### PREDICTING THE NUMBER OF HEXAGONAL SYSTEMS WITH 24 AND 25 HEXAGONS

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#### Abstract

We predict the number of hexagonal systems consisting of 24 and 25 hexagons to be  $H_{24} = 122237774262384$  and  $H_{25} = 606259305418149$ , with 6 and 5 significant digits, respectively. Further estimates for  $H_n$  up to n = 31 are also given.

#### Hexagonal Systems

Informally speaking, a *hexagonal system* can be viewed as a connected arrangement of hexagonal cells packed in the same way as the typical honeycomb arrangement in a beehive. More formally, it is a finite connected plane graph with no cut-vertices, in which all interior regions are mutually congruent regular hexagons [1]. Hexagonal systems have from time to time attracted the attention of mathematicians (and were named "hexagonal animals", "honeycomb systems", "polyhexes", etc.), in connection with statistical physics and applications to lattice gas models [2, 3, 4]. But the main interest in them comes from chemistry: hexagonal systems are the natural graph representations of benzenoid hydrocarbons, whence the names "benzenoid graphs", "benzenoid systems", and "fusenes" used in the chemical literature. An enormous literature exists on various chemical applications of hexagonal systems. We refer to [5, 6] for details and references.

One of the classical problems in the theory of hexagonal systems is their enumeration. In what follows, the number of non-isomorphic hexagonal systems consisting of n hexagons is denoted by  $H_n$ , where "non-isomorphic" means viewed up to translations, rotations, and symmetries. This in turn is equal to the number of n-cyclic benzenoid hydrocarbons. The first few values of  $H_n$  are given in Table 1.

The enumeration of hexagonal systems according to area stands as one of the most challenging unsolved problems of combinatorial theory (cf. Section 10.8.5 in [7]). In spite of numerous attempts, no one was successful in applying Pólya's theory [7, 8, 9] or any other technique of combinatorics to find  $H_n$  or, at least, in establishing the asymptotic behavior

| n              | 1       | 2        | 3        | 4         | 5          | 6      |
|----------------|---------|----------|----------|-----------|------------|--------|
| $H_n$          | 1       | 1        | 3        | 7         | 22         | 81     |
| $\overline{n}$ | 7       | 8        | 9        | 10        | 11         | 12     |
| $H_n$          | 331     | 1435     | 6505     | 30086     | 141229     | 669584 |
| $\overline{n}$ | 13      | 14       | 15       | 16        | 17         |        |
| $H_n$          | 3198256 | 15367577 | 74207910 | 359863778 | 1751594643 |        |

Table 1: Numbers  $H_n$  of hexagonal systems with n hexagons  $(1 \le n \le 17)$ 

of  $H_n$  as n goes to infinity. Consequently, the only way to evaluate  $H_n$  is to use a (more or less) brute-force computer-assisted constructive enumeration; details of these methods are outlined in the book [10], in the reviews [11, 12], and elsewhere [13, 14, 15, 16, 17, 18]. Recently, some very efficient algorithms for the construction and counting of hexagonal systems were designed [17, 18], but even with them the calculation of  $H_n$  is extremely time- and memory-consuming. For instance, in order to obtain  $H_{22}$ , more than 300 days of CPU time were needed; the analogous calculation of  $H_{23}$  required 2.4 years of CPU time [18].

The values of  $H_n$  for n between 13 and 16 were first reported in 1990 by Knop *et al.* ( $H_{13}$  and  $H_{14}$  in [13],  $H_{15}$  and  $H_{16}$  in [14]). Three years later Tošić *et al.* arrived at  $H_{17}$  [15, 16]. With this the limit of the performance of the currently available computers had been reached, and further progress had to wait until a completely new algorithm was developed by Caporossi and Hansen [17] and further enhanced by Brinkmann [18]. This enabled the determination of  $H_{18}$  to  $H_{21}$  [17] as well as  $H_{22}$  and  $H_{23}$  [18]. It seems to be unlikely that the application of the same technique will be feasible in the case of  $n \geq 24$ .

