## Trivial Object, Nontrivial Problems

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## Outline

Abstract

Computing Repetitions

The Mysterious Combinatorics of Overlapping Squares
Indeterminate Strings

Characterizing Strings using Regularities

Fast Computation of Global Data Structures

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## Abstract

In 1906 Axel Thue founded stringology (combinatorics on words) by describing an infinitely long sequence containing only three distinct letters (say, a, b, c) that contains no repetition; that is, no pair of adjacent equal substrings. Over the intervening century and a bit, thousands of papers have been written on various aspects, mathematical and computational, of this trivial mathematical object: the string (or word or text or sequence). Today more than ever does research flow - after all, DNA sequences are strings!

In this talk I discuss a collection of problem areas, easy to describe, not so easy to deal with:

- efficient (appropriate) computation of repetitions;
- the mysterious combinatorics of overlapping squares;
- efficient computation on "indeterminate" strings;
- characterizing strings by their "regularities";
- fast computation of global data structures.


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## Repetitions, Runs \& Periodicity

Repetitions arise out of local periodicity in strings:

$$
\boldsymbol{x}=\begin{array}{llllllllll}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10  \tag{1}\\
a & b & a & a & b & a & b & a & a & a
\end{array}
$$

has repetitions $a^{2}, a^{3},(a b)^{2},(b a)^{2}$ and $(a b a)^{2}$.
$(a b)^{2}$ and $(b a)^{2}$ arise out of the same maximal periodicity or run: ababa. The other repetitions are runs without a tail!

## Some Hard-Won Facts about Runs \& Repetitions

Suppose $\boldsymbol{x}=\boldsymbol{x}[1 . . n]$ is a string:

- There may be as many as $\Theta(n \log n)$ repetitions in $\boldsymbol{x}$ (Fibonacci string) and they can be computed in $\mathcal{O}(n \log n)$ time [Cro81, AP83, ML84].
- Let $\rho(n)$ be the maximum number of runs that can occur in any string of length $n$. Then [KK99] there exist universal positive constants $k_{1}, k_{2}$ such that $\rho(n) \leq k_{1} n-k_{2} \sqrt{n} \log _{2} n$. Furthermore the runs in $\boldsymbol{x}$ can be computed in $\Theta(n)$ time [Mai89, KK99].
- After many contributions by many researchers (for example, [FSS03, Ryt06, PSS08, Gir08, CIT08, MKI ${ }^{+}$08]), we now know [Sim10, BII ${ }^{+}$14, FSHIL15] that

$$
0.944575712 \cdots<\rho(n) / n<0.9565 \cdots
$$

So what is the big problem???

## There Oughta Be a Faster Simpler Way!

Runs are

- local (independent of other segments of $\boldsymbol{x}$ )
- sparse (expected number $0.4 n$ in binary strings, $0.02 n$ in strings on the English alphabet [PS08])
- independent of any ordering of the alphabet
but all current linear-time algorithms
- require heavy global data structures (suffix sorting)
- take no advantage of the expected sparsity of runs
- depend on an ordering of the alphabet


## Suffix Trees, Suffix Arrays, et al. ...

$$
\begin{array}{rl} 
& \begin{array}{llllllll}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
\boldsymbol{x} & =a & b & a & a & b & a & b \\
a \\
\mathrm{SA}_{\boldsymbol{X}} & =8 & 3 & 6 & 1 & 4 & 7 & 2
\end{array} \\
\mathrm{LCP}_{\boldsymbol{X}} & =0 \\
1 & 1 \\
3 & 3
\end{array} 0
$$



## . . then Lempel-Ziv [LZ77], finally Repetitions



Figure : From $\left[\mathrm{AHCl}^{+} 13\right]$

## A Recent Ray of Light: the Lyndon Array

If $\boldsymbol{x}$ is not a repetition, it is primitive. A Lyndon word is the unique least rotation of a primitive word in some total ordering of words.
F For example, in lexorder with $a \prec b, \boldsymbol{u}=a a b$ is least among its rotations $R_{0}(\boldsymbol{u})=a a b, R_{1}(\boldsymbol{u})=a b a, R_{2}(\boldsymbol{u})=b a a$.
In the Lyndon array $\boldsymbol{\lambda}_{\boldsymbol{x}}=\boldsymbol{\lambda}_{\boldsymbol{x}}[1 . . n]$ of a word $\boldsymbol{x}=\boldsymbol{x}[1 . . n], \boldsymbol{\lambda}_{\boldsymbol{x}}[i]$ is the length of the longest Lyndon word beginning at position $i$ of $\boldsymbol{x}$.

