Succinct Data Structures for Data Mining

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Overview

Big Data vs. big data

- Big Data: 10s of TB+.
    - Must be processed in streaming / parallel manner.
- Data mining is often done on big data: 10s-100s of GBs.
    - Graphs with 100s of millions of nodes, protein databases 100s of millions of compounds, 100s of genomes etc.
- Often, we use Big Data techniques to mine big data.
    - Parallelization is *hard* to do well [Canny, Zhao, *KDD'13*].
    - Streaming is inherently limiting.
- Why not use (tried and trusted, optimized) "vanilla" algorithms for classical DM problems?

Mining big data

- Essential that data fits in main memory.
  - Complex memory access patterns: out-of-core $\Rightarrow$ thrashing.
- Data stored accessed in a complex way is usually stored in a data structure that supports these access patterns.
  - Often data structure is MUCH LARGER than data!
  - Cannot mine big data if this is the case.
- Examples:
  - Suffix Tree (text pattern search).
  - Range Tree (geometric search).
  - FP-Tree (frequent pattern matching).
  - Multi-bit Tree (similarity search).
  - DOM Tree (XML processing).

Compressed Data Structures

Store data *in memory* in *compact* or *compressed* format and operate directly on it.

- (Usually) no need to decompress before operating.
- Better use of memory levels close to processor, processor-memory bandwidth.
  - Usually compensates for some overhead in CPU operations.

Programs = Algorithms + Data Structures

- If compressed data structure implements same/similar API to uncompressed data structure, can reuse existing code.

Compression vs. Data Structuring

Answering queries requires an *index* on the data that may be large:

- *Suffix tree:* data structure for indexing a text of n bytes.
    - Supports many indexing and search operations.
    - Careful implementation: $10n$ bytes of index data [Kurtz, *SPrEx '99*]
- *Range Trees:* data structures for answering 2-D orthogonal range queries on n points.
    - Good worst-case performance but $\Theta(n \log n)$ space.

Succinct/Compressed Data Structures

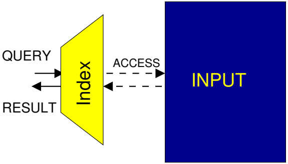
$$\text{Space usage} = \text{“space for data”} + \underbrace{\text{“space for index”}}_{\textit{redundancy}}.$$

Redundancy should be smaller than space for data.

Memory Usage Models

Indexing model

- Preprocess input to get *index*.
- Queries read index and *access* input (may be expensive).
- Redundancy = index size.



General model

- No restriction on access to data structure memory.
- Redundancy = memory usage − "space for data".

▷ Trade-off: redundancy vs. query time.

▷ Index or DS depends *crucially* on operations to be supported.

Space Measures

Data Size	Redundancy	
Naive	$O(1)$	(implicit/in-place)
Information-theoretic	lower-order	(succinct)
Entropy (H_0)	“lower-order”	(density-sensitive)
Entropy (H_k)	“lower-order”	(compressed)

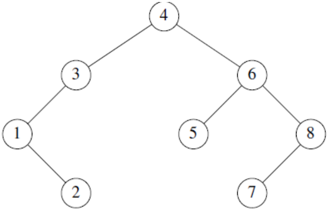
- Best known example of implicit data structure: array-based representation of binary heap.
- “Information-theoretic” count total number of instances of a given size; take the log base 2 (lg).
- “Entropy” is usually an *empirical* version of classical Shannon entropy.

Example: Sequences

$x \in \Sigma^n$ for some finite set of symbols $0, 1, \ldots, \sigma - 1$.

