

## TREES

BY

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*Dans ce cercle qui avance du même pas que moi, entrent les arbres, lentement, l'un après l'autre ou par groupes. J'aime à les voir émerger du néant, formes lourdes où se dessinent bientôt les membres figés, la résille cristallisée des rameaux. Ils s'avancent, lourds de leur mystère, plus chargés de poésie que jamais. Bientôt ils sont sur moi. Au dessus, à côté, derrière, enveloppants et amoureux. Est-il dans toute la mythologie quelques déesses qui font l'amour avec des arbres ? Sans doute.*

Bernard CLAVEL

### 1. Introduction

*Auprès de mon arbre, je vivais heureux...  
J'aurais jamais dû m'éloigner d'mon arbre.*  
Georges BRASSENS

The following picture shows a tree which has never existed except on the screen of a computer. It is a synthetic image of a tree which has been produced by an algorithm based on some combinatorial Mathematics.

The combinatorics underlying the algorithm producing such trees is very rich and forms the subject of this paper.

It started in *Hydrogeology* by HORTON [26] and STRAHLER [66] in some work about the morphological structure of river networks. Then analog studies have been made in other sciences (*Botanic, Anatomy, Neurophysiology,...*) where branching patterns appear. Underlying each branching pattern in nature, one

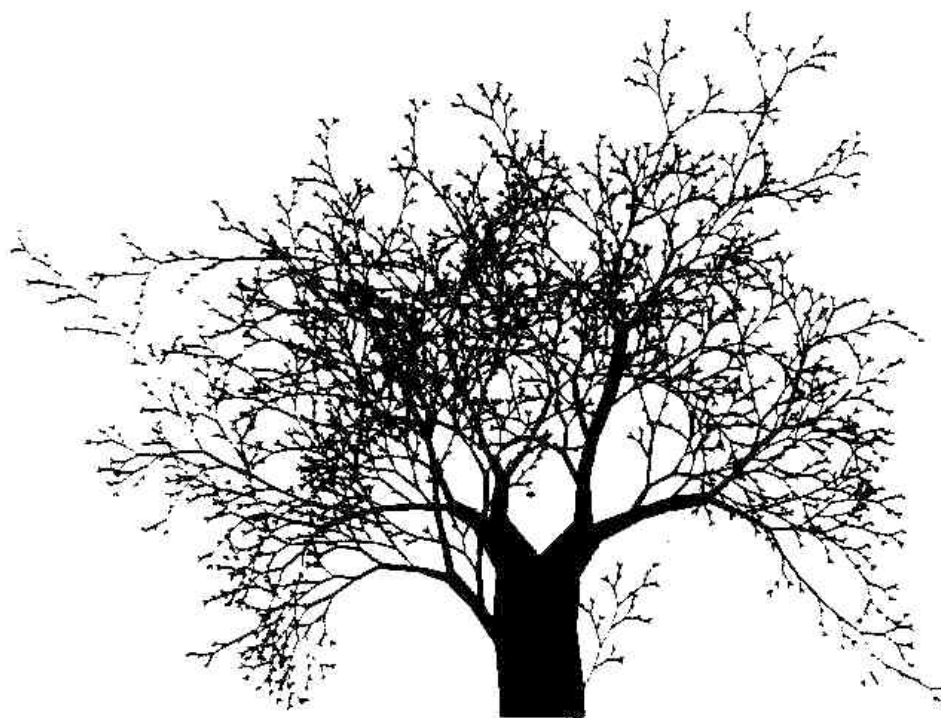


Fig. 1 : Combinatorics is beautiful

can define an abstract tree, by remembering only the "*topological*" structure of the ramifications, without considerations of the particular geometric details of the pattern. This abstract tree is a mathematical (*combinatorial*) object.

Horton Strahler analysis can be made for combinatorial trees. In particular, the determination of the mean, of the parameters for all trees with a given number of branching points involves deep *asymptotic analysis*, (see MEIR, MOON and POUNDER [36], [37], [41], KEMP [29], FLAJOLET, RAOULT, VUILLEMIN [19]). Some mathematical considerations appear, in relation with *Number Theory*. The famous zeta Riemann function is needed there.

In fact the last two papers quoted above are concerned about some optimization problems in *Computer Science* : what is the minimum number of *registers* needed to evaluate an arithmetic expression ? Curiously this problem involves the Horton Strahler parameter introduced in Hydrogeology.

The surprise is bigger when this parameter appears again in *Molecular Biology* in some theoretical considerations about secondary structures of single-stranded nucleic acids (see DE GENNES [8], MITIKO GO [40], VAUCHAUSSADE DE CHAUMONT, VIENNOT [69], [70], WATERMAN [75]).

For the determination of the *generating functions* for secondary structures (*i.e. partition functions* for physicists) we have used the methodology

SCHÜTZENBERGER introduced in [58] : coding of combinatorial objects with words of an *algebraic language* and introduction of systems of equations in non-commutative variables. This methodology have been very useful for many other problems, see CORI [5], DELEST, VIENNOT [10], [11], GOUYOU-BEAUCHAMPS [21], VIENNOT [72], [73].

Behind all the above studies related to the Horton-Strahler analysis is a beautiful combinatorial world, involving bijections and correspondences between paths and different families of trees (FRANÇON [20], KREWERAS [31], VAUCHAUSSADE DE CHAUMONT [69], VIENNOT [71], ZEILBERGER [79]).

The combinatorics of the Horton-Strahler analysis have been used in *Computer Graphics* for the creation of faithful synthetic images of trees, see EYROLLES [17], VIENNOT, EYROLLES, ARQUÈS, JANEY [84] and the pictures of trees in this paper.

The Horton-Strahler parameters (bifurcation ratios,...) can be considered as an attempt to give quantitative informations about the visual aspect, or "*shape*", of a tree. In relation with *fractals* theory, MANDELBROT [35], many works are done in *Physics* studying the "*shape*" of branching patterns occurring in nature or simulated on a computer, see for example NIEMEYER, PIETRONERO, WIESMANN [43] about *electric breakdown*, NITTMANN, DACCARD, STANLEY [45] about *viscous fingering*, SAWADA, DOUGHERTY, GOLLUB [53] about *electrolytic metal deposits* or WITTEN, SANDERS [76] about the *DLA* (diffusion limited aggregation).

To each tree, we associate a *stochastic* matrix, called *ramification matrix*. This notion can be considered as a refinement of the Horton-Strahler analysis and gives some pertinent quantitative informations about the "*shape*" of the tree. It is at the basis of the generation of the synthetic images of trees of this paper and [18]. To each matrix corresponds a family or "*species*" of synthetic trees. With VANNIMENUS, we are studying these ramifications matrices in *Physics* [81], and PENAUD [47] has just determined the ramification matrix of a *random binary tree*. Horton-Strahler analysis has also just been introduced in *Physics* by HINRICHSSEN, MALØY, FEDER and JØSSANG [83].

In a completely different context, Horton-Strahler parameter of binary trees appears again in the determination of a basis of the derived series of a free Lie algebra, REUTENAUER [80].

## 2. Horton-Strahler analysis in Hydrogeology

*Cette existence à l'abri de la cohue publique  
révèle des voix dans les arbres,  
des livres dans les ruisseaux qui coulent,  
des leçons dans les pierres  
et le bien en toute chose.*

SHAKESPEARE, Comme il vous plaira  
Acte II, scène I (trad. Victor HUGO).

The hydrogeologist HORTON introduced in [26] a process classifying the rivers of a fluvial network. The rule, modified by STRAHLER [66] is the following.

A river starting at a source point has order 0. Two rivers of order  $k$  joining together give rise to a river of order  $(k + 1)$ . A river of order  $i$  joining a river of order  $k$  with  $i < k$  gives rise to a river of order  $k$  (see Figure 2 next page). We have supposed that the river network has no island and that no more than two rivers join at the same point (as at Trois-Rivières in Canada).

Intuitively, the order of a river should reflect the "importance" of that river in the fluvial basin. On Figure 2, the reader will recognize the main rivers of the Garonne network : Dordogne, Lot, Tarn, Ariège, each having order 3. The orders are not increasing rapidly in the area of the Lannemezan plateau.

Many works have been done in Hydrogeology in order to discover certain laws about the frequency of rivers of given order and if there exists some correlation between length, width and order of river.

A *segment* of order  $k$  is a maximal portion of a river of order  $k$ . In other words, a segment of order  $k$  starts at the junction of two segments of order  $(k - 1)$  (unless if  $k = 0$ , it starts at a source point) and ends at the junction with a river of order  $k' > k$  (unless  $k$  is the maximum possible order, and then the segment ends in the sea). Let  $b_k$  be the number of segments of order  $k$ . The *bifurcation ratio*  $\beta_k$  of order  $k$  is defined by the relation

$$(1) \quad \beta_k = \frac{b_k}{b_{k+1}}.$$

Hydrogeologists have discovered that in general, the bifurcation ratios of a given river network are constant  $\beta_k = \beta$ . The constant  $\beta$  depends upon the particular network and is usually between 3 and 5.

