Trivial Object, Nontrivial Problems

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Outline

Abstract

Computing Repetitions

The Mysterious Combinatorics of Overlapping Squares

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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:

1	2	3	4	5	6	7	8	9	10	(1
x = a	b	а	а	b	а	b	а	а	а	(1

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has repetitions a^2 , a^3 , $(ab)^2$, $(ba)^2$ and $(aba)^2$.

 $(ab)^2$ and $(ba)^2$ 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 $\mathbf{x} = \mathbf{x}[1..n]$ is a string:

- There may be as many as ⊖(n log n) repetitions in x (Fibonacci string) and they can be computed in 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 $\rho(n) \le k_1 n - k_2 \sqrt{n} \log_2 n$. Furthermore the runs in **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 x)
- sparse (expected number 0.4n in binary strings, 0.02n 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. ...



··· then Lempel-Ziv [LZ77], finally Repetitions



Figure : From [AHCI+13]

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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.

For example, in lexorder with $a \prec b$, $\boldsymbol{u} = aab$ is least among its rotations $R_0(\boldsymbol{u}) = aab$, $R_1(\boldsymbol{u}) = aba$, $R_2(\boldsymbol{u}) = baa$.

In the Lyndon array $\lambda_{\mathbf{X}} = \lambda_{\mathbf{X}}[1..n]$ of a word $\mathbf{x} = \mathbf{x}[1..n]$, $\lambda_{\mathbf{X}}[i]$ is the length of the longest Lyndon word beginning at position *i* of \mathbf{x} .

In a remarkable recent result, [BII+14] used the computation of $\lambda_{\mathbf{X}}$ based on opposite orderings of the alphabet to show that $\rho(n) < n$, then went on to show that $\lambda_{\mathbf{X}}$ 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 $x = |\mathbf{x}|$):

Lemma ("Periodicity Lemma" [FW65])

Let p and q be two periods of \mathbf{x} , and let d = gcd(p, q). If $p+q \le x+d$, then d is also a period of \mathbf{x} .

It took 30 years to begin to think about a third square:

Lemma ("Three Squares Lemma" [CR95])

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

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

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 $\mathbf{x} = \mathbf{a} \ \mathbf{b} \ \mathbf{a} \ \mathbf{a} \ \mathbf{b} \ \mathbf{a} \ \mathbf{a} \ \mathbf{b} \ \mathbf{b} \ \mathbf{c} \ \mathbf{b} \ \mathbf{c} \ \mathbf{c} \ \mathbf{b} \ \mathbf{c} \ \mathbf$

The "New Periodicity Lemma"

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

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

Table : σ is the largest alphabet size consistent with u, v, k, w; d, d_1 and d_3 are prefixes of x with $d = \gcd(u, v, w)$, $d_1 = \gcd(u-w, v-u)$, $d_2 = \gcd(u, v-w)$, $d_3 = v \mod d_2$.

Subcases S	Conditions	Breakdown of x
1, 2, 5, 6, 8–10	$(\forall \mathbf{x}, \sigma = \mathbf{d})$	$\mathbf{x} = \mathbf{d}^{x/d}$
3.4.7	(∀ x)	$\mathbf{x} = \mathbf{d}_1^{u/d_1} \mathbf{d}_1^{v/d_1} \mathbf{d}_1^{(v-u)/d_1}$
-, .,.	specified cases	$\mathbf{x} - \mathbf{d}^{\mathbf{x}/d}$
		x - u
44 44	- dord < 0 u v	x ax/d
11-14	$\sigma = u \text{ or } u_2 \leq 2u - v$	$\mathbf{x} = \mathbf{a}^{\prime}$
	otherwise	$m{x} = \left((m{d}_3^{d_2/d_3})^{v/d_2} ight)^2$

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

"New Periodicity Lemma Revisited"

We call v^2 a double square DS(u, v) if it has proper prefix u^2 . We say that u is the primitive root of w if $w = u^e$ for some greatest integer $e \ge 1$ (for $w = (ab)^4$, u = ab, e = 4).

Lemma (NPLR [BFS16])

Consider a double square $DS(\boldsymbol{u}, \boldsymbol{v})$ with $\boldsymbol{v} = \boldsymbol{u}\boldsymbol{u}'$ for some nonempty \boldsymbol{u}' . Suppose that \boldsymbol{w}^2 is a proper substring of \boldsymbol{v}^2 . Then exactly one of the following holds:

- (a) w < u;
- (b) $u \le w < v$ and the primitive root of **w** is a rotation of the primitive root of **u**'.

NPLR applies to somewhat fewer 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 Σ ; an indeterminate string is defined on indeterminate letters — nonempty subsets of Σ .