It is a natural idea to somehow use the information contained in the sequence  $H_1$ ,  $H_2, \ldots, H_n$  to predict, at least approximately, the value of  $H_{n+1}$ . Early attempts in this direction [19, 20] were based on the assumption (without any theoretical justification, but in analogy with other results in graph enumeration) that for n being large enough,  $H_n$  can be approximated by some simple elementary function of n. This function was designed so as to depend on a few (usually two) adjustable parameters, the values of which were then determined from  $H_1, H_2, \ldots, H_n$ . The resulting values of  $H_{n+1}$  were eventually shown [13] to be quite accurate, but—of course—far from being exact. The same analysis was later applied to sequences of isomer counts of other homologous series of interest in chemistry [21, 22].

In this paper we report the results of an analogous approach, which, however, is much less arbitrary. Indeed, the class of sequences in which the approximation is searched for is much larger than those classes used so far, and allows for as many parameters as needed. The method is reminiscent of the methods of differential approximants [23] and algebraic approximants [24] used in statistical mechanics, and possesses the sound theoretical and algorithmic foundation of *holonomic functions*. This is the topic of the end of the introduction, which to a certain extend is independent from the rest of the text.

### Holonomic Guessing

Being faced with the first five entries 0, 1, 3, 6, and 10 of an infinite sequence of numbers, an obvious guess for the sixth one would be 15. One could even propose the formula n(n+1)/2

for the *n*th entry, but this refined guess cannot be proved unless further information is provided. For instance, such a proof would become an easy task if we knew in addition that we are dealing with the sums of the first n nonnegative integers.

Over the years various computer algebra tools have been developed in order to assist this process of guessing and proving. As far as guessing is concerned, this is reflected by the success of Sloane's classical book [25] and its enlarged revision [26]. Each book is basically a table of sequences of integers, collected from all branches of mathematics and sciences. The sequences are arranged in numerical order, and come each with a brief description and references. The mere existence of these "dictionaries" has allowed for a new process of research: after generating the first numbers of a sequence of combinatorial interest, one identifies them with the aid of the tables. The work by Sloane and Plouffe has recently found an electronic and algorithmic supplement [27]: the tables are now electronically available for human search; additionally the on-line system now has a facility where it will algorithmically try to guess a formula or to relate the input sequence to a tabulated one. In particular, the counting sequence of hexagonal systems is now to be found there (known as sequences number A000228, A018190, and A038148). With regard to proving, we only mention Zeilberger's "holonomic systems approach to special function identities" [28] and the developments described in [29].

In this article, the aspect of computer-assisted *holonomic guessing* plays the central role. The first systematic presentation of the underlying theory of univariate holonomic functions has been given by Stanley [30]. The first implementation of these ideas was realized in the form of the Maple package GFUN by Salvy and Zimmermann [31]; it is now used as part of [27]. Another package named GENERATINGFUNCTIONS provides Mathematica users with the same functionality [32].

A detailed description of holonomic theory (e.g., closure properties of holonomic functions, etc.) would go far beyond the scope of this note. Therefore we restrict to introduce only those notions that are relevant to the understanding of the method to be used for predicting the values  $H_{24}$  and  $H_{25}$ .

For many counting sequences  $(a_n)$ , the ordinary generating function and its exponential counterpart,

$$\sum_{n=0}^{\infty} a_n x^n \quad \text{and} \quad \sum_{n=0}^{\infty} \frac{a_n x^n}{n!},$$

respectively, are *holonomic*, which means that such a function or series satisfies a linear differential equation with polynomial coefficients. Examples of holonomic functions include many familiar power series such as algebraic functions (functions that are solution of a polynomial equation), the exponential function  $e^x$ , logarithmic function  $\log(1 + x)$ , and trigonometric functions like  $\sin x$ . For example, if  $b_n$  denotes the number of binary planar trees with n + 1 leaves (with the convention  $b_0 = 1$ ), then the ordinary generating function of the sequence  $(b_n)$  is holonomic since

$$\sum_{n=0}^{\infty} b_n x^n = \frac{1 - \sqrt{1 - 4x}}{2x}$$

is algebraic.

