The Goulden-Jackson Cluster Method: Extensions, Applications and Implementations $John\ NOONAN^1\ and\ Doron\ ZEILBERGER^1$

Abstract: The powerful (and so far under-utilized) Goulden-Jackson Cluster method for finding the generating function for the number of words avoiding, as factors, the members of a prescribed set of 'dirty words', is tutorialized and extended in various directions. The authors' Maple implementations, contained in several Maple packages available from this paper's website http://www.math.temple.edu/~ zeilberg/gj.html, are described and explained.

Preface

In New York City there is a hotel called ESSEX. Once in a while the bulbs of the first two letters of its neon sign go out, resulting in the wrong message. This motivates the following problem. Given a finite alphabet, and a finite set (lexicon) of 'bad words', find the number of *n*-lettered words in the alphabet that avoid as *factors* (i.e. strings of consecutive letters) any of the dirty words. More generally, count the number of such words with a prescribed number of occurrences of obscenities (the previous case being 0 bad words), and even more generally, count how many words are there with a prescribed number of occurrences of each letter of the alphabet, and a prescribed number of occurrences of each of the bad words.

Many problems in combinatorics, probability, statistics, computer science, engineering, and the natural and social sciences, are special cases of, or can be formulated in terms of, the above scenario. It is a rather well-kept secret that there exists a powerful method, the Goulden-Jackson Cluster method[GoJ1][GoJ2], to tackle it.

In this paper we start with a motivated and accessible account of the method, and then we generalize it in various directions. Most importantly, we describe our Maple implementations of both the original method and of our various extensions. These packages are obtainable, free of charge, from this paper's very own website http://www.math.temple.edu/~zeilberg/gj.html.

The Goulden-Jackson Cluster method is very similar, and in some sense, a generalization of, the method of Guibas and Odlyzko[GuiO], whose main motivation was Penney-ante games. However, philosophically, psychologically, and conceptually, the Goulden-Jackson and Guibas-Odlyzko methods are quite distinct, and we find that the former is more suitable for our purposes.

The Naive Approach

Before describing the Cluster method, let's review the naive approach. First, some notation. Given a word $w = w_1, \ldots, w_n$, a factor (burrowing the term from the theory of formal languages) is any of the $\binom{n+1}{2}$ words $w_i w_{i+1} \ldots w_{j-1} w_j$, for $1 \le i \le j \le n$. For example the factors of JOHN are J, O, H, N, JO, OH, HN, JOH, OHN, JOHN, while the factors of DORON are D, O, R, O, N, DO,

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OR, RO, ON, DOR, ORO, RON, DORO, ORON, DORON. Note that a given word may occur several times as a factor, for example the one-letter word O in DORON, or the two-letter words CA and TI in TITICACA. Also as in formal languages, given an alphabet V, we will denote the set of all possible words in V by V^* .

Consider a finite alphabet V with d letters, and suppose that we want to keep track of all factors of length $\leq R+1$, including individual letters. For every word w, of length $\leq R+1$, introduce a variable x[w]. All the x[w] commute with each other.

Define a weight on words $w = w_1, \dots, w_n$, by:

Weight(w) =
$$\prod_{r=1}^{R+1} \prod_{i=1}^{n-r+1} x[w_i, \dots, w_{i+r-1}]$$
.

For example, if R = 2, then Weight(SEXY) = x[S]x[E]x[X]x[Y]x[SE]x[EX]x[XY]x[SEX]x[EXY]. The weight of a set of words ('language') \mathcal{L} , $Weight(\mathcal{L})$, is defined as the sum of the weights of all the words belonging to that language. Also, given a language \mathcal{L} and a letter v, we will denote by $\mathcal{L}v$ the set of words obtained from \mathcal{L} by appending v at the end of each of the words of \mathcal{L} . Thus if $\mathcal{L} = \{SEX, LOON\}$, and R = 1, then $Weight(\mathcal{L}) = x[S]x[E]x[X]x[SE]x[EX] + x[L]x[O]^2x[N]x[LO]x[OO]x[ON]$, and $\mathcal{L}Y = \{SEXY, LOONY\}$.

The generating function

$$\Phi_R := \sum_{w \in V^*} Weight(w) \quad ,$$

stores all the information about the number of words with a prescribed number of factors of length $\leq R+1$. So, the number of words in V^* that have exactly n_u factors that are u for each $u \in V^*$ of $length(u) \leq R+1$, is the coefficient in Φ_R of the monomial $\prod x[u]^{n_u}$, where the product extends over the set $\{u \in V^*, length(u) \leq R+1\}$.

If we want the generating function for the number of words with a prescribed number of bad words and a prescribed number of letters, we may first compute Φ_R , (where R+1 is the maximum length of a bad word), and then set x[v] = s for each letter $v \in V$, and x[w] = t, if w is a bad word, and x[w] = 1 otherwise. The coefficient of $s^n t^m$ in the resulting generating function would be the number of n-letter words with exactly m instances of bad words occurring as factors. If we want the generating function for words with no occurrences of dirty words as factors, we set t = 0.