In a remarkable recent result, [BII ${ }^{+}$14] used the computation of $\lambda_{\boldsymbol{X}}$ based on opposite orderings of the alphabet to show that $\rho(n)<n$, then went on to show that $\lambda_{\boldsymbol{X}}$ could be used to compute all the runs.

More later...

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## The Periodicity Lemma

If there is a "fundamental theorem" of combinatorics on words, this is it (to avoid clutter, we write $x=|\boldsymbol{x}|$ ):
Lemma ("Periodicity Lemma" [FW65])
Let $p$ and $q$ be two periods of $\boldsymbol{x}$, and let $d=\operatorname{gcd}(p, q)$. If
$p+q \leq x+d$, then $d$ is also a period of $\boldsymbol{x}$.
It took 30 years to begin to think about a third square:

## Lemma ("Three Squares Lemma" [CR95])

Suppose $\boldsymbol{u}$ is primitive, and suppose $\boldsymbol{v} \neq \boldsymbol{u}^{j}$ for any $j \geq 1$. If $\boldsymbol{u}^{2}$ is a prefix of $\boldsymbol{v}^{2}$, in turn a proper prefix of $\boldsymbol{w}^{2}$, then $w \geq u+v$.

The Fibostring demonstrates that this result is best possible (squares ending at positions $6,10,16=6+10,26=10+16$ ):

$$
\boldsymbol{x}=\begin{array}{llllllllllllllllllllllllll}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 17 & 18 & 19 & 20 & 21 & 22 & 23 & 24 & 25 & 26 \\
a & b & a & a & b & \underline{a} & b & a & a & \underline{b} & a & a & b & a & b & \underline{a} & a & b & a & b & a & a & b & a & a & \underline{b}
\end{array}
$$

## The "New Periodicity Lemma"

## Lemma (NPL [FPST06, Sim07, FFSS12, KS12, BS15])

Suppose that $\boldsymbol{x}$ has prefixes $\boldsymbol{u}^{2}$ and $\boldsymbol{v}^{2}, 3 u / 2<v<2 u$, and that $\boldsymbol{w}^{2}$ occurs at position $k+1$ of $\boldsymbol{x}$, where $v-u<w<v, w \neq u$, and $0 \leq k<v-u$. Then for each of 14 subcases, the structure of $\boldsymbol{x}$ is given below:

Table : $\sigma$ is the largest alphabet size consistent with $u, v, k, w ; \boldsymbol{d}, \boldsymbol{d}_{1}$ and $d_{3}$ are prefixes of $\boldsymbol{x}$ with $d=\operatorname{gcd}(u, v, w), d_{1}=\operatorname{gcd}(u-w, v-u)$, $d_{2}=\operatorname{gcd}(u, v-w), d_{3}=v \bmod d_{2}$.

| Subcases $S$ | Conditions | Breakdown of $\boldsymbol{x}$ |
| :--- | :---: | :---: |
| $1,2,5,6,8-10$ | $(\forall \boldsymbol{x}, \sigma=d)$ | $\boldsymbol{x}=\boldsymbol{d}^{x / d}$ |
| $3,4,7$ | $(\forall \boldsymbol{x})$ <br> specified cases <br> $11-14$ | $\sigma=\boldsymbol{d}_{1}{ }^{u / d_{1}} \boldsymbol{d}_{1}{ }^{v / d_{1}} \boldsymbol{d}_{1}(v-u) / d_{1}$ <br> $\boldsymbol{x}=\boldsymbol{d}^{x / d}$ <br> otherwise $d_{2} \leq 2 u-v$ |
| $\boldsymbol{x}=\boldsymbol{d}^{x / d}$ |  |  |
|  | $\boldsymbol{x}=\left(\left(\boldsymbol{d}_{3}{ }^{d_{2} / d_{3}}\right)^{v / d_{2}}\right)^{2}$ |  |

(For $u<v \leq 3 u / 2$, a simpler result holds with even more structure.)

