## Accurate computation of the variance of the number of missing words in a random string

## Paul Leopardi

Thanks: Jörg Arndt, Richard Brent, Sylvain Forêt, Judy-anne Osborn.
Mathematical Sciences Institute, Australian National University.
For presentation at 4th International Conference on Combinatorial Mathematics and Combinatorial Computing, Auckland New Zealand, December 2008.

## Topics

- Overlapping serial tests
- Analysis of the problem: missing words in a string
- Word overlap correlations
- Enumeration of correlations (and generating functions)
- Open problems


## Overlapping serial tests (1993)

Overlapping serial tests (Marsaglia and Zaman, 1993) use an alphabet of size $\boldsymbol{\alpha}$, form a pseudorandom string of length $\boldsymbol{N}=\mathbf{2}^{\mathbf{2 1}}$, and examine the overlapping words of length $\boldsymbol{T}$.

Number of missing words should be approximately normal with mean $\mu$ and variance $\sigma^{2}$ :

| Test | $\boldsymbol{\alpha}$ | $\boldsymbol{T}$ | $\boldsymbol{\mu}$ | $\boldsymbol{\sigma}$ |
| :--- | ---: | ---: | :--- | :--- |
| OPSO: | $\mathbf{1 0 2 4}$ | $\mathbf{2}$ | $\mathbf{1 4 1 9 0 9 . 4 6 5 3}$ | $\mathbf{2 9 0 . 2 7}$ |
| OQSO: | $\mathbf{3 2}$ | $\mathbf{4}$ | $\mathbf{1 4 1 9 0 9 . 4 7 3 7}$ | $\mathbf{2 9 0}$ |
| DNA: | $\mathbf{4}$ | $\mathbf{1 0}$ | $\mathbf{1 4 1 9 1 0 . 5 3 7 8}$ | $\mathbf{2 9 0}$ |

## Overlapping serial tests (1995)

(Marsaglia, 1995) has the revised values:

| Test | $\boldsymbol{\alpha}$ | $\boldsymbol{T}$ | $\boldsymbol{\mu}$ | $\boldsymbol{\sigma}$ | $(\boldsymbol{\sigma}$ was $)$ |
| :--- | ---: | ---: | :--- | :--- | :--- |
| OPSO: | $\mathbf{1 0 2 4}$ | $\mathbf{2}$ | $\mathbf{1 4 1 9 0 9 . 6 0}$ | 290.46 | 290.27 |
| OQSO: | $\mathbf{3 2}$ | $\mathbf{4}$ | $\mathbf{1 4 1 9 0 9 . 4 7 3 7}$ | 295 | 290 |
| DNA: | $\mathbf{4}$ | $\mathbf{1 0}$ | $\mathbf{1 4 1 9 1 0 . 5 3 7 8}$ | 339 | 290 |

OQSO: "I don't know, and doubt that I ever will know, the true variance. There are just too many kinds of pairs of 4-letter words to undertake finding all the necessary generating functions."

DNA: "It appears a formidable task to find the exact variance for the DNA test."

## Overlapping serial tests (2008)

Values calculated using (Noonan, Zeilberger, 1999), (Rivals, Rahmann, 2003) and (Rahmann, Rivals, 2003):

| Test | $\boldsymbol{\alpha}$ | $\boldsymbol{T}$ | $\boldsymbol{\mu}$ | $\boldsymbol{\sigma}$ |
| :--- | ---: | ---: | :--- | :--- |
| OPSO: | $\mathbf{2}^{\mathbf{1 0}}$ | $\mathbf{2}$ | $\mathbf{1 4 1 9 0 9 . 3 2 9 9 5 5 0 0 6 9}$ | $\mathbf{2 9 0 . 4 6 2 2 6 3 4 0 3 8}$ |
| OQSO: | $\mathbf{3 2}$ | $\mathbf{4}$ | $\mathbf{1 4 1 9 0 9 . 6 0 0 5 3 2 1 3 1 6}$ | $\mathbf{2 9 4 . 6 5 5 8 7 2 3 6 5 8}$ |
| DNA: | $\mathbf{4}$ | $\mathbf{1 0}$ | $\mathbf{1 4 1 9 1 0 . 4 0 2 6 0 4 7 6 2 9}$ | $\mathbf{3 3 7 . 2 9 0 1 5 0 6 9 0 4}$ |

- Calculation of $\sigma$ for OPSO uses 6 generating functions;
- OQSO uses 55 ; DNA uses 4592.