How to compute Φ_R ? For each word $v \in V^*$, of length R, let Sof[v] be the subset of V^* of words that ends with v. Write $v = v_1, \ldots, v_R$. Every word in Sof[v] is either v itself or of length > R, in which case chopping the last letter results in an element of Sof[u], for one of the d u's of the form i, v_1, \ldots, v_{R-1} . In symbols

$$Sof[v] = \{v\} \bigcup_{i \in V} Sof[i, v_1, \dots, v_{R-1}] v_R \quad . \tag{SetEq}$$

Since, for any word $w = w_1, \dots, w_n \in V^*$, of length > R,

Weight(
$$w_1, ..., w_n$$
) = Weight($w_1, ..., w_{n-1}$) · $\prod_{r=1}^{R+1} x[w_{n-r+1}, ..., w_n]$,

the system of set equations (SetEq) translates to the linear system of (algebraic) equations

$$Weight(Sof[v]) = Weight(v) + \left(\prod_{r=1}^{R} x[v_{R-r+1}, \dots, v_{R}]\right) \sum_{i \in V} x[i, v_{1}, \dots, v_{R}] Weight(Sof[i, v_{1}, \dots, v_{R-1}]) \quad .$$

$$(Linear_Algebra_Eg)$$

We have a system of d^R linear equations for d^R unknowns $Weight(Sof[w]), w \in V^*, length(w) = R$, that obviously has a unique solution (on combinatorial grounds!). Since the coefficients are polynomials (in fact monomials) in the variables $x[w], w \in V^*, length(w) \leq R+1$, the solutions Weight(Sof[v]) must be rational functions in these variables.

After solving the system, we get Φ_R from

$$\Phi_R = \sum_{w \in V^*, \, length(w) < R} Weight(w) + \sum_{w \in V^*, \, length(w) = R} Weight(Sof[w]) \quad .$$

Since the first sum is a polynomial and the second sum is a finite sum of rational functions, it follows that Φ_R is a rational function. Hence every specialization, as described above, is also a rational function of its variables.

The Maple Implementation of the Naive Approach is contained in the package NAIVE. After downloading it from this paper's webpage to your working directory, go into Maple by typing maple, followed by [Enter]. Once in Maple, load the package by typing read NAIVE;. To get on-line help, type ezra();, for a list of the procedures, and ezra(procedure_name);, for instructions how to use a specific function. The most important function is PhiR that computes Φ_R . The function call is PhiR(Alphabet, R,x), where Alphabet is the set of letters, R is the non-negative integer R, and x is the variable-name for the indexed variables x[w]. For example, PhiR($\{1\},0,z$); should give 1/(1-z[1]).

The other procedures are Naivegf, Naivest, and Naives, that compute, the long way, what the procedures GJgf, GJst and GJs of the package DAVID_IAN, to be described shortly, compute fast. Their main purpose is to check the validity of DAVID_IAN and the other packages described later in this paper. The readers are warned only to use them for curiosity.

The Drawback of the Naive Approach

In order to get the generating function $\sum_{n=0}^{\infty} a(n)s^n$, where a(n) := number of words in $\{A, \ldots, Z\}^*$ of length n with no SEX in it (as a factor), we need to solve a system of 26^2 equations and 26^2 unknowns, then plug in $x[A] = \ldots = x[Z] = s$, $x[AA] = \ldots = x[ZZ] = 1$, $x[AAA] = \ldots = x[ZZZ] = 1$, except for x[SEX] = 0. For some economy, we could have made the substitution at

the equations themselves, before solving them, but we would still have to solve a system of that size.

If we wanted to find the generating function for SEX-less words with an arbitrary size alphabet, then the above method is not even valid in principle. Luckily, we have the powerful *Goulden-Jackson Cluster method*, that can handle such problems very efficiently.

The Most Basic Version of the Goulden-Jackson Cluster Method

Consider a finite alphabet V, and a finite set of bad words, B. It is required to find a(n) := the number of words of length n that do not contain, as factors, any of the members of the set of bad words B. For example if $V = \{E, S, X\}$, and $B = \{SEX, XE\}$, then $a(0) = 1, a(1) = 3, a(2) = 8, a(3) = 20, \ldots$

Of course we may assume that any factor of a bad word of B is not in B, since then the longer word would be superfluous, and can be deleted from the set of banned words. For example it is not necessary to ban both SEX and SEXY, since any word that contains SEXY in it would also contain SEX, and hence the set of words avoiding SEX and SEXY is identical to the set of words avoiding SEX.

As is often the case in combinatorics, we compute the generating function $f(s) = \sum_{n=0}^{\infty} a(n) s^n$ rather than a(n) directly. We know from the Naive section that this is a rational function of s, but this fact will emerge again from the Cluster algorithm, and this time the algorithm is efficient.

The methodology is the venerable Inclusion-Exclusion paradigm that, depending on one's specialty, is sometimes known as *Möbius Inversion* and *Sieve methods*. The essence of the method is to replace the straight counting of a hard-to-count set of 'good guys' by the weighted count of the much larger set of pairs

[arbitrary quy, arbitrary subset of his sins],

where the weight is (-1) to the power of the cardinality of the subset of his sins.