## "New Periodicity Lemma Revisited"

We call $\boldsymbol{v}^{2}$ a double square $\operatorname{DS}(\boldsymbol{u}, \boldsymbol{v})$ if it has proper prefix $\boldsymbol{u}^{2}$. We say that $\boldsymbol{u}$ is the primitive root of $\boldsymbol{w}$ if $\boldsymbol{w}=\boldsymbol{u}^{e}$ for some greatest integer $e \geq 1$ (for $\boldsymbol{w}=(a b)^{4}, \boldsymbol{u}=a b, e=4$ ).
Lemma (NPLR [BFS16])
Consider a double square $\operatorname{DS}(\boldsymbol{u}, \boldsymbol{v})$ with $\boldsymbol{v}=\boldsymbol{u} \boldsymbol{u}^{\prime}$ for some nonempty $\boldsymbol{u}^{\prime}$. Suppose that $\boldsymbol{w}^{2}$ is a proper substring of $\boldsymbol{v}^{2}$.
Then exactly one of the following holds:
(a) $w<u$;
(b) $u \leq w<v$ and the primitive root of $\boldsymbol{w}$ is a rotation of the primitive root of $\boldsymbol{u}^{\prime}$.

NPLR applies to somewhat fewer $\boldsymbol{w}$ than NPL, but is more precise in its characterization.

## Where Do We Go From Here?

As yet no algorithm makes use of these results.
But they clearly relate to the identification of runs.
Perhaps digestion is required!

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## Extending the Idea of a "String"

In DNA applications it can happen that a letter is not $a, c, g, t$, but some combination: $\{a, c\},\{g, t\}$. A regular string is defined on individual letters of an alphabet $\Sigma$; an indeterminate string is defined on indeterminate letters - nonempty subsets of $\Sigma$.

We say that $\lambda_{1}$ matches $\lambda_{2}$, written $\lambda_{1} \approx \lambda_{2}$, if $\lambda_{1} \cap \lambda_{2} \neq \emptyset$; thus $\{c\} \approx\{c\}$ and $\{a, c\} \approx\{c, g\}$.

The fundamental difficulty is nontransitivity of matching: possibly $\lambda_{1} \approx \lambda_{2} \approx \lambda_{3}$, but $\lambda_{1} \not \approx \lambda_{3}$. For example,

$$
\lambda_{1}=\{a, c\}, \lambda_{2}=\{c, g\}, \lambda_{3}=\{g, t\}
$$

Main goal: establish theory [SW09b], data structures [SW08, CRSW15] and algorithms [SW09a, ARS15, ARS16] for indeterminate strings that correspond to those for regular strings.

## The Prefix Array of an Indeterminate String - I

If $\boldsymbol{u}$ is a possibly empty proper prefix of $\boldsymbol{x}(0 \leq u<x)$ that matches a suffix $\boldsymbol{u}^{\prime}$ of $\boldsymbol{x}$, then $\boldsymbol{u}$ is said to be a border of $\boldsymbol{x}$. The border array $\boldsymbol{\beta}=\boldsymbol{\beta}_{\boldsymbol{X}}[1 . . n]$ gives in position $i \in 1 . . n$ the longest border of $\boldsymbol{x}[1 . . . i]$ :

$$
\begin{aligned}
& \boldsymbol{x}= \\
& \boldsymbol{\beta}= \\
& =
\end{aligned} \mathbf{\{ a , b \}} \begin{array}{ccc}
1 & 2 & 3 \\
\{b, c\} & c \\
1 & 2
\end{array}
$$

For regular strings, if $\beta[i]>0$, then $\beta[\beta[i]]$ is the second longest border of $\boldsymbol{x}[1 . . i]$, and so $\boldsymbol{\beta}$ gives all the borders of every prefix of $\boldsymbol{x}$. The border array can be easily computed in $\Theta(n)$ time and is ubiquitous in regular string algorithms.

Alas, due to the nontransitivity of matching, this is not true for indeterminate strings: to specify all the borders, a list needs to be stored at each position of $\boldsymbol{\beta}$.

## The Prefix Array of an Indeterminate String - II

The prefix array $\boldsymbol{\pi}=\pi_{\boldsymbol{X}}[1 . . n]$ gives in position $i$ the length of the longest substring beginning at $i$ that matches a prefix of $\boldsymbol{x}$.

$$
\begin{array}{lccc} 
& 1 & 2 & 3 \\
\boldsymbol{x}= & \{a, b\} & \{b, c\} & c \\
\boldsymbol{x}= & 3 & 2 & 0
\end{array}
$$

For regular strings, $\boldsymbol{\beta}$ and $\boldsymbol{\pi}$ are "equivalent": one can be computed from the other in linear time. But for indeterminate strings, the prefix array retains its useful properties: $\boldsymbol{\pi}_{\boldsymbol{X}}$ implicitly specifies all the borders of $\boldsymbol{x}$.