It is not difficult to prove that the series  $\sum_{n=0}^{\infty} a_n x^n$  is holonomic if and only if the sequence  $(a_n)$  satisfies a linear recurrence with polynomial coefficients, i.e.,

$$p_0(n)a_n + p_1(n)a_{n+1} + \dots + p_d(n)a_{n+d} = 0,$$

where the  $p_i$ 's are polynomials in the indeterminate n. This serves as a motivation to call the sequence  $(a_n)$  holonomic in this case. Algorithmically it is easy to convert each representation—differential equation and recurrence—into the other. Furthermore, both representations serve as the basis for computer-assisted guessing. For example, let us assume that we came up with the first six binary tree numbers  $(b_0, b_1, b_2, b_3, b_4, b_5) = (1, 1, 2, 5, 14, 42)$ . Then we could use GFUN (or GENERATINGFUNCTIONS) to automatically guess the recurrence

$$(n+2)b_{n+1} - 2(2n+1)b_n = 0.$$

The procedure to produce this guess is essentially based on a simple coefficient comparison method (namely differential Padé-Hermite approximants) for which one has to bound in advance the order of the recurrence and the degree of the polynomial coefficients involved: the product "order times degree" is essentially the number of undetermined coefficients used by the method.

As mentioned above, additional information is needed in order to prove such a guess. For instance, if one knows in advance that the generating function is algebraic, which implies the existence of a holonomic recurrence, then one only needs to know an upper bound for its order. Or, if the holonomic nature is not known in advance, one might observe the convolution recurrence

$$b_n = \sum_{k=0}^{n-1} b_k b_{n-k-1}.$$

In this case transforming the conjectured recurrence of order 1 into the closed form

$$b_n = \frac{1}{n+1} \binom{2n}{n}$$

and substituting it into the convolution formula leads to the verification of a binomial identity. This could again be left to the computer by appying a symbolic summation procedure from [29]. (The numbers  $b_n$  above are the well-known Catalan numbers, often denoted by  $C_n$ .)

Concerning the problem of enumerating hexagonal systems, we do not know up to now whether the corresponding generating function of  $(H_n)$  is holonomic or not. Therefore we would need additional information to actually prove the accuracy of our guess, which can only be considered as a "holonomic approximation". The information we use for our holonomic guessing solely consists in the values of  $H_n$  that have been computed so far. In order to provide further evidence, we present a detailed analysis of the stability of the prediction scheme.

Holonomic guessing could also be considered as a kind of computer-assisted "heuristic reasoning", meant in the spirit of Pólya. According to his dictionary of heuristics [33]: "We are often obliged to use heuristic reasoning. We shall attain complete certainty when we shall have obtained the complete solution, but before obtaining certainty we must often be satisfied with a more or less plausible guess."

In the present article we use the Maple package GFUN. Analogous procedures are available to Mathematica users [32] and could have been used as well.

# 1 Warming Up: Predicting the Number of Hexagonal Systems with n Hexagons for n between 18 and 23

When Tošić *et al.* gave the value 1751594643 for  $H_{17}$  [15, 16], only the values of  $H_1$ ,  $H_2$ , ...,  $H_{16}$  were known. All those results are summarized in Table 1. Using these initial 17 numbers as exclusive information about the sequence  $(H_n)$ , we proceed to guess a linear recurrence satisfied by a holonomic approximation of the sequence. By means of it we then predict further numbers  $H_n$  of hexagonal systems when  $18 \le n \le 23$ , before comparing them with the actual values already known at present.

### **Prediction Scheme**

We use the following prediction scheme:

Step 1. Load the package (as part of the standard distribution of Maple V Release 5), enter the list of numbers known after Tošić *et al.*, and set up a few package parameters.

Specifically, we require the package to consider equations of order 1 or 2 with polynomial coefficients of degree between 0 and 10.

Step 2. Guess a recurrence satisfied by the sequence which starts with the values above:

rec17:=listtorec(L,u(n));

which outputs:

$$\texttt{rec17} := [\{p_0(n)u(n) + p_1(n)u(n+1) + p_2(n)u(n+2), u(0) = 1, u(1) = 1\}, \texttt{ogf}]$$

where each  $p_i$  above is a polynomial of degree 5 in n with integer coefficients of 52 digits. The explicit values are available in Appendix A.