Introducing the weight on words $weight(w) := s^{length(w)}$, f(s), is the weight enumerator of the set of words, $\mathcal{L}(B)$ that avoid the members of B as factors, i.e.

$$f(s) = \sum_{w \in \mathcal{L}(B)} weight(w)$$
.

The trick is to add 0 to both sides and rewrite this as

$$f(s) = \sum_{w \in V^*} weight(w)0^{\lceil number \ of \ factors \ of \ w \ that \ belong \ to \ B \rceil}$$

and then use the following deep facts:

$$0 = 1 + (-1) \quad , \tag{i}$$

$$0^r = \begin{cases} 1, & \text{if } r = 0; \\ 0, & \text{if } r > 0. \end{cases}$$
 (ii)

and for any finite set A,

$$\prod_{a \in A} 0 = \prod_{a \in A} (1 + (-1)) = \sum_{S \subset A} (-1)^{|S|},$$

where as usual, |S| denotes the cardinality of S.

We now have,

$$f(s) = \sum_{w \in V^*} weight(w)0^{\lceil number\ of\ factors\ of\ w\ that\ belong\ to\ B \rceil} =$$

$$\sum_{w \in V^*} weight(w)(1+(-1))^{[number\ of\ factors\ of\ w\ that\ belong\ to\ B\,]} =$$

$$\sum_{w \in V^*} \sum_{S \subset Bad(w)} (-1)^{|S|} s^{length(w)} \quad ,$$

where Bad(w) is the set of factors of w that belong to B. For example if $B = \{SEX, EXE, XES\}$ and w = SEXES, then Bad(w) consists of the factors SEX (occupying the first three letters), EXE, (occupying letters 2,3,4), and XES (occupying the last three letters).

So the desired generating function is also the weight-enumerator of the much larger set consisting of pairs (w, S), where $S \subset Bad(w)$, and now the weight is defined by $weight(w, S) = (-1)^{|S|} s^{length(w)}$. Surprisingly, it is much easier to (weight-)count. We may think of them as 'marked words', where S denotes the subset consisting of those words that the censor, or teacher, was able to detect.

First, we need a convenient data-structure for these weird objects. Any word w, of length n, $w = w_1 \dots w_n$, has $\binom{n+1}{2}$ factors w_i, \dots, w_j , which we will denote by [i,j]. $1 \le i \le j \le n$. Hence any marked word may be represented by $(w; [i_1, j_1], [i_2, j_2], \dots, [i_l, j_l])$, where $w_{i_r} w_{i_r+1} \dots w_{j_r-1} w_{j_r} \in B$, for $r = 1, \dots, l$, and we make it canonical by ordering the j_r , i.e. we arrange the marked factors such that $j_1 < j_2 < \dots < j_l$. Since no bad word is a proper factor of another bad word, we can assume that all the i_r 's are distinct, and that there is no nesting.

For example if $B = \{SEX, EXE, XES\}$, and w = SEXES, then w gives rise to the following 2^3 marked words: (SEXES;), (SEXES; [1,3]), (SEXES; [2,4]), (SEXES; [3,5]), (SEXES; [1,3], [2,4]), (SEXES; [1,3], [3,5]), (SEXES; [2,4], [3,5]), (SEXES; [1,3], [2,4], [3,5]).

For human consumption, it is easier to portray a marked word by a 2-dimensional structure. The top line is the word itself, and then, we list each of the factors that are marked on a separate line, from right to left. For example the marked word (SEXES;), is simply

the marked word (SEXES; [2, 4]), is portrayed as

while the marked word (SEXES; [1,3], [2,4], [3,5]) is written as:

Given a word $w = w_1 \dots w_n$, we will say that two factors [i, j] and [i', j'] with j < j', overlap if they have at least one common letter, i.e. if $i < i' \le j$.

Let \mathcal{M} be the set of these marked words. How to (weight-)count them? Given a non-empty marked word $(w_1 \dots w_n; [i_1, j_1], [i_2, j_2], \dots, [i_l, j_l])$, there are two possibilities regarding the last letter.

Either $j_l < n$, in which case w_n is not part of any detected bad factor, and deleting it results in another, shorter, marked word $(w_1 \dots w_{n-1}; [i_1, j_1], [i_2, j_2], \dots, [i_l, j_l])$. We can always restore this last letter, and there is an obvious bijection between marked words of length n, in which $j_l < n$ and pairs (marked words of length n-1, letter of V).

The other possibility is that $j_l = n$, then we can't simply delete the last letter w_n . Let k be the smallest integer such that $[i_k, j_k]$ overlaps with $[i_{k+1}, j_{k+1}]$, $[i_{k+1}, j_{k+1}]$ overlaps with $[i_{k+2}, j_{k+2}]$, ..., $[i_{l-1}, j_{l-1}]$ overlaps with $[i_l, j_l]$, then removing the last $n - i_k + 1$ letters from w and the last l - k + 1 marked factors, results in a pair of marked words $(w_1 \dots w_{i_k-1}; [i_1, j_1], \dots, [i_{k-1}, j_{k-1}])$ and $(w_{i_k} \dots w_n; [1, j_k - i_k + 1], \dots, [i_l - i_k + 1, j_l - i_k + 1])$. The first of these two marked words could be arbitrary, but the second one has the special property that each of its letters belongs to at least one marked factor, and that neighboring marked factors overlap. Let's call such marked words clusters and denote the set of clusters by C.