- **Naive:** $n \lceil \lg \sigma \rceil$ bits [$\sigma = 3, 2n$ bits].
- **Information-Theoretic:**
  $\lg \sigma^n = \lceil n \lg \sigma \rceil$ bits. [$\sigma = 3, \sim 1.73n$ bits.]
  [Dodis, Patrascu, Thorup, *STOC'10*]
- **Entropy (0-th):** $H_0 \sim n_0 \lg(n/n_0) + n_1 \lg(n/n_1)$ $(\Sigma = \{0, 1\})$.
  - If $n_0 = n_1 = n/2$, $H_0 = n$. If $n_0 = 0.2n$, $H_0 \sim 0.72n$ bits.
  - Closely related to $\lg \binom{n}{n_1} = n_1 \lg \left(\frac{n}{n_1} \right) + O(n_1)$.
  - If $n_1 \ll n$, $H_0 \ll n$.
- **Entropy (k-th):** Count frequencies in all contexts of length k:
  $$\ldots 1011 \ldots 1010 \ldots 1011 \ldots$$
  - For $0^{n/2} 1^{n/2}$, $H_0 = n$ bits, $H_1 = O(\lg n)$ bits.

Example: Binary Trees



Given object x is an binary tree with n nodes.

- **Naive:** $\geq 2n$ pointers; $\Omega(n \lg n)$ bits.
- **Information-Theoretic:** $\lg \left(\frac{1}{n+1} \binom{2n}{n} \right) = 2n - O(\lg n)$ bits.
- **Entropy (0-th, k-th):** ?
  - Maybe define H_0 as $\sum_{i \in \{0,L,R,LR\}} n_i \lg(n/n_i)$, where $n_0 = \#$ leaves, $n_{LR} = \#$ nodes with both L and R child etc. [Davoodi et al., *PTRS-A '14*]

Bit Vectors

Data: Sequence X of n bits, $x_1, \ldots, x_n$. $m = n_1$. **Operations:**

- $rank1(i)$: number of 1s in $x_1, \ldots, x_i$.
- $select1(i)$: position of ith 1.

Also $rank0$, $select0$.

Example: $X = 01101001$, $rank1(4) = 2$, $select0(4) = 7$.

Want *rank* and *select* to take $O(1)$ time.

Operations introduced in [Elias, *J. ACM '75*], [Tarjan and Yao, *C. ACM '78*], [Chazelle, *SIAM J. Comput '85*], [Jacobson, *FOCS '89*].

Bit Vectors: Results

All operations $rank1, select0, select1$ in $O(1)$ time and:

- space $n + o(n)$ bits [Clark and Munro, *SODA '96*].
- space $H_0(X) + o(n)$ bits [RRR, *SODA '02*].
    - $H_0(X) + o(n) = \lg \binom{n}{m} + o(n) = m \lg(n/m) + O(m) + o(n)$.
    - n/m is roughly the average gap between 1s.
    - $m \ll n \Rightarrow H_0(X) \ll n$ bits.
    - $o(n)$ term is *not necessarily* a "lower-order" term.

Only $select1$ in $O(1)$ time and:

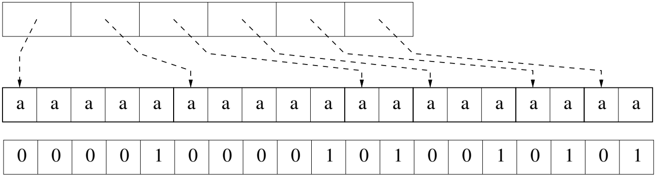
- space $H_0(X) + O(m)$ bits [Elias, *J. ACM '75*].

Called "Elias-Fano" representation.

Bit Vector Uses (1): Array of Strings

Data: m variable-length strings, total size n. Access i-th string.

- Naive: $8n$ bits (raw) $+ 64m$ bits
- Bitvector: $8n$ bits (raw) $+ n$ bits.
- Elias-Fano: $8n$ bits (raw) $+ m\log(n/m) + O(m)$ bits.

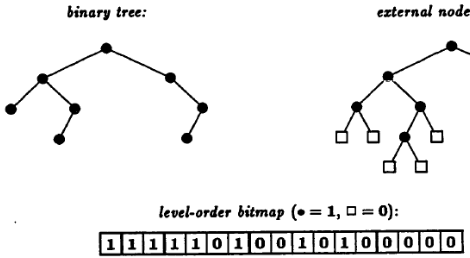


- XML textual data [Delpratt et al., *EDBT'08*], $n/m \sim 11$.
- Use to random-access any variable-length data encoding.

