

$$S_n(2) \sim \sqrt{\frac{1+\sqrt{2}}{\pi}} n^{-\frac{1}{2}} (1+\sqrt{2})^n.$$
 (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 $m \ge 3$, 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. $r(m) \rightarrow \frac{1}{2}$ from below as $m \rightarrow \infty$.

The behavior implied by these theorems is illustrated in Table 3

Table 3

3	r(m)	m	r(m)
0	0.333333333	13	0.497345948
_	0.381966011	14	0.498105305
2	0.414213562	15	0.498650302
w	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
00	0.486389036	21	0.499828048
9	0.490102038	22	0.499878286
0	0.492835560	23	0.499913869
<u></u>	0.494836199	24	0.499939061
2	0.496292071	25	0.499956892

6. Generalizations

The Catalan numbers themselves satisfy the recurrence rule

$$S_n = \sum_{j=0}^{n-1} S_j S_{n-1-j}, \quad S_0 = 1;$$

(29)

explicitly

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Solving Eq. (32) we obtain

$$y = \frac{1}{x^r} \left(-\frac{1}{2}(1 - \sqrt{1 - 4x^pT^2}), \quad T = T(m+1), \quad p = 2m+1-t.$$
 (33)

Eq. (11) gives the general solution

$$S_{n}(m,t) = \sum_{j=0}^{\infty} c_{j+1} f_{q}(m+1,2j+1), \qquad q = n - m - (2m+1-t)j, \quad n \geqslant m.$$
(34)

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

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

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

$$S_{j} = S_{j-1} + \sum_{i=0}^{j-1} S_{i}S_{j-1-i}, \qquad S_{0} = 1,$$
 (36)

and the functional equation is

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

From (34) we get the explicit solution

4) we get the explicit solution
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$$S_{n}(0,0) = \sum_{j=0}^{n} c_{j+1} \binom{n+j}{2j}. \qquad \left(\text{twice } (003) \right)$$
(3)

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 This sequence 1, 2, 6, 22, 90, 394, . . . is probably new; at least it cannot be found

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

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

$$S_{n+2}(2,0) \equiv S_{n+2} = S_{n+1} + S_n + S_{n-1} + \sum_{i=0}^{n-1} S_i S_{n-1-i},$$
(39)

From (32) and (34) we have

 $S_0 = S_1 = 0, S_2 = 1.$

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

$$S_n(2,0) = \sum_{i=0}^{\infty} c_{i+1} f_n^{1,2i+1}_{Si-2}.$$
 (41)

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

$$r = 1/s^2$$
, $s^5 - s^4 - s - 1 = 0$. (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

In conclusion, we want to thank our colleagues Jo Ann Howell and Myron Stein for several indispensible calculations. We also want to acknowledge the contributions of C.J. Everett; in addition to furnishing the Theorems of Section 5 and several identities (e.g. Eqs (11) and (17)), he provided detailed help whenever it was needed.

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