For a given river network, we can define the average length (in kilometers)  $\ell_k$  of the segments of order  $k$ . It has been observed that in general, the ratio  $\ell_{k+1}/\ell_k = \lambda_k$  is a constant for a given fluvial basin. This constant is  $\lambda \simeq \beta/2$ . Similar laws seem to have been observed for the width of rivers in correlation with their order.

Similar studies have been made for other branching patterns occurring in various natural sciences as Botany, MAC MAHON [34] or in Anatomy for

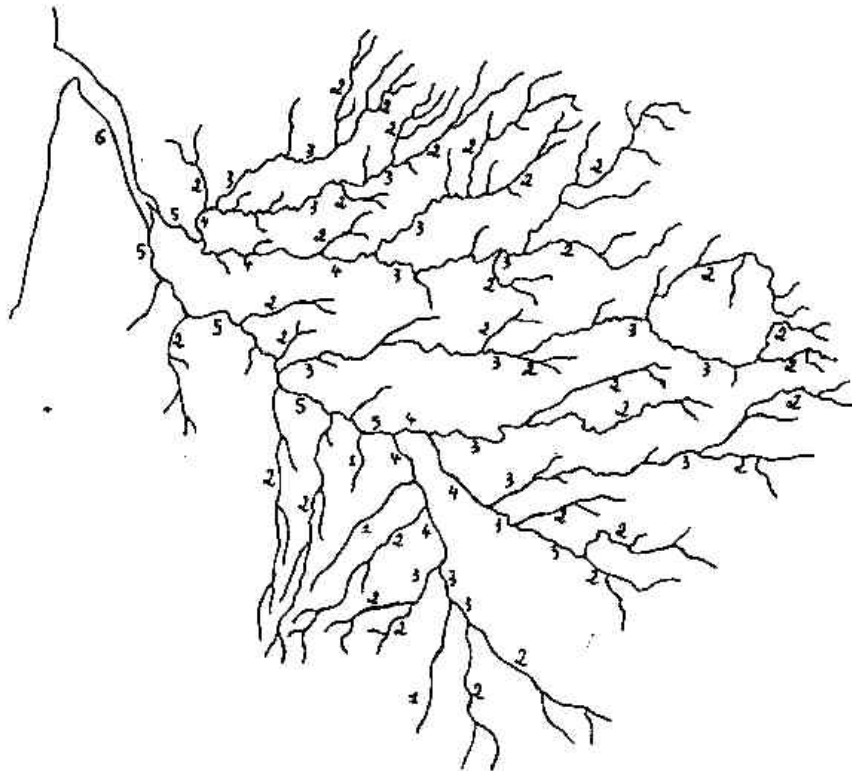


Fig. 2 : The Horton-Strahler rule for the Garonne river network

bronchial networks or arterial vessels, WOLDENBERG [78], or Neurophysiology, PERCHERON [48]. Similar laws seem to appear.

PRUD'HOMME, NAUDIN and VIGNEAUX [42], [49], [50] and GVIN [23] have studied possible correlations between the shape of rivers networks and the geological structure of the underground. More precisely, they introduce the *isolines of length-values* joining the points at the middle of each segment of given order  $k$  and labelled by the length of this segment (in the same way as one would draw some level curves joining some points of a map labelled by their altitude). They have shown some correlation between these curves and the structure of the underground. When the order  $k$  is increased, the curves change and the correlation appears deeper (until 2 km for big order). Their experiment have been done in the South-West of France and also for the golfe of Gascogne in the Atlantic Ocean. Some "river networks" can be defined on the submarine ground. A surprising continuity appears on *isolines of length-values* on both side of the seashore.

An interesting study can be made by comparing the above Horton-Strahler analysis of river networks with the analog analysis for random mathematical binary trees.

### 3. Horton Strahler analysis for random binary trees

A *binary tree*  $B$  is a very classical object in Combinatorics and in Computer Science. An example is visualized on Figure 3 below. If  $B$  has only one vertex, then  $B$  is reduced to this vertex. Else  $B$  is a triple  $B = (L, r, R)$  where  $r$  is a vertex of  $B$  called the *root* of  $B$ , and  $L$  (resp.  $R$ ) is a binary tree called the left (resp. right) subtree. There is two kinds of vertices : the *internal* vertices, each having two *sons* (a left son and a right son), and the *external* vertices, having no son. The internal (resp. external) vertices are marked by a "o" (resp. a "□") on Figure 3.

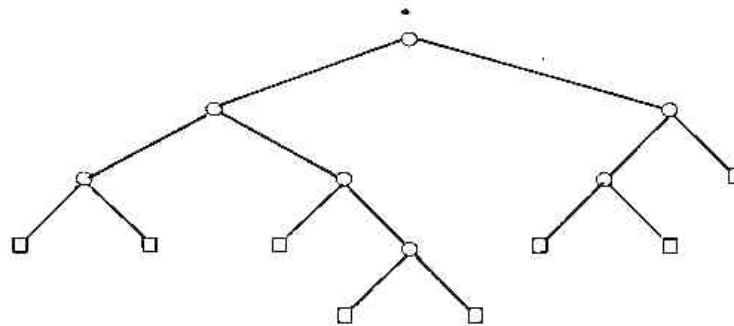


Fig. 3 : A binary tree

If a binary tree has  $n$  internal vertices, then it has  $(n + 1)$  external vertices. The total number of vertices is always an odd number  $2n + 1$ . The number of binary trees with  $n$  internal vertices is the classical Catalan number

$$(2) \quad C_n = \frac{1}{n+1} \binom{2n}{n},$$

with generating function  $y = \sum_{n \geq 0} C_n t^n$  solution of the following algebraic equation

$$(3) \quad y = t + y^2.$$

The first values of  $C_n$  are displayed on Table 1.

$n$	0	1	2	3	4	5	6	7	8	9	10
$C_n$	1	1	2	5	14	42	132	429	1430	4862	16796

Table 1 : The Catalan numbers.

On Figure 4 are displayed the five possible binary trees with 3 internal vertices.

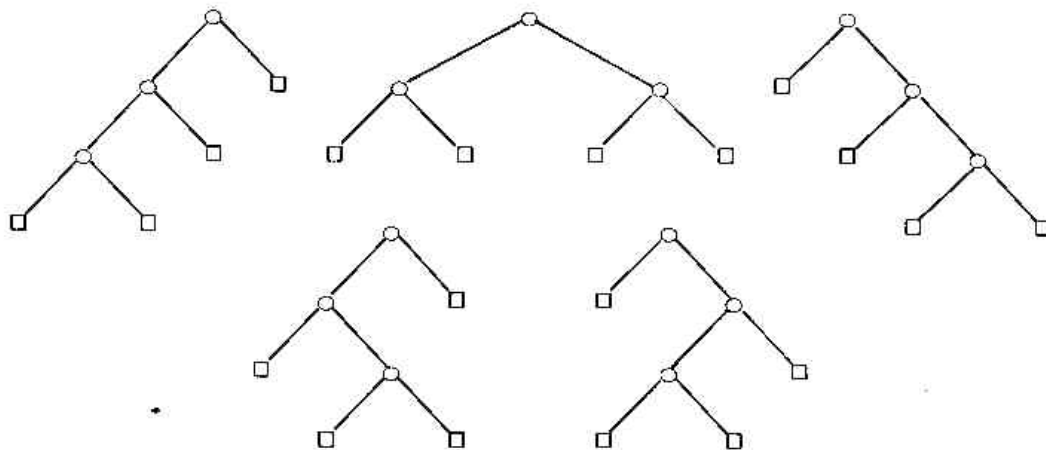


Fig. 4 : The five binary trees with 3 internal vertices

To each river network (having no island and no multiple branching point), one can associate a binary tree, when making abstraction of the real geometric details of the whole network and remembering only the mathematical arrangement of the different branchings. A natural question is to ask which kind of binary trees occurs in river networks. For example, there are approximatively  $10^{59}$  possible binary trees with 100 external vertices. Which choice is made among all possible river networks with 100 source points? Does a river network looks like a *random binary tree* (i.e. each binary tree with  $n + 1$  external vertices appears with the same probability  $1/C_n$ ), or does certain families of binary trees are privileged?