Bit Vector Uses (2): Binary Tree

Data: n-node binary tree. [Jacobson, *FOCS '89*]

- Add $n+1$ external nodes.
- Visit each node in level-order and write bitmap ($2n+1$ bits).



[Jacobson, *FOCS'89*]

- Number internal nodes by position of 1 in bit-string.
- Store bitmap as bit vector. Left child $= 2 * rank1(i)$, Right child $= 2 * rank1(i) + 1$, parent $= select1(\lfloor i/2 \rfloor)$.

Bit Vector Uses (3): Elias-Fano representation

Aim: Using represent bit-string X of lengusing $H_0(X) + O(m)$ bits support *only select*1 in $O(1)$ time.
[Elias, *J. ACM'75*], [Grossi/Vitter, *SICOMP'06*], [Raman et al., *TALG'07*].

- Space is always $O(nH_0)$.
- Consider bit-vector X as *subset* of $\{0, \ldots, n-1\}$, i.e. as characteristic vector of set $X = \{x_1, \ldots, x_m\}$.
- $select1(i) = x_i$.

Elias-Fano: MSB Bucketing

Bucket according to most significant b bits: $x \to \lfloor x/2^{\lceil \lg n \rceil - b} \rfloor$.

Example. $b = 3$, $\lceil \lg n \rceil = 5$, $m = 7$.

x_1	0	1	0	0	0
x_2	0	1	0	0	1
x_3	0	1	0	1	1
x_4	0	1	1	0	1
x_5	1	0	0	0	0
x_6	1	0	0	1	0
x_7	1	0	1	1	1

Bucket	Keys
000	—
001	—
010	x_1, x_2, x_3
011	x_4
100	x_5, x_6
101	x_7
110	—
111	—

Elias-Fano: Bucketing saves space

- ▷ Store only low-order bits.
- ▷ (Keep cumulative bucket sizes.)

Example

select(6)

bkt	sz	data
000	0	—
001	0	—
010	0	$\underbrace{00}_{x_1}, \underbrace{01}_{x_2}, \underbrace{11}_{x_3},$
011	3	$\underbrace{01}_{x_4}$
100	4	$\underbrace{00}_{x_5}, \underbrace{10}_{x_6}$
101	6	$\underbrace{11}_{x_7}$

Elias-Fano: Wrap up

- Choose $b = \lfloor \lg m \rfloor$ bits. In bucket: $\lceil \lg n \rceil - \lfloor \lg m \rfloor$-bit keys.
- $m \lg n - m \lg m + O(m)$ + space for cumulative bucket sizes.

Bucket no:	000	001	010	011	100	101	110	111
Bucket size:	0	0	3	1	2	1	0	0

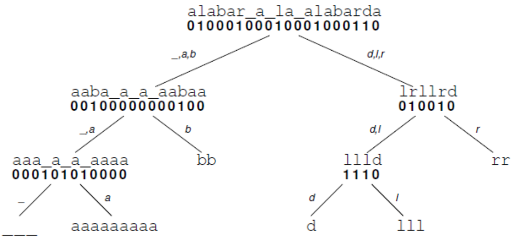
Unary encoding: $0, 0, 3, 1, 2, 1, 0, 0 \rightarrow$ 110001010010111.

z buckets, total size $m \Rightarrow m + z$ bits ($z = 2^{\lfloor \lg m \rfloor}$).

- Total space $= m \log(n/m) + O(m) = nH_0 + O(m)$ bits.
- In which bucket is the 6th key? ▷ "Index of 6th 0" $- 6$.

Bit Vector Uses (4): Wavelet Tree

Data: n-symbol string, alphabet size σ. [Grossi and Vitter, *SJC '05*]
Convert string into $\lg \sigma$ bit-vectors: $\underbrace{n \log \sigma}_{\text{raw size}} + o(n \log \sigma)$ bits.