Step 3. Convert this recurrence into a procedure which computes the nth term of the sequence:

pr17:=rectoproc(op(1,rec17),u(n));

Remarkably, the output procedure **pr17**, which is too large to be displayed here, has been *automatically generated* by GFUN. Additionally, GFUN *automatically optimized* it, in the sense of minimizing the number of arithmetical operations used in the procedure.

| n                  | 18                                   | 19                                   | 20                                     |
|--------------------|--------------------------------------|--------------------------------------|--|
| $H'_n$             | 8553612149                           | 41892180909                          | 205710300568                           |
| $H_n$              | 8553649747                           | 41892642772                          | 205714411986                           |
| $-\delta_n$        | $4.4 \cdot 10^{-6}$                  | $1.1\cdot 10^{-5}$                   | $2.0\cdot10^{-5}$                      |
|                    |                                      |                                      |  |
| n                  | 21                                   | 22                                   | 23                                     |
| $n \\ H'_n$        | $21 \\ 1012535580260$                | $\frac{22}{4994621421396}$           | 23<br>24686078283303                   |
| $n \\ H'_n \\ H_n$ | 21<br>1012535580260<br>1012565172403 | 22<br>4994621421396<br>4994807695197 | 23<br>24686078283303<br>24687124900540 |

Table 2: Predicted numbers  $H'_n$  of hexagonal systems with n hexagons, actual numbers  $H_n$ , and corresponding relative errors  $-\delta_n = -(H'_n - H_n)/H_n$  of prediction  $(18 \le n \le 23)$ 

Step 4. Compute predicted values for hexagonal systems with 18 to 23 hexagons. The predicted values  $H'_n$  are in fact rational numbers rounded to the nearest integer. Rather than displaying the Maple output, as obtained by the command

seq(i=trunc(pr17(i-1)+1/2),i=18..23);

we give the predicted results in Table 2.

#### **Comparison to Recent Results**

The numbers obtained in Step 4 of the previous scheme match with good accuracy those obtained by Caporossi and Hansen [17], and by Brinkmann, Caporossi and Hansen [18]. Indeed, the heavy computations described in [18, 17] proved the numbers  $H_n$  of hexagonal systems to be those given in Table 2. The table also gives the corresponding relative error

$$\delta_n = \frac{H'_n - H_n}{H_n}$$

of the predicted values  $H'_n$ .

In order to perform the calculations of rec17, pr17, and the estimates, not more than 3 seconds of CPU time were needed.

Note that other parameter settings could have been used in Step 1 above. Let us repeat that the number of undetermined coefficients used by the method is essentially the product "order times degree". The algorithm tries to detect equations with a small number of non-zero coefficients in the search space described by the parameters. The other setting

```
gfun['minordereqn']:=0: gfun['maxordereqn']:=20:
gfun['mindegcoeff']:=0: gfun['maxdegcoeff']:=2:
```

yields another equation with low polynomial degree but high order (specifically: order 8 instead of 2, degree 1 instead of 5, 25-digit instead of 52-digit integers). The latter recurrence results in different predicted numbers, which however approximate the actual ones with essentially the same good accuracy. This is why we will not discuss the choice of parameter settings any further.

| n                       | 4             | 5      | 6              | 7  | 8              | 9              | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
|-------------------------|---------------|--------|----------------|--|----------------|----------------|----|----|----|----|----|----|----|----|
| order                   | 2             | 2      | 2              | 2  | 2              | 2              | 2  | 2  | 1  | 2  | 2  | 1  | 2  | 2  |
| degree                  | 1             | 1      | 2              | 2  | 2              | 3              | 3  | 3  | 5  | 4  | 4  | 7  | 5  | 5  |
| $\operatorname{digits}$ | 1             | 1      | 3              | 4  | 5              | 9              | 13 | 17 | 26 | 28 | 33 | 47 | 48 | 52 |
| n                       | 18            | 19     | 20             | 21   | 22             | <u> </u>       |    |    |    |    |    |    |    |    |
|                         |               | 10     | 20             | <i>4</i> 1                                 |                | 20             |    |    |    |    |    |    |    |    |
| order                   | 1             | 2      | $\frac{20}{2}$ | $\frac{21}{1}$                             | $\frac{22}{2}$ | $\frac{23}{2}$ |    |    |    |    |    |    |    |    |
| order<br>degree         | $\frac{1}{8}$ | 2<br>6 | $\frac{20}{2}$ | $\begin{array}{c} 21\\ 1\\ 10 \end{array}$ | $\frac{22}{2}$ | $\frac{23}{2}$ |    |    |    |    |    |    |    |    |