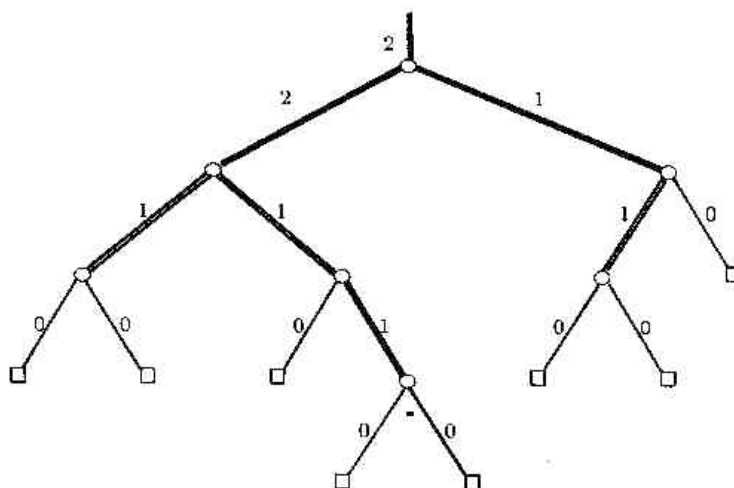
A partial answer can be given by comparing real quantitative measurement as the branching ratio  $\beta_k$  or the length segment ratio  $\lambda_k$  with their analog mean value for random binary trees.

In a river network, the notions of order and segment depend only of the underlying binary tree. An *edge* in a binary tree is pair  $(x, y)$  where  $y$  is a son of  $x$ . Each edge has an order. A *segment* is a maximal sequence of edges of the same order and going towards the root (see Figure 5 next page).

The *Strahler number*  $St(B)$  of the binary tree  $B$  is the maximal order of its edges. In other words, this parameter can be defined inductively by

$$(4) \quad \begin{aligned} St(\square) &= 0; \\ St(L, r, D) &= \text{if } St(L) = St(R) \text{ then } 1 + St(L) \\ &\quad \text{else } \max(St(L), St(r)). \end{aligned}$$





In the case of river networks the length of a segment was measured in kilometers. Here we will define the (abstract) length as the number of edges of the segment.

On the opposite, the binary tree of Figure 6b looks like the so-called "gourmand de la vigne". They grow in springtime on the bottom part of the winetrees and has to be cut in order to get better quality and quantity of wine. Such binary tree has only one segment of order 1 and the bifurcation ratio  $\beta_1$  of order 1 is the number of external vertices of the binary tree. Thus  $\beta_1$  can be as large as possible. Combining these two extreme cases, the reader will imagine how to construct families of binary trees where the bifurcation ratio  $\beta_k$  is as large as possible for any  $k$ .



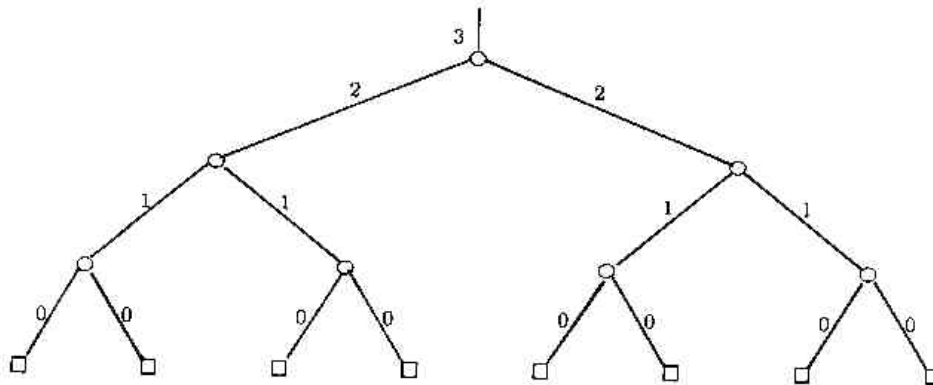


Fig. 6a : Perfect tree

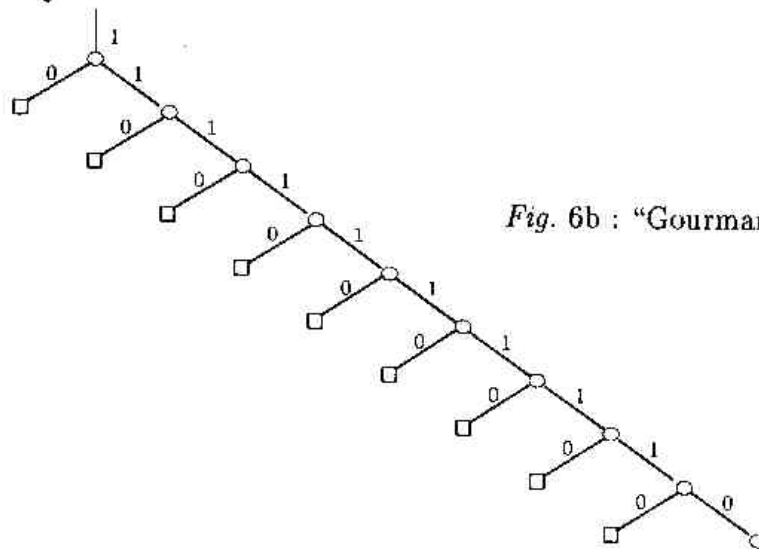


Fig. 6b : "Gourmand de la vigne"

Fig. 6 : Two extreme cases of binary trees : perfect tree and "gourmand de la vigne"

The bifurcation ratios seem to be a good quantitative information about the "shape" of the binary tree. SHREVE [61] generated the number of segments for large binary trees and found similar empirical laws for these numbers. As in the case of river networks, they tend to approximate geometric series. Rigorous asymptotic studies have been made by MEIER, MOON and POUNDER [36], [37] and [41].

Let  $s_k^n$  be the mean number of segments of order  $k$  among all binary trees with  $n$  internal vertices. MOON [41] proved the following result

$$(5) \quad s_k^n = \frac{n}{4^k} + \frac{1}{6} \left( \frac{1}{4^k} \right) + O\left(\frac{1}{n}\right)$$

for fixed integer  $k$  as  $n \rightarrow \infty$ . This relation implies

$$(6) \quad \frac{s_k^n}{s_{k+1}^n} = 4 - \frac{4^k}{2n} + O\left(\frac{1}{n^2}\right).$$

It is a good surprise that all the bifurcation ratios  $\beta_k$  of a large random binary trees tend to be equal to 4, which is just between the two values 3 and 5 coming from Hydrogeology.

Let  $L_k(B)$  be the total length of all segments of order  $k$  in the binary tree  $B$ . Let  $L_k^n$  be the mean of  $L_k(B)$  among all binary trees with  $n$  internal vertices. Then MEIER and MOON proved [36] the following relations (for a fixed  $k$  and  $n \rightarrow \infty$ ) :

$$(7) \quad L_k^n = \frac{n}{2^k} + \frac{1}{3} \left( 2^k - \frac{1}{2^k} \right) + O\left(\frac{1}{n}\right),$$

$$(8) \quad \frac{L_k^n}{s_k^n} = 2^k \left( 1 + \frac{4^k - 1}{6n} \right) + O\left(\frac{1}{n^2}\right).$$

Thus analogous Horton Strahler laws exist for large random binary trees. All the length segment ratios tends to  $\lambda = 2$ , which is half of  $\beta = 4$ . According to bifurcation ratio and length of segments, river networks tend to have the same behaviour as random binary trees.

#### 4. Optimization problems in Theoretical Computer Science

Strahler number of binary trees have reappeared in Computer Science. We consider arithmetical expressions involving only binary laws. Such expressions can be identified with labelled binary trees. Each internal vertex corresponds to a binary law, each external vertex corresponds to a variable, see Figure 7.

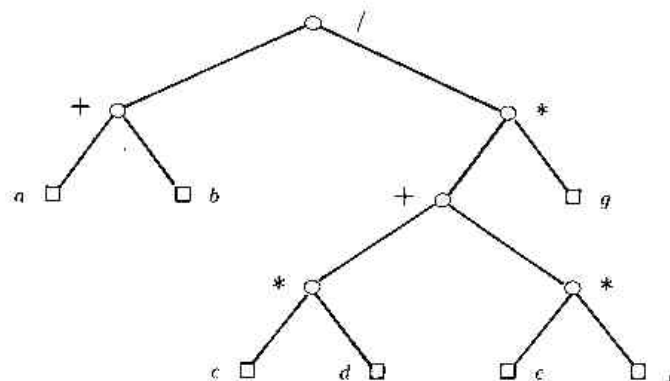


Fig. 7 : The binary tree associated to the arithmetical expression  
 $(a + b) / ((c * d + e * f) * g)$

The computation with a computer of an arithmetical expression requires a certain number of *registers* where are performed the arithmetical operations. Here is an example of a possible computation of the arithmetical expression displayed on Figure 7 using 4 registers.

$$\begin{aligned} R_1 &\leftarrow a; & R_2 &\leftarrow b; & R_1 &\leftarrow R_1 + R_2; \\ R_2 &\leftarrow c; & R_3 &\leftarrow d; & R_2 &\leftarrow R_2 * R_3; \\ R_3 &\leftarrow e; & R_4 &\leftarrow f; & R_3 &\leftarrow R_3 * R_4; \\ R_2 &\leftarrow R_2 + R_3; & R_3 &\leftarrow g; & R_2 &\leftarrow R_2 * R_3; \\ R_1 &\leftarrow R_1 / R_2. \end{aligned}$$

In fact it would have been possible to use only 3 registers, and this number is the minimum possible.