## Strings, words, indicator variable

We analyze the problem: find the distribution of the number of missing words in a random string.

Alphabet size is $\alpha$, equally likely.
String length is $N$. Word length is $T$.

Words overlap. The string $S$ contains $N-T+1$ words.
There are $\boldsymbol{\alpha}^{\boldsymbol{N}}$ possible strings $\boldsymbol{S}_{\boldsymbol{i}}, \boldsymbol{\alpha}^{\boldsymbol{T}}$ possible words $\boldsymbol{W}_{\boldsymbol{j}}$.
Define indicator $\boldsymbol{v}_{i, j}:=1 \Leftrightarrow$ word $\boldsymbol{W}_{\boldsymbol{j}}$ is missing from string $\boldsymbol{S}_{\boldsymbol{i}}$.

## Number of missing words $X$

The number of words missing from string $\boldsymbol{S}_{\boldsymbol{i}}$ is

$$
X_{i}:=\sum_{j} v_{i, j}
$$

$\boldsymbol{X}$ is the number of words missing from a random string $S$.
For constant $\boldsymbol{\lambda}:=\boldsymbol{N} / \boldsymbol{\alpha}^{\boldsymbol{T}}$ as $\boldsymbol{N} \rightarrow \infty$, $\boldsymbol{X}$ is asymptotically normal. (Rukhin 2002)

## Pair absence probability, generating functions

The probability that both words $\boldsymbol{W}_{\boldsymbol{j}}$ and $\boldsymbol{W}_{\boldsymbol{k}}$ are missing from a random string $S$ is

$$
a_{j, k}:=\alpha^{-N} \sum_{i} v_{i, j} v_{i, k}
$$

Generating functions:

$$
\begin{gathered}
A_{j, k}:\left[z^{N}\right] A_{j, k}(z)=a_{j, k} \\
A_{j}:\left[z^{N}\right] A_{j}(z)=a_{j, j}
\end{gathered}
$$

## Expected value, variance

The expected value of $\boldsymbol{X}$ is

$$
\begin{aligned}
\mathrm{E}[X] & =\alpha^{-N} \sum_{i} X_{i}=\alpha^{-N} \sum_{i} \sum_{j} v_{i, j} \\
& =\sum_{j} a_{j, j}
\end{aligned}
$$

The variance is $\operatorname{var}[\boldsymbol{X}]=\mathbf{E}\left[\boldsymbol{X}^{2}-\boldsymbol{X}\right]-\mathbf{E}[\boldsymbol{X}]-\mathbf{E}[\boldsymbol{X}]^{2}$, with

$$
\begin{aligned}
\mathrm{E}\left[X^{2}-X\right] & =\alpha^{-N} \sum_{i} \sum_{j \neq k} v_{i, j} v_{i, k} \\
& =\sum_{j \neq k} a_{j, k}
\end{aligned}
$$

## Word overlap correlation vectors

Words $\boldsymbol{B}, \boldsymbol{C}$ of length $\boldsymbol{T}, \boldsymbol{B}_{\mathbf{0}} \ldots \boldsymbol{B}_{\boldsymbol{T}-1}$ etc.
(Word overlap) correlation vector $B C$ :

$$
B C_{s}=1 \Leftrightarrow B_{r+s}=C_{r}, r=0 \ldots T-S-1
$$

$B$ :

| D | A | N | G | E | R |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  |  |
| A | N | G | E | R | S |
|  |  |  |  |  |  |
|  |  | A | N | G | E |
| R | S |  |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |

$B C: \begin{array}{lllllll} & 0 & 1 & 0 & 0 & 0 & 0\end{array}$

Correlation vectors $B B, C C$ are called autocorrelations.
(Guibas and Odlyzko 1981; Rivals and Rahmann 2003)