Table 3: Parameters for the recurrence obtained by the scheme at nth stage  $(4 \le n \le 23)$ 

# 2 Predicting the Number of Hexagonal Systems with 24 or More Hexagons

In the previous section, we started from a list of known values for the  $H_n$  (up to n = 17), and derived a *single* recurrence to predict *several* further values (up to n = 23). In this section, we follow a more incremental strategy: from a list of known or already predicted values for  $H_1, \ldots, H_n$ , we derive a recurrence to predict a *single* further value for  $H_{n+1}$ . Adjoining it to the initial list, we then iterate the process  $\ell$  times, ending with *several* recurrences, one for each value predicted for  $H_{n+1}, \ldots, H_{n+\ell}$ .

Prior to this, we provide good numerical evidence for the stability of our incremental prediction scheme, which makes it possible to obtain values for  $H_{24}$  and  $H_{25}$  of credibly good accuracy.

### Stability of the Prediction Scheme

Using all known values  $H_1, \ldots, H_n$  for a number  $n \leq 23$ , one can predict the numbers  $H_{n+p}$  for  $p \geq 1$  following the same scheme as previously outlined for n = 17. This is readily implemented in Maple:

Setting the order and degree parameters as indicated in the Maple code above, the recurrences obtained are of small order (1 or 2), but involve polynomials in n of degree linear in n (typically,  $\lfloor n/3 \rfloor$ ) and integers of (experimentally)  $O(n \ln n)$  digits. This is summarized in Table 3. Denote by  $H_n^{(p)}$  the value for  $H_{n+p}$  predicted p steps ahead by the

| n              | 10                   | 11                 | 12                   | 13                   | 14                   | 15                 |
|----------------|----------------------|--------------------|----------------------|----------------------|----------------------|--------------------|
| p = 1          | $9.9\cdot10^{-4}$    | $4.8\cdot10^{-3}$  | $7.8\cdot10^{-4}$    | $-1.2 \cdot 10^{-5}$ | $-4.3 \cdot 10^{-5}$ | $1.6\cdot 10^{-5}$ |
| p = 2          | $7.2\cdot 10^{-3}$   | $1.6\cdot 10^{-2}$ | $3.1 \cdot 10^{-3}$  | $-9.3 \cdot 10^{-5}$ | $-1.8\cdot10^{-4}$   | $7.1\cdot 10^{-5}$ |
| $\overline{n}$ | 16                   | 17                 | 18                   | 19                   | 20                   | 21                 |
| p = 1          | $-2.0 \cdot 10^{-6}$ | $4.4\cdot10^{-6}$  | $-5.2 \cdot 10^{-6}$ | $8.6 \cdot 10^{-6}$  | $-1.9 \cdot 10^{-6}$ | $3.7\cdot 10^{-6}$ |
| p = 2          | $-3.8 \cdot 10^{-6}$ | $1.1\cdot 10^{-5}$ | $-1.9 \cdot 10^{-5}$ | $3.4\cdot10^{-5}$    | $-6.7 \cdot 10^{-6}$ | $2.0\cdot 10^{-5}$ |
| $\overline{n}$ | 22                   |                    |                      |                      |                      |                    |
| p = 1          | $-7.6 \cdot 10^{-7}$ |                    |                      |                      |                      |                    |

Table 4: Relative errors  $-\delta_n^{(p)}$  of prediction  $(1 \le p \le 2, 4 \le n \le 22)$ 

scheme at the *n*th stage (i.e., by using the known  $H_k$ 's for  $1 \le k \le n$ ). This value  $H_n^{(p)}$  is obtained as the result of the following Maple command (again, a rational number rounded to the nearest integer):

Here, n and p are replaced by the corresponding integers.