The following result is due to ERSHOV [16]: the minimum number of registers required in the evaluation of an arithmetic expression is exactly the Strahler number, increased by one, of the corresponding binary tree. Such problem is equivalent to a *pebbles* problem. Given a binary tree  $B$ , one can put pebbles on the vertices of  $B$  with the following rule. A pebble can be put on a vertex  $x$  in the following two possible cases: else  $x$  is an external vertex, else  $x$  has two sons each having a pebble. What is the minimum number of pebbles required to put a pebble on the root of  $B$ ? Pebbles correspond to registers and the computation of the arithmetical expression corresponds to a possible movement of the pebbles.

FLAJOLET, RAOULT, VUILLEMIN [19] and independently KEMP [29] have solved the problem of finding an asymptotic expression for the minimum number of registers required to evaluate a long random arithmetical expression (in other words, the mean  $St_n$  of the Strahler number of binary trees with  $n$  internal vertices, when  $n \rightarrow \infty$ ). They found the following beautiful result

$$(9) \quad St_n = \log_4 n + D(\log_4 n) + O(1),$$

where  $D(t)$  is a continuous periodic function with period one.

This function can be defined as follows. Let  $T(n)$  be the number of ones in the binary expansions of all integers  $0, 1, \dots, n-1$ . A result of DELANGE [9] is that there exist a real function  $F$  such that for all  $n \geq 0$ ,

$$(10) \quad T(n) = \frac{1}{2}n \log n + nF(\log n),$$

with  $F$  continuous and periodic with period 1.

Let  $H_4(x)$  be the 4th Hermite polynomial, that is  $e^{t^2}(d^4/dt^4)(e^{-t^2})$ . Let  $\gamma$  be the Euler constant. Then the function  $D(t)$  appearing in the relation (9) is defined by

$$(11) \quad D(t) = 1 - \frac{\gamma}{2 \log 2} - \int_0^\infty t H_4(t) F(\log t + u) e^{-t^2} dt.$$

Explicit expressions can be given for the coefficients of the Fourier transform of  $D(t)$ . These coefficients involve the famous Riemann zeta function.

Strahler numbers of binary trees are also related to optimum procedures for traversing all vertices of a binary tree. A very classical procedure called *preorder*, exists in programming (see for example KNUTH [30]). This procedure can be implemented in a non recursive way by using a stack. If the number of internal vertices is  $n$ , then the maximal possible height of this stack is  $n$  and the average is in  $n^{1/2}$ . Using Strahler numbers of subtrees and a rule very similar to the above pebbles or registers problem, one can define an optimal procedure called *economic order* in [19]. The maximum height of the stack is in  $\log_2 n$  and the average in  $\log_4 n$ .

## 5. Combinatorics of Strahler numbers

*Arbres de la forêt, vous connaissez mon âme  
Au gré des envieux, la foule loue et blâme  
Vous me connaissez, vous! Vous m'avez vu souvent,  
Seul dans vos profondeurs, regardant et rêvant.*  
Victor HUGO

The proof of relation (9) relies on an explicit expression for the generating function of binary trees having a given Strahler number.

Let  $S_{n,k}$  (resp.  $S_{n,\leq k}$ ) be the number of binary trees  $B$  with  $n$  internal vertices and Strahler number  $\text{St}(B) = k$  (resp.  $\text{St}(B) \leq k$ ). We denote the corresponding generating functions by

$$(12) \quad S_k(t) = \sum_{n \geq 0} S_{n,k} t^n \quad \text{and} \quad S_{\leq k}(t) = \sum_{n \geq 0} S_{n,\leq k} t^n.$$

Let  $U_n(t)$  be the  $n^{\text{th}}$  Tchebycheff polynomial of second kind, that is the polynomial defined by the relation

$$(13) \quad \sin(n+1)\theta = \sin \theta U_n(\cos \theta).$$

We denote by  $F_n(t)$  the polynomial

$$(14) \quad F_n(t) = U_n\left(\frac{1}{2}t\right).$$

This polynomial is a *monic* (i.e. coefficient of  $x^n$  is 1) polynomial of degree  $n$ . The reciprocal  $F_n^*(t) = t^n F_n(t^{-1})$  is an even polynomial and we can define  $R_n(t)$  by the relation

$$(15) \quad R_n(t^2) = t^n F_n\left(\frac{1}{t}\right).$$

These polynomials satisfies the recurrence

$$(16) \quad R_{n+1}(t) = R_n(t) - tR_{n-1}(t); \quad R_0(t) = 1, \quad R_1(t) = 1.$$

We have the following explicit expression for the generating function of binary trees  $B$  with  $\text{St}(B) \leq k$  (see [19], [29])

$$(17) \quad S_{\leq k}(t) = \frac{R_{2k-2}(t)}{R_{2k-1}(t)}.$$

Using some identity on Tchebycheff polynomials, one can deduce the relation

$$(18) \quad S_k(t) = \frac{t^{2^k-1}}{R_{2^k-1}(t)}.$$

In fact, very interesting combinatorics appear behind identities (17) and (18).

Define a *Dyck word* as a word  $w$  on the alphabet  $\{x, \bar{x}\}$  satisfying the two following conditions

$$(19) \quad \begin{cases} \text{(i)} & |w|_x = |w|_{\bar{x}}, \\ \text{(ii)} & \text{for every factorization } w = uv, \quad |u|_x \geq |u|_{\bar{x}}, \end{cases}$$

where  $|w|_z$  denotes the number of occurrences of the letter  $z$  in the word  $w$ .

Such Dyck word (classically called restricted Dyck word on two letters) can be visualized by what I call a *Dyck path*, that is a sequence of points  $(s_0, \dots, s_{2n})$  of  $\mathbb{N} \times \mathbb{N}$  such that  $s_0 = (0, 0)$ ,  $s_{2n} = (2n, 0)$  and each "elementary step"  $(s_i, s_{i+1})$  is North-East or South-East (see Figure 8).

The number of Dyck paths (or words) of length  $2n$  is again the Catalan number  $C_n$ . A classical bijection is defined between binary trees with  $(2n+1)$  vertices and Dyck words of length  $2n$ . This bijection is obtained by traversing the binary tree in prefix order, and writing  $x$  (resp.  $\bar{x}$ ) when one encounters an internal (resp. external) vertex. An example is displayed on Figure 8 next page.

The *height*  $H(\omega)$  of a Dyck path (or Dyck word)  $\omega$  is the maximal height of its vertices, that is

$$(20) \quad H(\omega) = \max_{0 \leq i \leq 2n} \{y_i \mid s_i = (x_i, y_i)\}.$$

Classically, the generating function for Dyck paths  $\omega$  with bounded height  $H(\omega) \leq p$  is given by the relation (KREWERAS [31])

$$(21) \quad \sum_{\substack{\omega \text{ Dyck paths} \\ H(\omega) \leq p}} t^{|\omega|/2} = \frac{R_p(t)}{R_{p+1}(t)}.$$