For example if $V = \{E, S, X\}$ and $B = \{SEX, ESE, XES\}$, the marked word

which in one-dimensional notation is (SEXESEX; [1, 3], [4, 6], [5, 7]), is not a cluster (since [1, 3] and [4, 6] don't overlap), while

which in one-dimensional notation is written (SEXESEX; [1, 3], [3, 5], [4, 6], [5, 7]), is a cluster.

Hence any member of \mathcal{M} (i.e. marked word) is either empty (weight 1), or ends with a letter that is not part of a cluster, or ends with a cluster. Peeling off the maximal cluster, results in a smaller marked word (by definition of maximality). Hence we have the decomposition:

$$\mathcal{M} = \{empty_word\} \cup \mathcal{M}V \cup \mathcal{M}C \quad .$$

Taking weights we have,

$$weight(\mathcal{M}) = 1 + weight(\mathcal{M})ds + weight(\mathcal{M})weight(\mathcal{C})$$
.

Since $weight(\mathcal{M}) = f(s)$, solving for f(s) yields

$$f(s) = \frac{1}{1 - ds - weight(C)} .$$

It remains to find the weight-enumerator of C, weight(C).

Let's examine how two bad words u and v can be the last two members of a cluster. This happens when a proper suffix (tail) of u coincides with a proper prefix(head) of v.

For any word $w = w_1 \dots w_n$, let HEAD(w) be the set of all proper prefixes:

$$HEAD(w_1 \ldots w_n) := \{ w_1, w_1 w_2, w_1 w_2 w_3, \ldots, w_1 w_2 \ldots w_{n-1} \}$$
,

and let TAIL(w) be the set of all proper suffixes

$$TAIL(w_1 ... w_n) := \{ w_n, w_{n-1} w_n, w_{n-2} w_{n-1} w_n, ..., w_2 ... w_n \}$$
.

Given two words u and v, define the set $OVERLAP(u,v) := TAIL(u) \cap HEAD(v)$.

For example $OVERLAP(PICACA, CACACA) = \{CA, CACA\}.$

If $x \in HEAD(v)$, then we can write v = xx', where x' is the word obtained from v be chopping off its head x. Let's denote x' by v/x. For example SEXYSEX/SEX = YSEX.

Adopting the notation of [GrKP], section 8.4, let's define

$$u: v := \sum_{x \in OVERLAP(u,v)} weight(v/x)$$
 ,

which is a certain polynomial in s. For example

$$SEXSEX : EXSEXS = s + s^4$$
,

corresponding to the following two ways in which SEXSEX can be followed by EXSEXS at the end of a cluster:

giving rise to weight s, since the leftover is the one-letter S, and

giving rise to the term s^4 , since the leftover is the four-letter string SEXS.

Now the set of clusters \mathcal{C} , can be partitioned into

$$\mathcal{C} = \bigcup_{v \in B} \mathcal{C}[v] \quad ,$$

where C[v] $(v \in B)$, is the set of clusters whose last (top) entry is v.

Given a cluster in C[v], it either consists of just v, or else, chopping v results in a smaller cluster that may end with any bad word u for which OVERLAP(u,v) is non-empty. This means that there is a word $x \in OVERLAP(u,v)$ for which u = x''x and v = xx', for some non-empty words x'' and x'. By removing v from the cluster, we lose its tail, x' = v/x, from the underlying word. Conversely, given a cluster in C[u] and one of the elements x, of OVERLAP(u,v), we can reconstitute the bigger cluster in C[v] by adding v to the end of the cluster, and appending the word v/x into the underlying word of the cluster.

For example, if once again, $V = \{E, S, X\}$, and $B = \{SEX, ESE, XES\}$, then the cluster

belongs to C[SEX]. Chopping the top SEX, results in the smaller cluster

that belongs to C[ESE], and so in this example x = SE, and x' = SEX/SE = X.

We have just established a bijection

$$\mathcal{C}[v] \leftrightarrow \{(v, [1, length(v)])\} \bigcup_{u \in B} \mathcal{C}[u] \times OVERLAP(u, v) \quad , \qquad (Set_Equations)$$

where if $C \in C[v]$ has more than one bad word, and is mapped by the above bijection to (C', x), then weight(C) = (-1)weight(C')weight(v/x).

Taking weights, we have

$$weight(\mathcal{C}[v]) = (-1)weight(v) - \sum_{u \in B} (u:v) \cdot weight(\mathcal{C}[u]) \quad . \tag{Linear_Equations}$$

This is a system of |B| linear equations in the |B| unknowns weight(C[v]). Furthermore, it is usually rather sparse, since for most pair of bad words u and v, OVERLAP(u, v) is empty. In fact, let's

denote by Comp(v) the set of bad words $u \in B$ for which OVERLAP(u, v) is non-empty, then the above system can be rewritten:

$$weight(\mathcal{C}[v]) = -weight(v) - \sum_{u \in Comp(v)} (u:v) \cdot weight(\mathcal{C}[u]) \quad . \tag{Linear_Equations'}$$

Note that in general |B| is much smaller than d^R (where d is the number of letters in your alphabet V, and R+1 is the maximal length of a bad word in B), the number of equations in the system of linear equations required by the naive approach described at the beginning. So the Goulden-Jackson method is much more efficient, in general.