The comparison of the estimate  $H_n^{(p)}$  with the actual value  $H_{n+p}$  is achieved via the relative error

$$\delta_n^{(p)} = \frac{H_n^{(p)} - H_{n+p}}{H_{n+p}},$$

which is given in Table 4. Our calculations suggest that for a fixed p, each sequence of the absolute value  $|\delta_n^{(p)}|$  of the errors made when predicting p steps ahead decreases with (possibly) some small oscillation.

The errors  $\delta_n^{(p)}$  for higher values of p are given in Table 7 (Appendix B). The same remark about their decrease with small oscillation applies to values of p up to 8. Besides, the data in the table also strongly suggests a slow and monotonic variation of  $-\delta_n^{(p)}$  with the parameter p (at least when n is greater than 8). More specifically, when  $n \ge 8$  the ratio  $\mu_n = \delta_n^{(8)} / \delta_n^{(1)}$  never exceeds a few hundreds.

#### Predictions

Following our calculation scheme and the recurrence computed for n = 23, we obtain the predictions for the next values of  $H_n$  that are given in Table 5. Note that the predicted values  $H''_n = H_n^{(1)}$  for n > 23 have been obtained by defining  $H_n^{(p)}$  by the recurrence computed using the known values  $H_1$  to  $H_{23}$  together with the successively predicted ones  $H_{23}^{(1)}, H_{24}^{(1)}, \ldots, H_{n-1}^{(1)}$ .

The validity of these predictions for n = 24 and n = 25 is suggested by the stability of the scheme, as described in the previous section (see Table 4). A similar analysis of Table 7 vindicates the further values and the bounds on the errors to be found in Table 5.

In order to perform the calculations of the recurrences, evaluation procedures, and estimates for each n between 1 and 23, not more than 60 seconds of CPU time were needed.

| n                      | 24                  | 25                  | 26                 |
|------------------------|---------------------|---------------------|--------------------|
| $H_n''$                | 122237774262384     | 606259305418149     | 3011424390300379   |
| $\operatorname{error}$ | $10^{-6}$           | $10^{-5}$           | $10^{-5}$          |
| n                      | 27                  | 28                  | 29                 |
| $H_n''$                | 14979449994317356   | 74608167670480920   | 372053203099446920 |
| error                  | $10^{-5}$           | $10^{-4}$           | $10^{-4}$          |
| n                      | 30                  | 31                  |                    |
| $H_n''$                | 1857452345893521033 | 9283108148442320346 |                    |
| $\operatorname{error}$ | $10^{-3}$           | $10^{-3}$           |                    |

Table 5: Predicted numbers  $H''_n$  of hexagonal systems with n hexagons and presumable relative error bounds  $(24 \le n \le 31)$ 

| n              | 5     | 6     | 7     | 8     | 9     | 10    | 11    | 12    | 13    |
|----------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| $\rho_n$       | 3.682 | 4.086 | 4.335 | 4.533 | 4.625 | 4.694 | 4.741 | 4.776 | 4.805 |
| $\overline{n}$ | 14    | 15    | 16    | 17    | 18    | 19    | 20    | 21    | 22    |
| $\rho_n$       | 4.829 | 4.849 | 4.867 | 4.883 | 4.898 | 4.911 | 4.922 | 4.933 | 4.943 |
| n              | 23    | 24    | 25    | 26    | 27    | 28    | 29    | 30    |       |
| $\rho_n$       | 4.951 | 4.960 | 4.967 | 4.974 | 4.981 | 4.987 | 4.992 | 4.998 |       |

Table 6: Observed ratios  $\rho_n = H_{n+1}/H_n$  (5  $\leq n \leq 22$ ), as well as predicted ratios  $\rho''_n = H''_{n+1}/H''_n$  (23  $\leq n \leq 30$ )

Again, the other parameter setting suggested at the end of Section 1 yields a different recurrence (order 11 instead of 2, degree 1 instead of 7, 46-digit instead of 116-digit integers). However, the numbers predicted by this alternative recurrence remain close to the ones in Table 5.

### **3** Exponential Asymptotic Part

A natural idea is to consider the ratio  $\rho_n = H_{n+1}/H_n$  of two successive terms of the sequence of observed numbers of hexagonal systems. Table 6 provides further evidence to corroborate the conjecture of Aboav and Gutman that the limiting value is remarkably close (or exactly equal) to 5 [20].