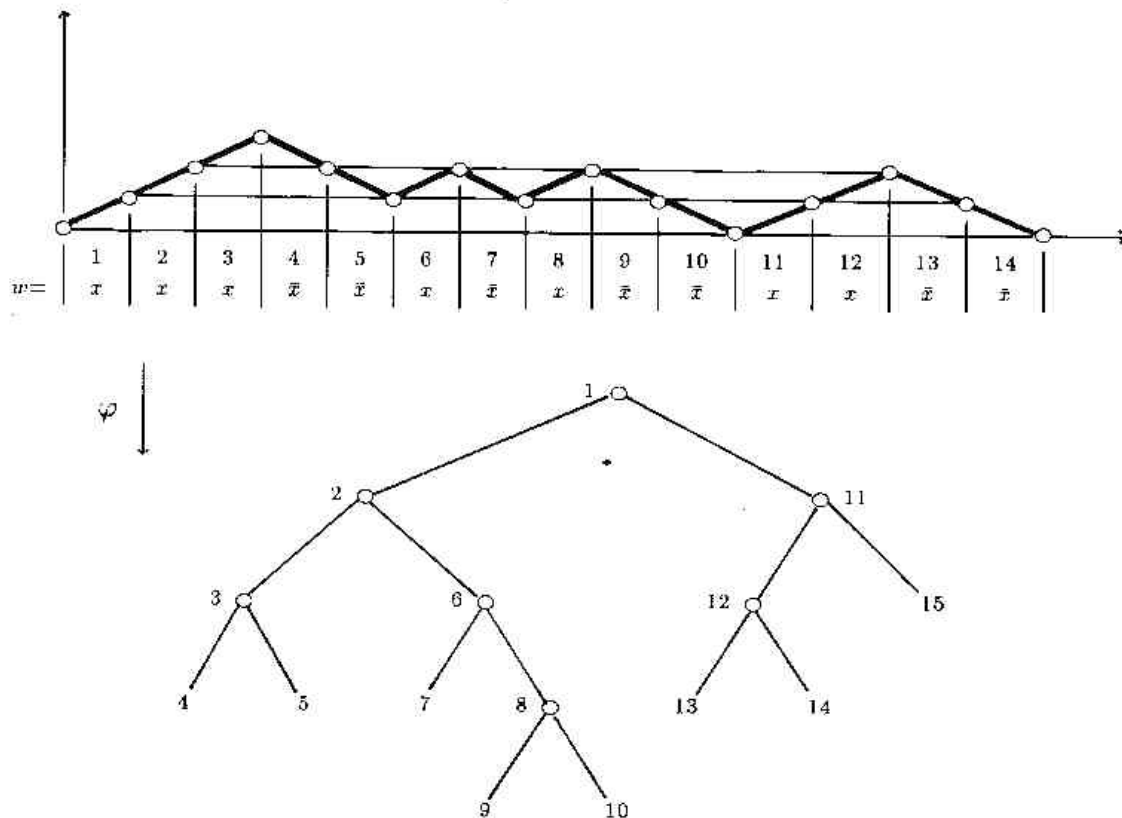


Fig. 8 : The correspondence between binary trees and Dyck paths

A bijective proof of this last identity can be given (see VIENNOT [71]) using the fact that  $F_n(t)$  is the *matching polynomial* of the graph  $\text{Seg}_n$  formed by a segment of length  $n$ . The matching polynomial of a graph  $G$  is defined as

$$(22) \quad P_G(t) = \sum_{\alpha \text{ matchings of } G} (-1)^{|\alpha|} t^{n-2\alpha},$$

where  $n$  is the number of vertices of  $G$  and  $\alpha$  is a matching of  $G$ , that is a set of two by two disjoint edges of  $G$  (no common vertices), see an example on Figure 9.

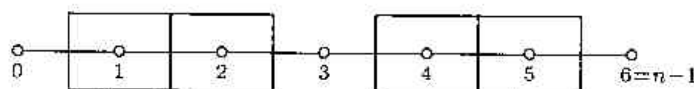


Fig. 9 : A matching of the graph  $\text{Seg}_n$

Identity (17) says that the two following parameters have the same distribution : Strahler number  $St(B)$  of binary trees having  $(2n + 1)$  vertices and  $\lfloor \log_2(1 + H(\omega)) \rfloor$  (integer part of the logarithm of the height) for Dyck paths  $\omega$  having length  $2n$ . It is difficult to find a bijection between binary trees and Dyck paths (words) transforming one parameter into the other. Such a bijection has been defined recursively by FRANÇON [20], using the so-called *Motzkin* paths and the operator *contraction* of Motzkin path (see also VIENNOT [71] in connection with the notion of contraction in a continued fraction).

## 6. Secondary structures in Molecular Biology

More recently, Strahler numbers have appeared again in some theoretical problems in Molecular Biology.

We consider molecules of single-stranded nucleic acids as for example RNA, mRNA (messenger RNA) or tRNA (transfert RNA). The *primary structure* of such molecule is the sequence of bases linked by phosphodiester bonds. There are four possible bases in RNAs : *A* (Adenine), *U* (Uracyl), *G* (Guanine) and *C* (Cytosine). A primary structure is encoded by a word on the alphabet  $\{A, U, G, C\}$ . Such bases can be linked together by hydrogen bonds (*A* with *U*, *G* with *C*). The primary structure is thus folded into a planar graph called the *secondary structure*. The vertices of this graph are the bases and the edges are the primary and secondary bonds, see *Figure 10* next page.

The spatial *ternary structure* of the molecule will not be considered here. Many works have been made in Molecular Biology about the prediction of the secondary structure from the knowledge of the primary structure. The notion of *order* of an hydrogen bond has been introduced, in relation with the computation of the energy of the secondary structure, see MITIKO GÔ [40], DE GENNES [8], WATERMAN [75]. It is convenient to introduce a certain *forest of trees* associated to each secondary structure. The vertices of the forest are the hydrogen bonds of the secondary structure. The edges of the forest are defined according to the "adjacency" of hydrogen bonds, as shown on *Figure 10*.

Such forests are not classical in Molecular Biology. They have been introduced by VAUCHAUSSADE, DE CHAUMONT and VIENNOT [69], [70]. They can be very useful in the study of the *homologies* of secondary structures, that is the common features of the same molecule in different species. These forests appear precisely to be the relevant information needed in the study of homologies. For example, the homologies stated in the work [67] can be formulated by saying that the corresponding forests have a certain common "subforest". Now we define the order of a vertex in a forest.

A *planar rooted tree*  $T$  (or *tree* for short) is : if  $T$  has only one vertex, then  $T$  is reduced to this point (which is the *root*); else  $T = (r; T_1, \dots, T_p)$  where  $r$  is a vertex called the *root* and  $T_1, \dots, T_p$  is an ordered sequence of (planar rooted)



trees. A *forest* of (planar rooted) *trees* is an ordered sequence of trees, see an example on Figure 10.

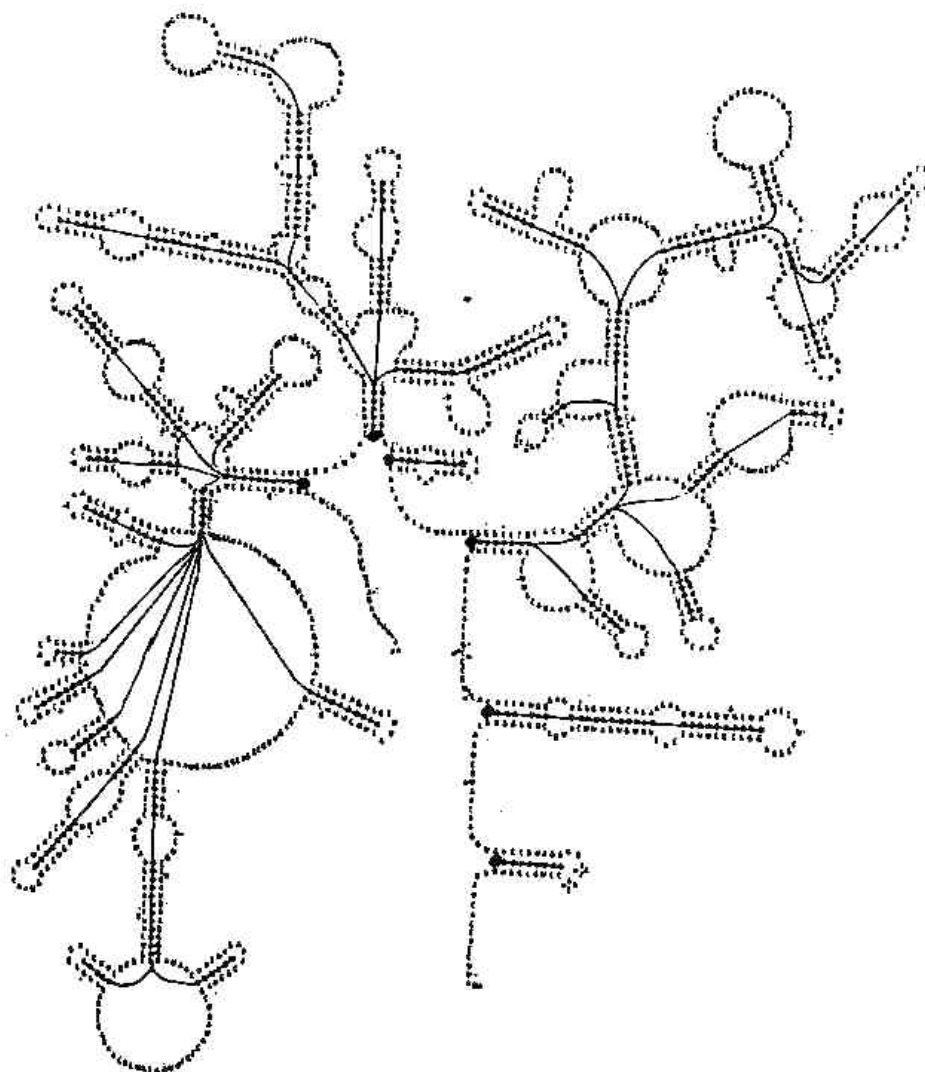


Fig. 10 : Secondary structure of 16S-RNA of E. Coli— (from [67])  
with its associated forest.