After solving ($Linear_Equations'$), we get weight(C), by using

$$weight(\mathcal{C}) = \sum_{v \in B} weight(\mathcal{C}[v])$$
 ,

which we plug into

$$f(s) = \frac{1}{1 - ds - weight(C)} .$$

Example: Find the generating function of all words in $\{A, B, C, \dots, X, Y, Z\}$ that avoid the dirty words PIPI and CACA.

Answer: d = 26, and the system is

(i)
$$weight(C[PIPI]) = -s^4 - s^2 weight(C[PIPI])$$

(ii)
$$weight(C[CACA]) = -s^4 - s^2 weight(C[CACA])$$

from which

$$weight(\mathcal{C}[PIPI]) = weight(\mathcal{C}[CACA]) = -s^4/(1+s^2) \quad ,$$

and hence $weight(\mathcal{C}) = -2s^4/(1+s^2)$, and hence

$$f(s) = \frac{1}{1 - 26s + 2s^4/(1 + s^2)} = \frac{1 + s^2}{1 - 26s + s^2 - 26s^3 + 2s^4}$$

Another Example: Find the generating function of all words in $\{A, B, C, \dots, X, Y, Z\}$ that avoid the dirty words PIPI, CACA, PICA and CAPI.

Answer: d = 26, and the system is

$$(i)\ weight(\mathcal{C}[PIPI]) = -s^4 - s^2 weight(\mathcal{C}[PIPI]) - s^2 weight(\mathcal{C}[CAPI])$$

(ii)
$$weight(C[CACA]) = -s^4 - s^2 weight(C[CACA]) - s^2 weight(C[PICA])$$

$$(iii)\ weight(\mathcal{C}[PICA]) = -s^4 - s^2 weight(\mathcal{C}[PIPI]) - s^2 weight(\mathcal{C}[CAPI])$$

$$(iv)\ weight(\mathcal{C}[CAPI]) = -s^4 - s^2 weight(\mathcal{C}[CACA]) - s^2 weight(\mathcal{C}[PICA])$$

from which

$$f(s) = \frac{1 + 2s^2}{1 - 26s + 2s^2 - 52s^3 + 4s^4} \quad .$$

Maple Implementation

A Maple implementation of this is contained in the package DAVID_IAN, downloadable from this paper's website http://www.math.temple.edu/~zeilberg/gj.html.

The function call is $GJs(Alphabet,Set_of_bad_words,s)$. For example, to get the generating function $f(x) = \sum_{n=0}^{\infty} a(n)x^n$, where a(n) is the number of ways of spinning a dreidel n times, without having a run of length 4 of any of Gimel, Heh, Nun, or Shin, do $GJs(\{G,H,N,S\},\{[G,G,G,G],[H,H,H,H],[N,N,N,N],[S,S,S,S]\},x)$;

Penney-Ante

The system of equations (Linear_Equations') is identical to the one occurring in so-called Penney-Ante games, in which each player picks a word, and a coin (or die), with as many faces as letters, is tossed (or rolled) until a string matching that of one of the players is encountered, in which case, she won. Since the special case of two players and two letters is so beautifully described in [GrKP], section 8.4, and the general case is just as beautifully described in Guibas and Odlyzko's paper [GuiO], we will only mention here how to use our Maple implementation. The function call, in the package DAVID_IAN, is Penney(List_of_letters,List_of_words,Probs). The output is the list of probabilities of winning corresponding to the list of words List_of_words. Prob is the way the die is loaded, i.e. the probabilities of the respective letters in the list List_of_letters.

For example, to treat the original example in Walter Penney's paper [P] (see also [GrKP], p. 394), in which Alice and Bob flip a coin until either HHT or HTT occurs, and Alice wins in the former case while Bob wins in the later case, do (in DAVID_IAN), Penney([H,T],[[H,H,T],[H,T,T]],[1/2,1/2]);, getting the output: [2/3,1/3]. If the probability of a Head is p, then do Penney([H,T],[[H,H,T],[H,T,T]],[p,1-p]);, getting $[p/(p^2-p+1),(1-p)^2/(p^2-p+1)]$.

In order to check the validity of Penney, we have also written a procedure PenneyGames that simulates many Penney-Ante games, and gives the scores of each player. The function call is PenneyGames(List_of_letters,List_of_words,Probs,K), where K is the number of individual games. Thus typing PenneyGames([H,T],[[H,H,T],[H,T,T]],[1/2,1/2],300); should give something close to [200,100], but the exact outcome changes, of course, for each new batch of 300 games, according to the whims of Lady Luck.

Be sure to try also BestLastPlay, which will tell you the best counter-move.