An integer array $\boldsymbol{y}=\boldsymbol{y}[1 . . n]$ is said to be feasible if $\boldsymbol{y}[1]=n$ and for every $i \in 2 . . n, 0 \leq y[i] \leq n+1-i$.
Lemma
Every feasible array is the prefix array of some (indeterminate) string.

## The Prefix Array of an Indeterminate String - III

## Problem

Given a feasible array $\boldsymbol{y}$, find a lexicographically least string $\boldsymbol{x}$ (regular if possible) whose prefix array $\pi_{\boldsymbol{x}}=\boldsymbol{y}$.

In [CCR09] a linear-time algorithm is described that, given a feasible array $\boldsymbol{y}$, computes a lexicographically least corresponding regular string $\boldsymbol{x}$, whenever this is possible, and otherwise returns an error message.

In [BSBW14] it is shown that a lexicographically least indeterminate string whose prefix array is $\boldsymbol{y}$ has alphabet size $\sigma \leq n+\sqrt{n}$. Then in [ARS15] an $\mathcal{O}\left(\sigma n^{2}\right)$-time algorithm is described that computes a lexicographically least indeterminate string whose prefix array is $\boldsymbol{y}$.

## Question

Can this calculation be done any quicker? Can it be done in less than $\mathcal{O}\left(n^{2}\right)$ (worst case, average case) time?

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## Periodicity \& Quasiperiodicity

A string $\boldsymbol{x}=\boldsymbol{x}[1 . . n]$ is said to have period $p=n-b$ whenever it has a border of length $b$. Sometimes (especially when $\boldsymbol{x}$ is a repetition or near-repetition), the minimum period can be a good descriptor of $\boldsymbol{x}$ :

$$
\begin{equation*}
\boldsymbol{x}=(a b)^{m},(a b a c)^{m} a b \tag{2}
\end{equation*}
$$

usually not:

$$
\begin{equation*}
\boldsymbol{x}=a b b a b a a, a b a c a b a d \tag{3}
\end{equation*}
$$

even when there is a lot of "regularity" in $\boldsymbol{x}$.
In [AFI91] a quasiperiod $q$ of $\boldsymbol{x}$ was introduced: the length of a border of $\boldsymbol{x}$ such that every position of $\boldsymbol{x}$ is contained in some occurrence of $\boldsymbol{q}=\boldsymbol{x}[1 . . q]$. Then $\boldsymbol{q}$ is called a cover of $\boldsymbol{x}$.
[LS02] showed that the cover array $\gamma_{\boldsymbol{x}}$ [1..n] of $\boldsymbol{x}$ could be computed in $\Theta(n)$ time from the border array, specifying all the covers of every prefix of $\boldsymbol{x}$. [ARS16] showed how to compute $\gamma_{\boldsymbol{X}}$ using the prefix array, and thus extended the result to indeterminate strings using $\mathcal{O}(n)$ time on average.

## Seeds \& $k$-Covers

Unfortunately, the quasiperiod doesn't help very much: $\boldsymbol{x}=(a b a c)^{m} a b$ in (2) has no cover, nor do the strings of (3).

A seed of $\boldsymbol{x}$ is a minimum cover of a superstring of $\boldsymbol{x}$ and can be computed in $\mathcal{O}(n \log n)$ time [IMP93]. Every periodic string has a seed - for example, $(a b a c)^{m} a b$ has seed abac. But a seed may not help very much: in (3), abbabaa has seed abbaba and the only seed of abacabad is itself.

These deficiencies led to the idea of a $k$-cover: a minimum cardinality collection of strings, each of length $k$, that covers a given string $\boldsymbol{x}$. For example, both the strings of (3) have a 4-cover of size 2, perhaps not very helpful. Unfortunately, computing a $k$-cover is NP-complete [CIMS05], though it can be approximated to within a factor $k$ in polynomial time [IMS11].

## Enhanced/Partial String Covering

An enhanced cover $\boldsymbol{u}$ of $\boldsymbol{x}$ is a border of $\boldsymbol{x}$ that, over all the borders of $\boldsymbol{x}$, covers a maximum number of positions in $\boldsymbol{x}$. The enhanced cover array EC[1..n] gives the enhanced cover of every nonempty prefix of $\boldsymbol{x}$. EC can be computed in $\mathcal{O}(n \log n)$ worst-case time $\left[\right.$ FIK ${ }^{+}$13] and in $\mathcal{O}(n)$ expected time, both for regular and indeterminate strings [AIR $\left.{ }^{+} 16\right]$. No help for strings such as (3), whose borders are short and scarce.