## Correlation polynomials

For correlation vector $\boldsymbol{v}$, the correlation polynomial $\boldsymbol{P}_{\boldsymbol{v}}$ is

$$
P_{v}(z):=v_{0}+v_{1} z+\ldots+v_{T-1} z^{T-1}
$$

For $\boldsymbol{P}_{\boldsymbol{j}}:=\boldsymbol{P}_{\boldsymbol{W}_{\boldsymbol{j}} \boldsymbol{W}_{\boldsymbol{j}}}$, the generating function $\boldsymbol{A}_{\boldsymbol{j}}$ is

$$
A_{j}(z)=\frac{P_{j}(z / \alpha)}{(z / \alpha)^{T}+(1-z) P_{j}(z / \alpha)}
$$

(Guibas and Odlyzko 1981; Rahmann and Rivals 2003, Lemma 2.1)

## Correlation matrices and correlation classes

For $\boldsymbol{P}_{\boldsymbol{j}, \boldsymbol{k}}:=\boldsymbol{P}_{\boldsymbol{W}_{\boldsymbol{j}}, \boldsymbol{W}_{\boldsymbol{k}}}$ etc. the correlation matrix is

$$
M_{j, k}(z):=\left[\begin{array}{ll}
P_{j, j}(z) & P_{j, k}(z) \\
P_{k, j}(z) & P_{k, k}(z)
\end{array}\right]
$$

Given $M:=\left[\begin{array}{ll}m_{11} & m_{12} \\ m_{21} & m_{22}\end{array}\right] \quad$ define $M^{V}:=\left[\begin{array}{ll}m_{22} & m_{21} \\ m_{12} & m_{11}\end{array}\right]$,

$$
R(M):=m_{11}+m_{22}-m_{12}-m_{21} .
$$

Define the equivalence class $[M]:=\left\{M, M^{T}, M^{V}, M^{T V}\right\}$, so

$$
\left[M_{j, k}(z)=M_{j, k}(z), M_{j, k}^{T}(z), M_{k, j}(z), M_{k, j}^{T}(z)\right\}
$$

Note $M^{\prime} \in[M] \Rightarrow \operatorname{det} M^{\prime}=\operatorname{det} M$ and $R\left(M^{\prime}\right)=\boldsymbol{R}(M)$.
(Rahmann and Rivals 2003, Lemma 3.2)

## Generating function for pairs of words

For $Q_{j, k}(z):=\operatorname{det} M_{j, k}(z), \quad R_{j, k}(z):=R\left(M_{j, k}(z)\right)$, the generating function $\boldsymbol{A}_{\boldsymbol{j}, \boldsymbol{k}}$ for the pair $\boldsymbol{W}_{\boldsymbol{j}}, \boldsymbol{W}_{\boldsymbol{k}}$ is given by

$$
A_{j, k}(z)=\frac{Q_{j, k}(z / \alpha)}{(1-z) Q_{j, k}(z / \alpha)+(z / \alpha)^{T} R_{j, k}(z / \alpha)}
$$

(Rahmann and Rivals 2003, Lemma 3.2)
Also (Goulden and Jackson 1979, 1983; Guibas and Odlyzko 1981; Noonan and Zeilberger 1997; Rukhin 2002).

## Set partitions, restricted growth strings

We could simply sum $a_{j, k}$ for all $\alpha^{2 T}-\alpha^{T}$ word pairs $W_{j} \neq W_{k}$, but for Marsaglia's tests, $\alpha^{2 T}=2^{40}$.
So instead we enumerate correlation classes and count the word pairs for each class.

Word pairs $\boldsymbol{W}_{\boldsymbol{j}}, \boldsymbol{W}_{\boldsymbol{k}}$ with $\boldsymbol{\beta}$ different letters $\rightarrow$ partition of $\{0, \ldots, 2 T-1\}$ into $\beta$ nonempty subsets $\leftrightarrow$ restricted growth string of length $\mathbf{2 T}$ with $\boldsymbol{\beta}$ different letters.
$S$ is a restricted growth string if $S_{k} \leqslant S_{j}+1$ for each $\boldsymbol{j}$ from $\mathbf{0}$ to $\boldsymbol{k}-\mathbf{1}$, for $\boldsymbol{k}$ from $\mathbf{1}$ to $\mathbf{2 T} \mathbf{- 1}$.