In the same vein, we observed that each predicted recurrence of the  $H_n^{(p)}$  for fixed n asymptotically behaves exponentially, namely  $H_n^{(p)} \sim K_n \alpha_n^p$  for a constant  $K_n$  and a parameter  $\alpha_n$  that is an explicit algebraic number close to, but greater than 5. Furthermore, the greater n is, the closer to 5 the exponential parameter  $\alpha_n$  is.

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## A Explicit Value for the Recurrence of Section 1

The second-order recurrence in Step 2 of the prediction scheme described in Section 1 involves the following polynomials of degree 5 in n with integer coefficients of 52 digits:

 $p_0 = -1867772898049832297838775598964134957166764980189512$ 

- 10884556829407079968697291551132882484933172548220036n
- $+\ 12721533878650287528554902964949356722769733250349510n^2$
- $-\ 3253475329234326006503819920315214439352035172000985n^3$
- $+\ 318101006316857306412246953850890000013322435689442n^4$
- $-10942967863460680674924857755657134350847957422779n^5$ ,
- $p_1 = 5111812422122801926839613693662870834533658464707872$ 
  - $+\ 35469788015542951395105181875419339475240204323784n$
  - $-\ 3367129112115264514741892953382392619519869487897336n^2$
  - $+\ 770288443670151618651821390139171124785671163970316n^3$
  - $-\ 17497962137475978810591830043300350924099002352308n^4$
  - $-\ 3188835391221555958813481750811329757447934182008n^5,$

 $p_2 = -1081346508024323209666946031566245292455631161506120$ 

- $+\ 182573229867847718790436477380820200105219280204290n$
- $+\ 296672275392575104755387719895756498293914347320231n^2$
- $-\ 50732258097471360256894519492471993600238207615036n^3$
- $-\ 7073106935049620643525597754441192257088974124079n^4$
- $+\ 1027640238414335110389952660120536662439679446914n^5.$

# **B** More Numerical Results Supporting the Prediction Accuracy

Table 7 is an extended version of Table 4. It suggests that the calculation method proposed in this paper is very stable, far beyond the prediction of the first next two values  $H_{24}$  and  $H_{25}$  of the sequence.