We say that λ_1 matches λ_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 **u** is a possibly empty proper prefix of **x** ($0 \le u < x$) that matches a suffix **u'** of **x**, then **u** is said to be a border of **x**. The border array $\beta = \beta_{\mathbf{X}}[1..n]$ gives in position $i \in 1..n$ the longest border of **x**[1..*i*]:

For regular strings, if $\beta[i] > 0$, then $\beta[\beta[i]]$ is the second longest border of $\mathbf{x}[1..i]$, and so β gives all the borders of every prefix of \mathbf{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 β .

The Prefix Array of an Indeterminate String - II

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

$$egin{array}{cccc} & 1 & 2 & 3 \ m{x} = & \{a,b\} & \{b,c\} & c \ m{\pi} = & 3 & 2 & 0 \end{array}$$

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

An integer array y = y[1..n] is said to be feasible if y[1] = nand for every $i \in 2..n$, $0 \le y[i] \le n+1-i$.

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

In [CCR09] a linear-time algorithm is described that, given a feasible array y, computes a lexicographically least corresponding regular string 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 y has alphabet size $\sigma \leq n + \sqrt{n}$. Then in [ARS15] an $\mathcal{O}(\sigma n^2)$ -time algorithm is described that computes a lexicographically least indeterminate string whose prefix array is y.

Question

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

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Periodicity & Quasiperiodicity

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

$$\boldsymbol{x} = (ab)^m, \ (abac)^m ab; \tag{2}$$

usually not:

$$\mathbf{x} = abbabaa, abacabad,$$
 (3)

even when there is a lot of "regularity" in x.

In [AFI91] a quasiperiod q of x was introduced: the length of a border of x such that every position of x is contained in some occurrence of q = x[1..q]. Then q is called a cover of x.

[LS02] showed that the cover array $\gamma_{\mathbf{X}}[1..n]$ of \mathbf{x} could be computed in $\Theta(n)$ time from the border array, specifying all the covers of every prefix of \mathbf{x} . [ARS16] showed how to compute $\gamma_{\mathbf{X}}$ 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: $\mathbf{x} = (abac)^m ab$ in (2) has no cover, nor do the strings of (3).

A seed of **x** is a minimum cover of a superstring of **x** and can be computed in $\mathcal{O}(n \log n)$ time [IMP93]. Every periodic string has a seed — for example, $(abac)^m ab$ 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 **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 u of x is a border of x that, over all the borders of x, covers a maximum number of positions in x. The enhanced cover array EC[1..n] gives the enhanced cover of every nonempty prefix of x. EC can be computed in $\mathcal{O}(n \log n)$ worst-case time [FIK⁺13] and in $\mathcal{O}(n)$ expected time, both for regular and indeterminate strings [AIR⁺16]. No help for strings such as (3), whose borders are short and scarce.

Given an integer $\alpha \in 1..n$, an α -partial cover of \mathbf{x} is a substring of \mathbf{x} that covers at least α positions in \mathbf{x} ; the shortest α -partial cover can be computed for all α in $\mathcal{O}(n \log n)$ time [KPR⁺15]. Similarly there are α -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 $\mathbf{x} = \mathbf{x}[1..n]$, the suffix array $SA = SA_{\mathbf{x}}[1..n]$ is such that for every $i \in 1..n$, SA[i] = j iff $\mathbf{x}[j..n]$ is the *i*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 *x* is equivalent to computing its Lyndon brackets, mentioned in [Lot83].
- 2003 [SR03] describes an $\mathcal{O}(n^2)$ -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 **x** in linear time.
- 2016 [FHI⁺16] describes half a dozen algorithms to compute $\lambda_{\mathbf{X}}$, but none of them is both linear-time and "elementary".

 $\lambda_{\mathbf{X}} = \text{NSV}(ISA_{\mathbf{X}})$

Definition (Next Smaller Value) Given an array $\mathbf{x}[1..n]$ of ordered values, NSV = NSV $_{\mathbf{x}}[1..n]$ is the **next smaller value array** of \mathbf{x} if and only if for every $i \in 1..n$, NSV[i] = j, where

- (a) for every $h \in 1..j-1$, $x[i] \le x[i+h]$; and
- (b) either i+j = n+1 or x[i] > x[i+j].

procedure NSVISA(x[1..n]) : $\lambda_x[1..n]$ Compute SA_x ([NZC09, PST07]) Compute ISA_x in place [PST07] $\lambda_x \leftarrow NSV(ISA_x)$ (in place) [FHI⁺16] Hey Presto — linear time!



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

Why should we need to use SA to compute λ in linear time? Why isn't there a simpler (and linear-time) algorithm?

Will we find more applications for λ as we did for SA?

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