## Set partitions, restricted growth strings

Each permutation of the alphabet preserves the correlation matrix. The set of word pairs with $\boldsymbol{\beta}$ different letters splits into orbits under $\mathbb{S}_{\boldsymbol{\alpha}}$ of size

$$
\frac{\alpha!}{(\alpha-\beta)!}
$$

The number of partitions of $\{\mathbf{0}, \ldots, \mathbf{2 T}-\mathbf{1}\}$ into exactly $\boldsymbol{\beta}$ nonempty subsets is the second kind Stirling number $S(2 T, \beta)$.

If $\alpha \leqslant \mathbf{2 T}$, the total number of word pairs is

$$
\alpha^{2 T}=\sum_{\beta=1}^{\alpha} \frac{\alpha!}{(\alpha-\beta)!} S(2 T, \beta)
$$

## Enumeration by set partitions

Define $n[M](\alpha)=\sharp\left\{(j, k) \mid M_{j, k}=[M]\right\}$, the number of word pairs for correlation class $[M]$.

For $\boldsymbol{\alpha} \leqslant \boldsymbol{2 T}$, to determine all correlation classes [ $\boldsymbol{M}]$, and find $\boldsymbol{n}[\boldsymbol{M}](\boldsymbol{\alpha})$ for each,

Keep a count for each correlation class encountered so far; For each $\boldsymbol{\beta}$ from 1 to $\boldsymbol{\alpha}$ :

- For each restricted growth string of length $2 T$ with exactly $\boldsymbol{\beta}$ different letters:

1. Find the correlation class for the corresponding word pair;
2. Add $\frac{\alpha!}{(\alpha-\beta)!}$ to the count for the class.

## Population of each correlation class

For each correlation class [ $M$ ], $n[M](\alpha)$ is a polynomial in $\alpha$ of maximum degree $2 T$.

For $\alpha>2 T$, to find $n[M](\alpha)$, first find $n[M](\gamma)$ for $\gamma$ from 1 to $2 T$ and interpolate the polynomial.

In the case of Marsaglia's tests:

| Test | $\boldsymbol{\alpha}$ | $\boldsymbol{T}$ | Classes | Method |
| :--- | ---: | ---: | ---: | :--- |
| OPSO: | $\mathbf{1 0 2 4}$ | $\mathbf{2}$ | 6 | (Rahmann and Rivals 2003) |
| OQSO: | $\mathbf{3 2}$ | $\mathbf{4}$ | 55 | Polynomial interpolation |
| DNA: | $\mathbf{4}$ | $\mathbf{1 0}$ | 4592 | Exhaustive enumeration |

## Number of correlation classes

Define $b(T, \alpha)$ to be the number of correlation classes for unequal strings of length $\boldsymbol{T}$ and alphabet size $\boldsymbol{\alpha}$.

The set of classes remains unchanged for $\alpha>2 \boldsymbol{T}$.

The number of classes $\boldsymbol{b}(\boldsymbol{T}, \boldsymbol{\alpha})$ for small $\boldsymbol{T}$ is:

| $\alpha$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| :---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 2 | 1 | 3 | 11 | 31 | 87 | 193 | 415 | 839 | 1632 | 3004 |
| 3 | 1 | 6 | 20 | 54 | 141 | 322 | 655 | 1322 | 2506 | 4577 |
| 4 | 1 | 6 | 20 | 55 | 141 | 324 | 657 | 1329 | 2515 | 4592 |
| $2 T$ | 1 | 6 | 20 | 55 | 141 | 324 | 657 | $? ? ? ?$ | $? ? ? ?$ | $? ? ? ?$ |

See A152139, A152959, Online Encyclopedia of Integer Sequences.

## Some open problems

1. "Characterize and efficiently enumerate $2 \times 2$, and more generally, $\boldsymbol{k} \times \boldsymbol{k}$ matrices of correlation vectors between $\boldsymbol{k}$ pairwise different [words], and find the number of such matrices.
Compute the number of $\boldsymbol{k}$-tuples of words that share a given correlation matrix."
(Rahmann and Rivals 2003)
2. For $\boldsymbol{T}>2, \lambda:=N / \alpha^{T}$ constant as $N \rightarrow \infty$, find a high order asymptotic expansion for $\operatorname{var}[\boldsymbol{X}]$. (Rukhin 2002; Rahmann and Rivals 2003)
3. Does $b(T, 4)=b(T, 2 T)$ for all $T$ ?