The number of forests of trees with  $n$  vertices is the Catalan number (which is also the number of trees with  $(n + 1)$  vertices). Very classical bijections are

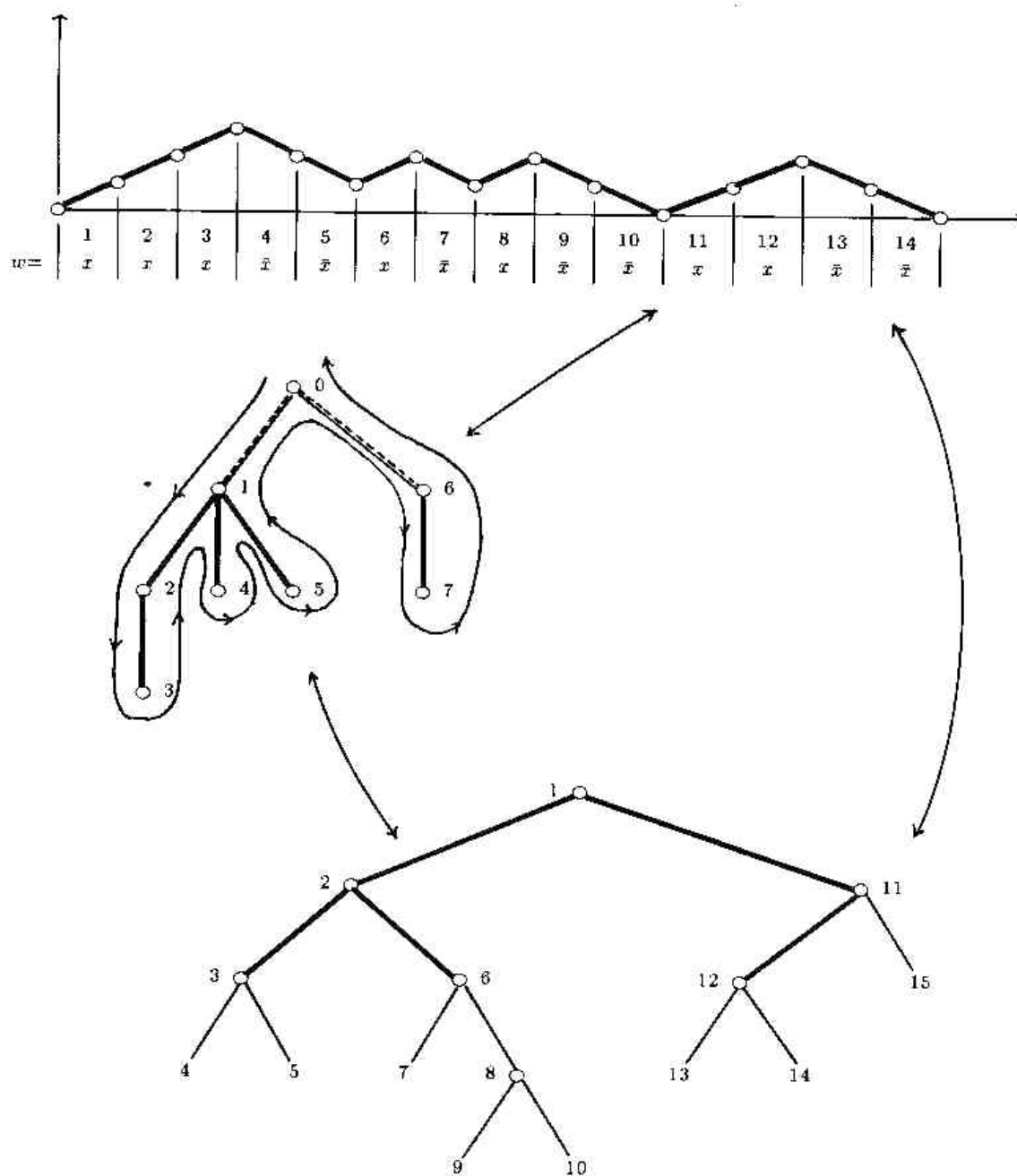


Fig. 11 : The Golden Triangle : binary trees, forests of trees and Dyck paths

known between forests of trees and Dyck words (or paths) and between these forests and binary trees (called *fundamental transform* by KNUTH [30]). Examples are given in Figure 11 above. The triangle formed by these classical bijections is commutative.

A *filament* of a forest is a maximal sequence of vertices  $(s_1, \dots, s_p)$  such that for  $i = 1, \dots, p-1$ ,  $s_i$  has only one son and this son is  $s_{i+1}$ , and  $s_p$  is a *leaf* of the forest (i.e. no son). The filaments are two by two disjoint. We introduce the operator  $\delta$  "deletion of filaments" :  $\delta(F)$  is the forest obtained from  $F$  by deleting all the vertices of all the filaments of  $F$ . If a vertex is deleted at stage  $i$ , then this integer  $i$  is called the *order* of the vertex. The maximal order possible in a forest  $F$ , that is the minimal integer  $k$  such that  $\delta^k(F) = \emptyset$ , is called the *order* of the forest.

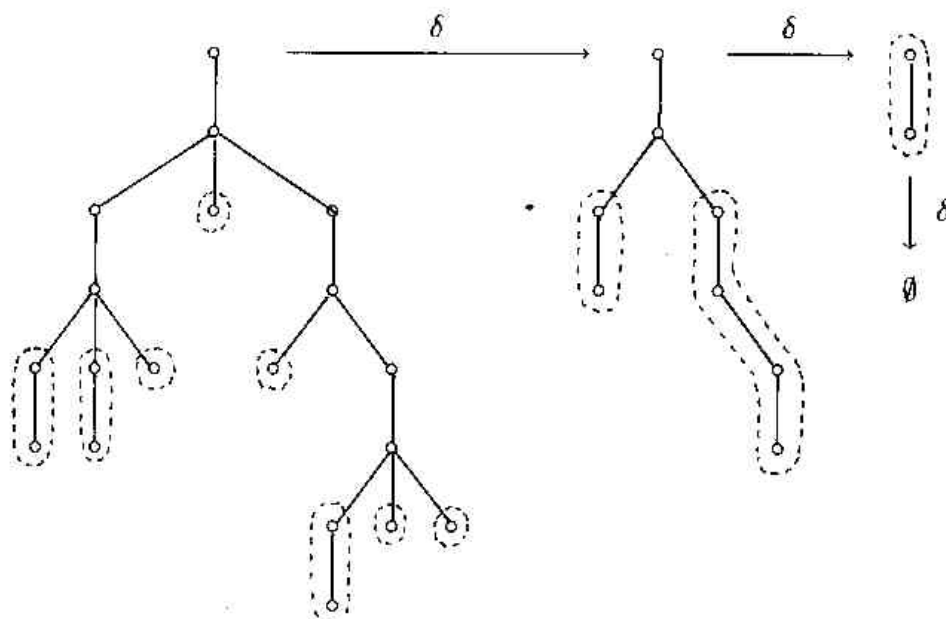


Fig. 12 : Filaments, order of a forest and the operator  $\delta$

In a secondary structure, the order of an hydrogen bond is the order of the corresponding vertex in the underlying forest of the molecule. The order of the secondary structure is the order of the underlying forest. These definitions are equivalent to the ones given in [8], [40], [75].

WATERMAN [75] raised the problem of finding the generating function for all possible secondary structures of order  $k$  (that is all planar graphs representing possible secondary structures). This problem has been solved in VAUCHAUSSADE DE CHAUMONT, VIENNOT [69], [70]. The solution applies a methodology introduced by SCHÜTZENBERGER in [58] and [59] more than 25 years ago.

Secondary structures of order  $k$  are encoded by words of an algebraic language. Then we write down a system of algebraic equations satisfied by the non-commutative generating function of such words. Each equation is equivalent to a certain combinatorial lemma on the objects. Then, by sending all

the non-commutative variables onto a single variable, we get an ordinary algebraic system. This system may be solved. Usually this methodology have been used in order to explain the algebricity of generating functions, once formulæ are known by classical enumerative method (Lagrange inversion formula, ...). A deep example is given in the numerous work of CORI and VAUQUELIN [5], [6] following some work by TUTTE on the enumeration of *planar maps*.

Here the method is reversed in order to get new enumerative formulæ. Such methodology, combined with an intensive use of MACSYMA, has been successively applied in *polyominoes* and *animals* enumerations by DELEST, DULUCQ, GOLYOU-BEAUCHAMPS and VIENNOT [10], [11], [21], [22], [72], [73]. In the case of secondary structures, the coding with words of algebraic languages is very simple. The difficult part is in solving the commutative algebraic system. Some analogues of the Tchebycheff polynomials with on parameter have to be used, together with the combinatorial theory of orthogonal polynomial introduced in VIENNOT [71]. The explicit solution is the following.