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| n              | 4                    | 5                   | 6                    | 7                    | 8                    | 9                    |
|----------------|----------------------|---------------------|----------------------|----------------------|----------------------|----------------------|
| p = 1          | 0.22                 | 0.24                | $3.6 \cdot 10^{-2}$  | $-2.7 \cdot 10^{-2}$ | $4.7 \cdot 10^{-2}$  | $-7.5 \cdot 10^{-3}$ |
| p = 2          | 0.47                 | 0.42                | $9.0\cdot10^{-2}$    | $1.3 \cdot 10^{-2}$  | 0.22                 | $-2.2 \cdot 10^{-2}$ |
| p = 3          | 0.68                 | 0.60                | 0.16                 | 3.7                  | 0.65                 | $-4.2 \cdot 10^{-2}$ |
| p = 4          | 0.81                 | 0.72                | 0.22                 | 44.                  | 1.6                  | $-6.7 \cdot 10^{-2}$ |
| p = 5          | 0.90                 | 0.81                | 0.28                 | 320.                 | 3.3                  | $-9.6 \cdot 10^{-2}$ |
| p = 6          | 0.94                 | 0.87                | 0.33                 | 1800.                | 6.3                  | 0.13                 |
| p = 7          | 0.97                 | 0.91                | 0.38                 | 8000.                | 11.                  | 0.17                 |
| p = 8          | 0.98                 | 0.94                | 0.43                 | 31000.               | 17.                  | 0.20                 |
| $\mu_n$        | 4.4                  | 3.9                 | 12.                  | $11 \cdot 10^{7}$    | 360.                 | 26.                  |
| n              | 10                   | 11                  | 12                   | 13                   | 14                   | 15                   |
| p = 1          | $9.9\cdot10^{-4}$    | $4.8 \cdot 10^{-3}$ | $7.8\cdot10^{-4}$    | $-1.2 \cdot 10^{-5}$ | $-4.3 \cdot 10^{-5}$ | $1.6\cdot 10^{-5}$   |
| p = 2          | $7.2\cdot10^{-3}$    | $1.6 \cdot 10^{-2}$ | $3.1\cdot10^{-3}$    | $-9.3 \cdot 10^{-5}$ | $-1.8 \cdot 10^{-4}$ | $7.1\cdot 10^{-5}$   |
| p = 3          | $2.1 \cdot 10^{-2}$  | $3.5\cdot10^{-2}$   | $7.5\cdot10^{-3}$    | $-3.0 \cdot 10^{-4}$ | $-4.4 \cdot 10^{-4}$ | $1.9\cdot 10^{-4}$   |
| p = 4          | $4.3\cdot10^{-2}$    | $6.2\cdot10^{-2}$   | $1.4\cdot10^{-2}$    | $-6.9 \cdot 10^{-4}$ | $-8.5\cdot10^{-4}$   | $3.9\cdot10^{-4}$    |
| p = 5          | $7.5\cdot10^{-2}$    | $9.9\cdot10^{-2}$   | $2.4\cdot10^{-2}$    | $-1.3 \cdot 10^{-3}$ | $-1.4 \cdot 10^{-3}$ | $6.9\cdot 10^{-4}$   |
| p = 6          | 0.12                 | 0.14                | $3.6\cdot10^{-2}$    | $-2.1 \cdot 10^{-3}$ | $-2.2 \cdot 10^{-3}$ | $1.1 \cdot 10^{-3}$  |
| p = 7          | 0.17                 | 0.19                | $5.0\cdot10^{-2}$    | $-3.2 \cdot 10^{-3}$ | $-3.1 \cdot 10^{-3}$ | $1.6 \cdot 10^{-3}$  |
| p = 8          | 0.22                 | 0.25                | $6.7\cdot10^{-2}$    | $-4.5 \cdot 10^{-3}$ | $-4.3 \cdot 10^{-3}$ | $2.2 \cdot 10^{-3}$  |
| $\mu_n$        | 220.                 | 53.                 | 87.                  | 370.                 | 99.                  | 140.                 |
| n              | 16                   | 17                  | 18                   | 19                   | 20                   | 21                   |
| p = 1          | $-2.0 \cdot 10^{-6}$ | $4.4\cdot 10^{-6}$  | $-5.2 \cdot 10^{-6}$ | $8.6 \cdot 10^{-6}$  | $-1.9 \cdot 10^{-6}$ | $3.7\cdot10^{-6}$    |
| p=2            | $-3.8 \cdot 10^{-6}$ | $1.1\cdot 10^{-5}$  | $-1.9 \cdot 10^{-5}$ | $3.4\cdot 10^{-5}$   | $-6.7 \cdot 10^{-6}$ | $2.0\cdot 10^{-5}$   |
| p = 3          | $-8.8 \cdot 10^{-6}$ | $2.0\cdot10^{-5}$   | $-4.6 \cdot 10^{-5}$ | $8.3\cdot10^{-5}$    | $-1.6 \cdot 10^{-5}$ |                      |
| p = 4          | $-1.7 \cdot 10^{-5}$ | $2.9 \cdot 10^{-5}$ | $-9.0 \cdot 10^{-5}$ | $1.6 \cdot 10^{-4}$  |                      |                      |
| p = 5          | $-3.0 \cdot 10^{-5}$ | $3.7\cdot10^{-5}$   | $-1.6 \cdot 10^{-4}$ |                      |                      |                      |
| p = 6          | $-4.9 \cdot 10^{-5}$ | $4.2\cdot10^{-5}$   |                      |                      |                      |                      |
| p = 7          | $-7.3 \cdot 10^{-5}$ |                     |                      |                      |                      |                      |
| $\overline{n}$ | 22                   |                     |                      |                      |                      |                      |
| p = 1          | $-7.6 \cdot 10^{-7}$ |                     |                      |                      |                      |                      |

Table 7: Error  $-\delta_n^{(p)}$  of the prediction and measure  $\mu_n = \delta_n^{(8)}/\delta_n^{(1)}$  of its variation with p  $(1 \le p \le 8, 4 \le n \le 23)$ 

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