Keeping Track of the Number of Bad Words

Almost nobody is perfect. It is extremely unlikely that a long word would contain no bad factors. A more general question is to find the number of words $a_m(n)$ in the alphabet V with exactly m occurrences of factors that belong to B. Let's define the generating function

$$F(s,t) := \sum_{n=0}^{\infty} \sum_{m=0}^{n} a_m(n) s^n t^m$$
.

F(s,t) generalizes f(s) since, obviously, f(s) = F(s,0).

The above analysis goes almost verbatim. Now we have:

$$F(s,t) = \sum_{w \in V^*} weight(w)t^{[number\ of\ factors\ of\ w\ that\ belong\ to\ B]}$$

and then use the following deep facts:

$$t = 1 + (t - 1) \quad ,$$

and for any finite set A,

$$\prod_{a \in A} t = \prod_{a \in A} (1 + (t - 1)) = \sum_{S \subset A} (t - 1)^{|S|},$$

where as usual, |S| denotes the cardinality of S.

We now have,

$$\begin{split} f(s) &= \sum_{w \in V^*} weight(w) t^{\lceil number\ of\ factors\ of\ w\ that\ belong\ to\ B \rceil} \\ &= \sum_{w \in V^*} weight(w) (1 + (t-1))^{\lceil number\ of\ factors\ of\ w\ that\ belong\ to\ B \rceil} \\ &= \sum_{w \in V^*} \sum_{S \subset Bad(w)} (t-1)^{|S|} s^{length(w)} \quad , \end{split}$$

where Bad(w) is the set of factors of w that belong to B.

The set of linear equations (Linear_Equations') now becomes:

$$weight(\mathcal{C}[v]) = (t-1)weight(v) + (t-1)\sum_{u \in Comp(v)} (u:v) \cdot weight(\mathcal{C}[u]) \quad , \ (Linear_Equations'')$$

and the rest stays the same.

Maple Implementation: In the package DAVID_IAN, the function that finds F(s,t) is GJst. For example let a(n,m) be the number of ways of arranging n children in a line in such a way that exactly m boys are isolated (surrounded by girls on both sides, see [CoGuy], p. 205). To find the generating function $F(s,t) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} a(n,m) s^n t^m$ do GJst({B,G},{[G,B,G]},s,t);

Keeping Track of the Individual Counts of Each Obscenity

Suppose we want to know how many words of length n has m_1 occurrences of b_1 , m_2 occurrences of b_2 , ..., m_f occurrences of b_f , where the set of bad words is $B = \{b_1, b_2, \dots b_f\}$, we need to keep track of the individuality of each bad word. Introducing the variable t[b] for each bad word $b \in B$, we now require

$$F(s; t[b_1], \ldots, t[b_f]) = \sum_{w \in V^*} weight(w) \prod_{b \text{ is a bad factor of } w} t[b]$$
,

and then use the following:

$$t[b] = 1 + (t[b] - 1) \quad ,$$

and for any finite set A,

$$\prod_{a \in A} t[a] = \prod_{a \in A} (1 + (t[a] - 1)) = \sum_{S \subset A} \prod_{a \in S} (t[a] - 1) \quad .$$

We now have,

$$\begin{split} F(s\,;\,t[1]\,,\,\ldots\,,\,t[f]\,) &= \sum_{w\in V^*} weight(w) \prod_{b\ is\ a\ bad\ factor} t[b] \\ &= \sum_{w\in V^*} \sum_{S\subset Bad(w)} \left(\prod_{b\in S} (t[b]-1)\right) s^{length(w)} \quad, \end{split}$$

where Bad(w) is the set of factors of w that belong to B.

The set of linear equations (Linear_Equations") now becomes:

$$weight(\mathcal{C}[v]) = (t[v] - 1) \cdot weight(v) + (t[v] - 1) \cdot \sum_{u \in Comp(v)} (u : v) \cdot weight(\mathcal{C}[u]) \quad ,$$

$$(Linear_Equations''')$$

and the rest stays the same.

Maple Implementation: In the package DAVID_IAN, the function that finds $F(s;t[b_1],\ldots,t[b_f])$ is GJstDetail. For example, to number of ways of arranging n kids in line such that there are a isolated boys and b isolated girls is the coefficient of $s^n t[G,B,G]^a t[B,G,B]^b$ in the Maclaurin expansion of the rational function GJstDetail({B,G},{[G,B,G], [B,G,B]},s,t);

Keeping Track of the Letters as well

If you want to know the above information, but also wish to know the individual count of the letters, do exactly as above, with the only difference that weight(w) is no longer simply $s^{length(w)}$, but rather (if $w = w_1 \dots w_n$):

$$weight(w) := \prod_{i=1}^{n} x[w_i]$$
 .

(For example $weight(ESSEX) = x[E]^2x[S]^2x[X]$). The function calls are GJgf and GJgfDetail. We refer the reader to the on-line documentation in the package DAVID_IAN for instructions.

Generalizing to the Case of an Arbitrary Set of Bad Words

What happens if we remove the condition, on the set of bad words B, that no bad word can be a proper factor of another bad word? As we saw above, if all we want is the generating function for the number of n-letter words that avoid (as factors) the members of B, then we can easily remove all members of B that have another member of B as a factor, until we get a set of banned words

B', that meets the above condition, and that gives the same enumeration. So, as far as applying GJs in DAVID_IAN, i.e. finding the generating function f(s), we don't need to generalize.