The generating function for the number  $a_{n,k}$  of (unlabelled) secondary structures of order  $k$  is given by

$$(23) \quad \sum_{n \geq 0} a_{n,k} t^n = \frac{t^{p(k)}}{(1-t)V_1 \cdots V_k}, \quad \text{with } p(k) = 5 \times 2^{k-1} - 2,$$

and  $V_i$  is the sequence of polynomials defined by the recurrence

$$(24) \quad V_{k+1} = (V_k)^2 - 2t^{p(k)}, \quad V_1 = 1 - 2t - t^3.$$

The problem of enumerating all forests having a given order is simpler and can be solved using the same methodology. The surprise is that we get exactly the generating function (18) enumerating binary trees having a given Strahler number. Thus we have the remarkable fact :

The number of forests of (planar rooted) trees having  $n$  vertices and order  $k$  is the same as the number of binary trees having  $n$  internal vertices and Strahler number  $k$ .

Remark that the binary trees considered in this paper can be viewed as particular cases of planar rooted trees. When applying the definition of order with filaments, one get the Strahler number of the binary tree. But this trivial fact is no help in the previous proposition.

I have proposed a prize of ten bottles of *Domaine des Mates* 1981 (red wine produced by myself at Isle-Saint-Georges near Bordeaux) for a bijective proof of this fact. D. ZEILBERGER [79] get a (recursive) bijection (and get the ten bottles of wine). BENDER and CANFIELD get also a bijection.

Thus we have three parameters having the same distribution : Strahler number,  $\lfloor \log_2(1 + H(w)) \rfloor$  and order, with non-trivial bijections relating them. In fact more can be said. The following double distributions are the same :

— for binary trees  $B$  with  $n$  internal vertices, Strahler number  $St(B)$  and the number left external vertices (i.e. vertices  $\circ$ );

□

for Dyck paths  $\omega$  having length  $2n \lfloor \log_2(1 + H(\omega)) \rfloor$  and number of South-East steps going from an even level to an odd level;

— for forests  $F$  of (planar rooted) trees, Order  $Or(F)$  and number of leaves of the forest.

## 7. Ramification matrix

In relation with some considerations in Computer Graphics (see below Paragraph 8), we have introduced the notion of *ramification matrix* of a binary tree. It appears as a refinement of the Horton Strahler considerations.

Let  $B$  be a binary tree with  $St(B) = k$  and  $x$  be an internal vertex of  $B$ . The *order* of the vertex  $x$  is  $St(B)$  if  $x$  is the root of  $B$ , else is the order of the edge  $\{x, y\}$  where  $y$  is the father of  $x$  ( $x$  is the son of  $y$ ). The *biorder* of the vertex  $x$  is the pair formed by the order of the edges joining  $x$  to its two sons.

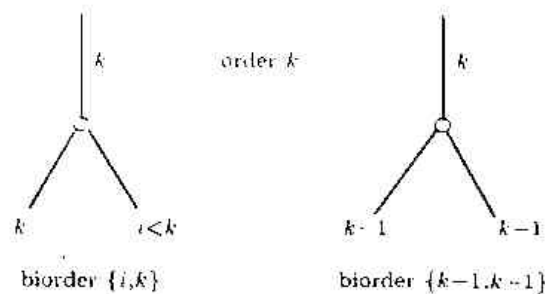


Fig. 13 : Order and biorder of an internal vertex in a binary tree

We define successively the following quantities

- (25)  $a_k$  is the number of internal vertices having order  $k$ ;
- (26)  $\begin{cases} b_{k,i} \text{ is the number of vertices of biorder } (k, i), \text{ for } 0 \leq i < k, \\ b_{k,k} \text{ is the number of vertices of biorder } (k-1, k-1), \text{ for } 1 \leq k; \end{cases}$
- (27)  $p_{k,j} = b_{k,j}/a_k$  for  $0 \leq j \leq k$  and  $1 \leq k$ .

The number  $p_{k,j}$  is the probability for a vertex of order  $k$  to have a biorder  $(k, j)$ .

The *ramification matrix*  $R(B)$  of the binary tree  $B$  is the  $\kappa \times (\kappa+1)$  stochastic matrix

$$(28) \quad R(B) = (p_{k,j})_{0 \leq j \leq k \leq \kappa, 1 \leq k \leq \kappa}.$$

This matrix gives quantitative informations about the "shape" of a binary tree. For example, the ramification matrix of a perfect tree is

$$R = \begin{pmatrix} 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

PENAUD [47] has just proved that the ramification matrix of a random binary tree looks like

$$R = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \frac{1}{16} & \frac{1}{16} \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$

Table 2. Ramification matrix of a large random binary tree.

More precisely, he proves that the mean value of the biorder probability  $p_{k,i}$  among all binary trees with  $n$  internal vertices tends (for fixed  $k$  and  $i$ , as  $n \rightarrow \infty$ ) to the value  $1/2^{i+1}$  (for  $0 \leq i < k$ ) and to  $1/2^k$  for  $i = k$ .

Recently, following the ideas of MANDELBROT [35], many works have been done in Physics about the study of branching patterns occurring in some experiments or in computer simulation. Branching patterns are considered as fractals and the measurement of the "shape" is considered by giving a fractal dimension. Trees coming from real experimentations are digitalized and one considers the number of points of the pattern in concentric circles of radius  $R$ . This number is expected to behave like  $R^D$ , where  $D$  is a fixed exponent called the (fractal) *mass dimension*.

Such measurements have been made for *electric breakdown*, see for example NIEMEYER, PIETRONERO, WIESMANN [43], for the so-called *viscous fingers*, see for example NITTMANN, DACCARD, STANLEY [45], for *electrolytic metal*

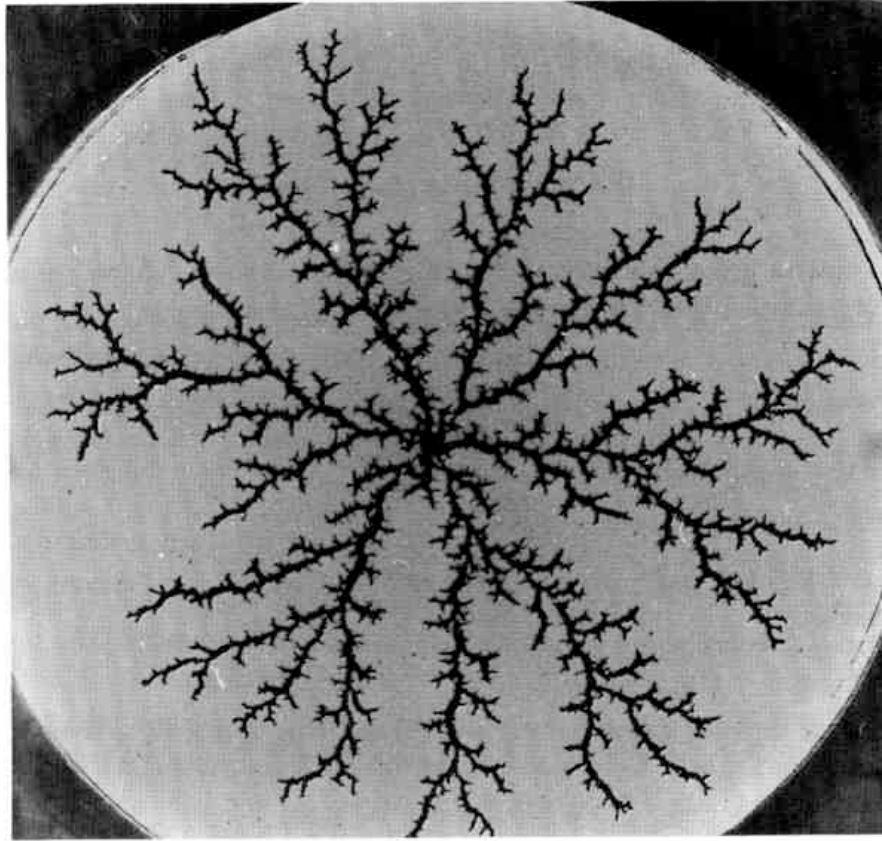


Fig. 14 : Viscous fingers (courtesy from Van Damme and LaRoche, Laboratoire CNRS CRSOCI, Orléans)

*deposit*, see for example SAWADA, DOUGHERTY, GOLLUB [53], or for *Diffusion Aggregation Process* (DLA) of WITTEN and SANDERS [76].

As for river networks, one can associate a binary tree underlying all these branching patterns. The mass fractal dimension give some information about the geometry of this pattern, but this notion can be applied for any pattern, not necessarily branching. It should be of great interest to give a quantitative measurement of the "shape" of such branching pattern which make emphasis of the fact that the pattern is branching. We claim that the ramification matrix should be of interest in such considerations. With VANNIMENUS, we are investing such matrices for branching patterns occuring in Physics [81], [82].