Given an integer $\alpha \in 1$..n, an $\alpha$-partial cover of $\boldsymbol{x}$ is a substring of $\boldsymbol{x}$ that covers at least $\alpha$ positions in $\boldsymbol{x}$; the shortest $\alpha$-partial cover can be computed for all $\alpha$ in $\mathcal{O}(n \log n)$ time [KPR $\left.{ }^{+} 15\right]$. Similarly there are $\alpha$-partial seeds [KPR ${ }^{+}$14], but computation time increases.

New ideas (new regularities) are needed: both strings (3) are one letter change away from being periodic!

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## The Tale of the Suffix Array

Given $\boldsymbol{x}=\boldsymbol{x}[1 . . n]$, the suffix array $\mathrm{SA}=\mathrm{SA}_{\boldsymbol{X}}[1 . . n]$ is such that for every $i \in 1 . . n, \mathrm{SA}[i]=j$ iff $\boldsymbol{x}[j . . n]$ is the $i^{\text {th }}$ suffix in some global order (such as lexorder).

1990 SA invented [MM90, MM93] hopefully to supplement the suffix tree [Wei73].
1995-2002 About 15 SACAs proposed, none of them linear-time, none lightweight [PST07].
2003 Three linear-time SACAs proposed, all recursive, all slow [KA03, KS03, KSPP03].
2004 SAs can do anything STs can do! [AKO04]
2009 A fast, recursive, linear-time, lightweight SACA is discovered [NZC09], an efficient implementation is made available on-line [Mor09].
2010- SA applications multiply, in bioinformatics and elsewhere.

## What about the Lyndon Array?

1983 Computing the Lyndon array of $\boldsymbol{x}$ is equivalent to computing its Lyndon brackets, mentioned in [Lot83].
2003 [SR03] describes an $\mathcal{O}\left(n^{2}\right)$-time algorithm to compute Lyndon brackets, [HR03] hints at an algorithm to compute the Lyndon array from the suffix array.
2014 [BII ${ }^{+}$14] uses the Lyndon array to show $\rho(n)<n$ and to compute all the runs in given $\boldsymbol{x}$ in linear time.
2016 [ $\mathrm{FHI}^{+}$16] describes half a dozen algorithms to compute $\boldsymbol{\lambda}_{\boldsymbol{X}}$, but none of them is both linear-time and "elementary".

## $\lambda_{\boldsymbol{x}}=\operatorname{NSV}\left(I S A_{\boldsymbol{x}}\right)$

## Definition (Next Smaller Value)

Given an array $\boldsymbol{x}[1 . . n]$ of ordered values, $\mathrm{NSV}=\mathrm{NSV}_{\boldsymbol{X}}[1 . . n]$ is the next smaller value array of $\boldsymbol{x}$ if and only if for every
$i \in 1 . . n$, NSV $[i]=j$, where
(a) for every $h \in 1 . . j-1, \boldsymbol{x}[i] \leq \boldsymbol{x}[i+h]$; and
(b) either $i+j=n+1$ or $\boldsymbol{x}[i]>\boldsymbol{x}[i+j]$.

$$
\begin{array}{rl}
\boldsymbol{r} & 2 \\
\boldsymbol{x} & =3 \\
3 & 8 \\
\hline & 4 \\
10 & 5 \\
2 & 6 \\
\hline & 4 \\
8 & 8 \\
\hline
\end{array}
$$

procedure $\operatorname{NSVISA}(\boldsymbol{x}[1 \ldots n]): \lambda_{\boldsymbol{x}}[1 \ldots n]$
Compute $S A_{\boldsymbol{X}} \quad$ ([NZC09, PST07])
Compute ISA $\boldsymbol{X}_{\boldsymbol{x}}$ in place [PST07]
$\boldsymbol{\lambda}_{\boldsymbol{x}} \leftarrow$ NSV(ISA $\boldsymbol{x}$ ) (in place) [FHI+16]
Hey Presto - linear time!

## BUT ...

The suffix array $\mathrm{SA}_{\boldsymbol{X}}$ is more "global", less "elementary" than the Lyndon array $\lambda_{\boldsymbol{x}}$ : SA sorts all the suffixes of the string, $\lambda$ just computes a local property at each position $i$.

Why should we need to use SA to compute $\lambda$ in linear time?
Why isn't there a simpler (and linear-time) algorithm?
Will we find more applications for $\lambda$ as we did for SA?
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