But if we are interested in the more general F(s,t), i.e. in GJst, then the original Cluster method fails. We will now describe how to modify it.

Everything goes as before, but now the clusters look different. Given a marked word $(w_1 \ldots w_n; [i_1, j_1], [i_2, j_2], \ldots, [i_l, j_l])$, we may no longer assume that $j_1 < j_2 < \ldots < j_l$, only that $j_1 \le j_2 \le \ldots \le j_l$, and now we may have nesting: i.e.: it is possible to have: $i_r < i_s < j_s < j_r$, for some s < r. Since the second component of a marked word $(w_1 \ldots w_n; [i_1, j_1], [i_2, j_2], \ldots, [i_l, j_l])$ is a set, we may arrange the $[i_r, j_r]$ in such a way that $j_r \le j_{r+1}$ for $r = 1, \ldots, l-1$, and if $j_r = j_{r+1}$, then $i_r < i_{r+1}$. For example if $B = \{AC, CA, CACA, ICAC, TICA, TIT, TI\}$ then the following marked word is a cluster:

In one-dimensional notation it is written: (TITICACA; [1, 2], [1, 3], [3, 6], [4, 7], [6, 7], [5, 8], [7, 8]).

In the original case, it was easy to enumerate clusters, since removing the rightmost (i.e. top) bad word resulted in a smaller cluster. This is no longer true. We are hence forced to introduce the larger set of *committed clusters*.

The above marked word is a member of C[CA]. Chopping the rightmost bad factor, CA, is still a cluster:

which belongs to C[CACA], but note that the underlying word has not changed, so the weight stays the same, except for a factor of (t-1). If we chop the rightmost factor again, which is now CACA, we get the following cluster

which belongs to C[AC], BUT, unlike the previous scenario, in which ANY cluster in C[AC] could have been gotten, now we MUST have the 3^{rd} letter from the end be a C.

Such a situation occurs whenever we have $u, v \in B$ such that v = xuy, where both x and y are non-empty words in the alphabet V. For each such pair, we introduce the set $\mathcal{C}'[x, u]$, which is the set of clusters whose rightmost bad word is u, and the underlying word ends with xu. Now we have many more unknowns and many more equations, we set them up in an analogous way. But at the end, after solving the system, when we compute $weight(\mathcal{C})$, we only sum $weight(\mathcal{C}[v])$, and ignore all the $weight(\mathcal{C}'[u,x])$. Note that $weight(\mathcal{C}'[u,x])$ play the roles of catalysts, that enable the chemical reaction, but at the end are discarded.

We leave it to the readers to fill in the details. The readers may get a clue from examining the Maple implementation JODO, that does the job, and which we will now describe.

JODO: The Maple implementation of the Generalized Cluster Method

The main routine is GJNZst that computes the generating function F(s,t). For example to find the number of 10-letter words in the alphabet, $\{P,I\}$ containing exactly 13 factors that are either PI, or PIPI, take the coefficient of $s^{10}t^{13}$ in the Taylor expansion of GJNZst($\{I,P\},\{[P,I],[P,I]\},s,t$);.

An Interesting Application of JODO to Counting Runs

A run in a word, is a string of a repeated letter. Given a set of bad words B, it is of interest to know how many words are there avoiding B as factors and having a specified number of maximal runs. It is also of interest to know the average number of maximal runs. It can be shown that for any finite set of bad words B, the average number of runs in an n-letter word avoiding the words of B as factors is asymptotically C(B)n, where C(B) is a certain algebraic number that depends, of course, on B.

Note that a new maximal run starts whenever we have an occurrence of any two-letter word ab, with $a \neq b$. So all we have to do is append to B these words, giving them the variable t, and then use a variant of GJNZ to find the generating function. The relevant functions are Runs and AvRuns. The implementation details may be found in the package.

Generalizing to Non-Consecutive Bad Words

So far, we wanted to avoid factors, i.e. the occurrence of a bad word occurring as consecutive letters. Suppose we want to avoid SEX but also the possibility that SEX would appear when the letters are separated by one place, i.e., in addition to SEX, we don't want factors of the form S?E?X, or S?EX, or SE?X, where a question-mark could stand for any character. Hence SHEXY would be censored as would ASELX, but ASHOEOOX would be allowed. In other words, we want to include as our set of bad words, words including a blank, where, for example, [T, BL, T], means that whenever two T's are separated by exactly one letter, we count it as a bad word. The analysis goes almost verbatim, and the details can be found by examining the source code of the Maple package

BLANKS, that is yet another Maple package that accompanies this paper.

The Maple Package BLANKS

The principal routines are BLANKSst and BLANKSs0. The function calls are BLANKSst(alphabet, BL, MISTAKES) and BLANKSs0(alphabet, BL, MISTAKES), where alphabet is the set of letters, BL is the symbol denoting the blank, and MISTAKES is the set of bad words, that are lists in the alphabet $V \cup \{BL\}$.