## 8. Synthetic images of trees using Combinatorics

*Je suis sur la montagne, dessinant un vieux sapin de pâturage. Je découvre une loi. "Voyez, dis-je, à mon maître : à la plus vieille branche, on peut reconnaître l'âge de l'arbre" (...). La plus vieille branche, la première à partir du sol, propose une série croissante, probablement incontestable. Et l'arbre entier est une pure fonction mathématique.*

LE CORBUSIER

Very recently, many people have been interested in the creation of faithful synthetic images of trees generated with a computer. A great variety of methods have been considered :  $L$ -langages and "graftals", stochastic models, fractals, botanical models, see AONO, KUNII [1], BLOOMENTAL [2], DEMKO, HODGES, NAYLOR [13], DE REFFY & al. [14], KAWAGUCHI [28], OPPENHEIMER [46], REEVES, BLAU [52], SMITH [64].

With EYROLLES, we have used purely combinatorial methods based on Horton-Strahler ideas and the introduction of ramifications matrices.

We only construct binary trees in 2 dimensions. The "geometry" of the tree is extremely simplified and we do not try to create realistic details as bark, leaves or flowers,... Once a (mathematical) binary tree have been generated, the geometric parameters defining the image are : the width and length of each edges (which is drawn as a rectangle), the branching and deviation angles for each internal vertex of the binary tree (see Figure 15).

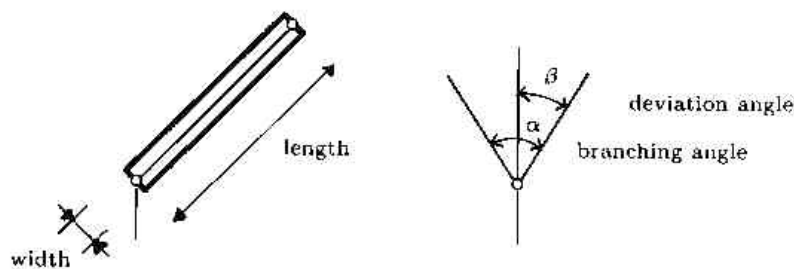


Fig. 15 : Geometric parameters for synthetic 2D trees

The idea is that a branch having a big order in the tree is important, and thus emphasis must be made on this branch by a judicious choice of the geometric parameters. In our program, the width and length of each branches depend only of the order of the corresponding edge of the binary tree. The branching and deviation angles of a branching point depend only of the biorder of the corresponding internal vertex. Usually we have taken simple laws : linear, polynomial or exponential.

The inputs of the program are a number  $k$  (which will be the Strahler number of the tree) and a stochastic matrix having at least  $k$  rows. The program generates at random a binary tree having  $k$  as Strahler number and (approximately) the given matrix for ramification matrix. All the trees which can be generated belong to a same family or species, characterized by the same ramification matrix. Then with a given choice for the geometrical laws ruling the width, length and angles as functions of the order and biorder, the program draws the geometrical tree on the screen. An option can introduced some "regularities" in the tree.

Contrarily to all previous methods, emphasis is made on the choice of the underlying binary tree, and not on the geometry of the tree. With a very simple and poor geometry, a great variety of trees can be obtained. This fact tends to show that the ramification matrix is a pertinent parameter in the tree. Also an advantage of this method is that ramification matrices give an efficient way for controlling the general shape of the tree.

In particular, by taking linear combination of matrices, one can go continuously from one species to another species. One can also mix together two or three ramification matrices, as for example on Figure 16 : the tree behave differently near the main branches (large order) and at the tip of the branches (small order). Such trees can be called non *self-similar*. In fact, the notion of *self-similarity* can be considered for trees, analogously to self-similarity of fractal patterns. A possible characteristic should be that all the rows of the ramification represent the same function. In this sense, random binary trees are self-similar.

A complete system for the generation, drawing and manipulation of synthetic images of realistic trees and leaves of trees has been developped in VIENNOT, EYROLLES, JANEY, ARQUÈS [84]. The pictures are in colour and the system includes the creation of landscapes.

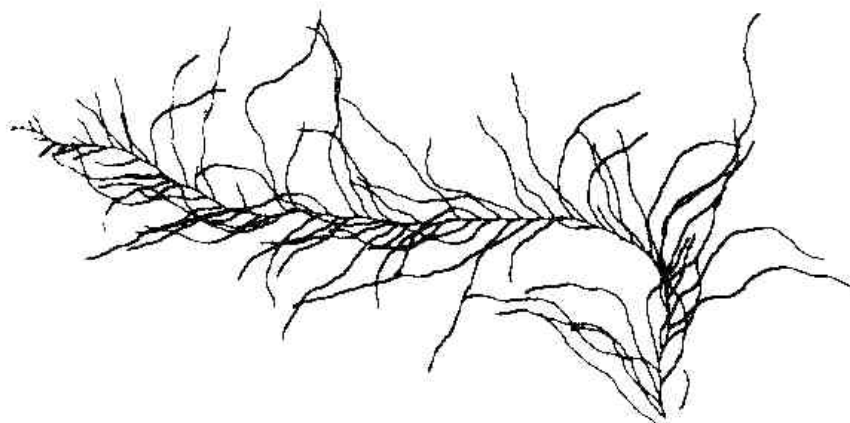


Fig. 16 : Non self-similar tree

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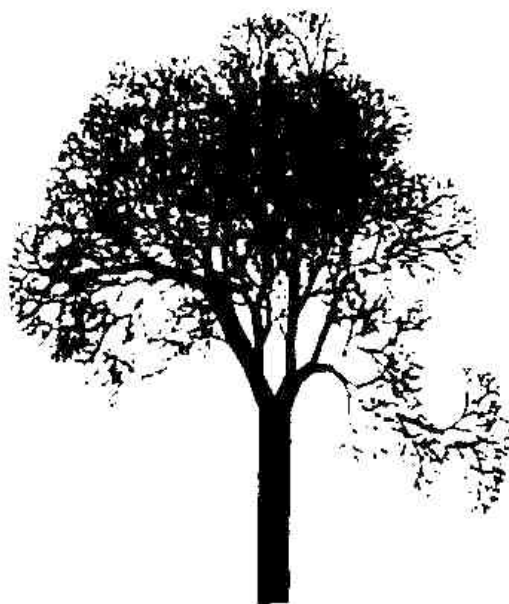
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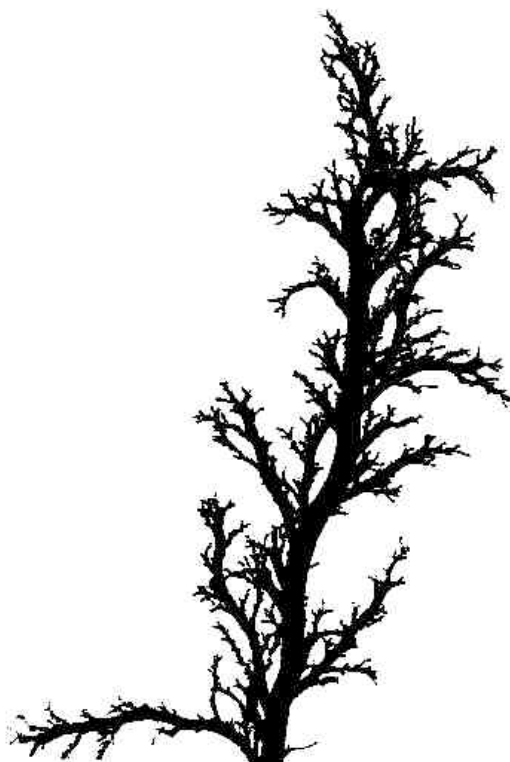
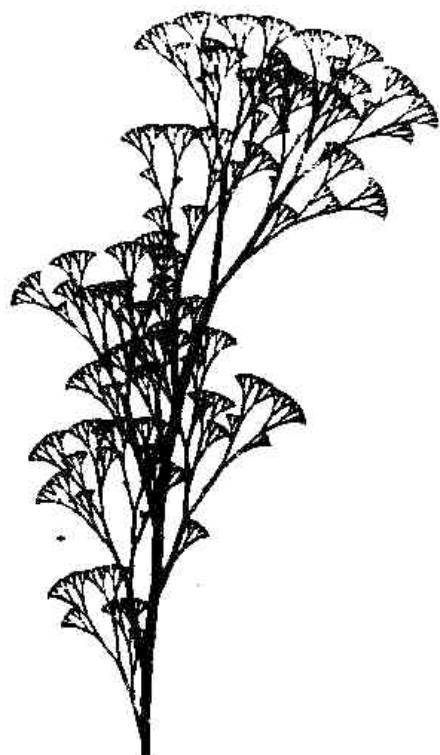


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