For example, to find the generating function

$$F(s,t) := \sum_{n} \sum_{m} a(n,m) s^{n} t^{m} \quad ,$$

for a(n, m), the number of 0-1 sequences of length $n, w = w_1, \ldots, w_n$, that have exactly m occurrences of either $w_i = w_{i+1} = w_{i+2}$ or $w_i = w_{i+2} = w_{i+4}$ or $w_i = w_{i+3} = w_{i+6}$, type, in BLANKS, BLANKSst({0,1},B,{[0,0,0], [1,1,1], [0,B,0,B,0], [1,B,1,B,1], [0,B,B,0,B,B,0], [1,B,B,1,B,B,1]}).

If you want F(s,0), the generating function for a(n) := the number of 0-1 sequences of length n with none of the above (i.e. the number of ways of 2-coloring the integers $\{1,2,\ldots,n\}$ such that you don't have a mono-chromatic arithmetic sequence of length 3 and difference ≤ 3 , then type: BLANKSsO($\{1,2\}$,B, $\{[0,0,0]$, [1,1,1], [0,B,0,B,0], [1,B,1,B,1], [0,B,B,0,B,B,0], [1,B,B,1,B,B,1] $\}$).

Exploiting Symmetry

Often the set of bad words is invariant either under the action of the symmetric group (in case when the alphabet is, say, $\{1, 2, ..., n\}$), or under the action of the group of signed permutations, (when the alphabet is, $\{-1, 1, -2, 2, ..., -n, n\}$). Then by symmetry, the Cluster generating functions $weight(\mathcal{C}[w])$ only depend on the equivalence class of w, and there are many fewer equations, and many fewer unknowns. The two Maple packages SYMGJ and SPGJ implement these two cases respectively. We refer the readers to the on-line documentation for details.

Series Expansions

Many times the set of equations is too big for Maple to solve exactly. Nevertheless, using the set of equations (*Linear_Equations'*) or its analogs, we can iteratively get series expansions for the Cluster generating function, and hence for the generating function itself, to any desired number of terms. The procedure GJseries in DAVID_IAN handles this. The package GJseries is a more efficient implementation of these ideas.

Applications

The applications to Self-Avoiding Walks (see [MS] for a very readable introduction to this subject) is described in [N]. The package GJSAW, that also comes with this paper, is a targeted implementation.

Another application is to the computation of the number of ternary square-free words (e.g. [B],[Cu]), which are sequences in the alphabet $\{1,2,3\}$ that do not contain a 'square' i.e. a factor of the form uu where u is a word of any length. As such, the set of bad words, B, is infinite, and the present theory would have to be extended. However, we can find upper bounds and exact series expansions, by limiting the length of u. In particular, taking the set of bad words to be uu, where u is of length ≤ 23 , the first 48 terms of the sequence a(n) := number of n-letter words in the alphabet $\{1,2,3\}$ that avoid uu with length(u) ≤ 22 coincides with the first 46 terms of the real thing (i.e. a(0) through a(45)), and using GJsqfree (which is a Maple package targeted to deal with square-free words), we were able to extend sequence M2550 of [SP], to 46 terms:

M2250 1, 3, 6, 12, 18, 30, 42, 60, 78, 108, 144, 204, 264, 342, 456, 618, 798, 1044, 1392, 1830, 2388, 3180, 4146, 5418, 7032, 9198, 11892, 15486, 20220, 26424, 34422, 44862, 58446, 76122, 99276, 129516, 168546, 219516, 285750, 372204, 484446, 630666, 821154, 1069512, 1392270, 1812876, 2359710, 3072486.

It is well known and easy to see (e.g. [MS], p. 9) that the obvious inequality $a(n+m) \le a(n)a(m)$ implies that $\mu := \lim_{n \to \infty} a(n)^{1/n}$ exists.

Using Zinn-Justin's method, described in [Gut], we were able to estimate that $\mu \approx 1.302$, and that if, as is reasonable to conjecture, $a(n) \sim \mu^n n^{\theta}$, then $\theta \approx 0$.

Hence we have ample evidence to the following:

Conjecture: The number of *n*-letter square-free ternary words is given, asymptotically by $a(n) \sim C\mu^n$, where $\mu := \lim_{n \to \infty} a(n)^{1/n}$.

In [B] it is shown that $2^{1/24} \approx 1.03 < \mu$, and the upper bound $\mu \leq 1.316$ is stated. Using the series expansion for 'finite-memory' (memory 23) square-free words, as above, we found the sharper upper bound $\mu \leq 1.30201064$.

The Maple package GJsqfree

The Maple package GJsqfree, that is also available from this paper's website, is a targeted implementation to the case of counting square-free words. The main procedure is Series, that gives the first NUTERMS + 1 terms of the sequence enumerating the number of words in an alphabet of DIM letters that avoid factors of the form uu, where the length of u is $\leq MEMO$. In particular, the first 2(MEMO+1) terms of this sequence coincide with those of the sequence of square-free words. The function call is: Series(MEMO,DIM,NUTERMS); . For example to get the sequence above, we entered Series(23,3,47);

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