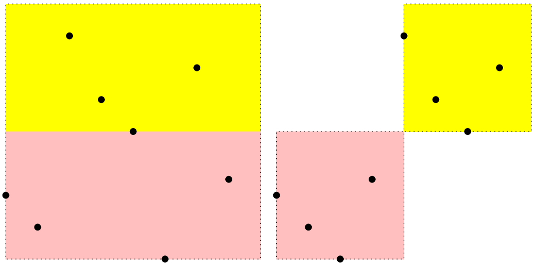


[Navarro, *CPM'12*]

rank and *select* operations on any character in $O(\log \sigma)$ time.

Bit Vector Uses (4): Wavelet Tree (cont'd)

Data: Permutation over $\{1, \ldots, n\}$ (string over alphabet of size n). View as 2-D point set on $n \times n$ integer grid [Chazelle, *SJC '88*]:



Represent as wavelet tree: using $n + o(n)$ bits, in $O(1)$ time reduce to $n/2 \times n/2$ integer grid.

▷ Range tree in disguise, but takes only $O(n)$ words of space, not $O(n \lg n)$ words. Orthogonal range queries in $O(\lg n)$ time.

Bit Vector Uses (4): Wavelet Tree (cont'd)

A wavelet tree can represent any array of (integer) values from an alphabet of size σ. A huge number of complex queries can be supported in $O(\log \sigma)$ time:

- range queries
- positional inverted indexes
- graph representation
- permutations
- numeric sequences
- document retrieval
- binary relations
- similarity search

▷ Very flexible and space-efficient data representation.

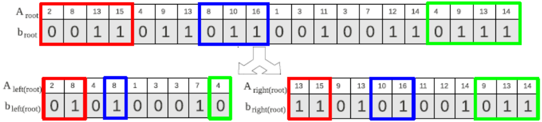
▷ Adequately fast for most applications (a few memory accesses).

▷ Well supported by libraries.

Graph Similarity Search [Tabei and Tsuda, *SDM 2011*]

- View chemical compound as a feature vector / bag of words.
- Database of compounds: $W_1, W_2, \ldots$.
- Given query Q, find all compounds at small Jaccard distance
- Filtering criterion: find all W_i s.t. $|Q \cap W_i| \geq k$.
- Like text search, but $|Q|$ is large.

A	2,8,13,15
B	4,9,13
C	8,10,16
D	1,3,11
E	3,7,12,14
F	4,9,13,14

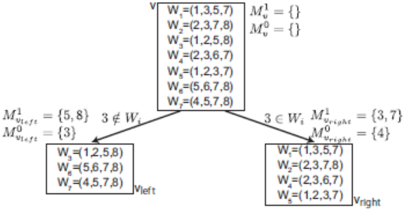


[Tabei and Tsuda, *SDM'11*]

- Inverted list as wavelet tree.
- Fairly fast, fairly memory-efficient, *much* better scalability.

Similarity Search (2) [Tabei, *WABI 2012*]

- View chemical compound as a feature vector / bag of words.
- Given query Q, find all compounds at small Jaccard distance
- Filtering criterion: find all W_i s.t. $|Q \cap W_i| \geq k$.
- Based on *multi-bit tree* [Kristensen et al., *WABI '09*].



- Fast, but memory-hungry.
- Represent tree structure succinctly.
- Represent original fingerprints with VLE and bit-vectors.
- 10x reduction in space, scaled to 30 million compounds.

Compound-Protein Pair Similarity [Tabei et al., *KDD '13*]

- View chemical compound as a feature vector / bag of words.
- Given query Q, find all compounds at small Jaccard distance
- Database: $W_1, W_2, \ldots$.
- New constraint: each W_i has a real number $F(W_i)$ giving its *functionality*.
  - Filtering criterion: find all W_i s.t. $|Q \cap W_i| \geq k$.
  - In addition, we only want those W_i s.t. $|F(W_i) - F(Q)| \leq \delta$.
- Idea is similar to the wavelet-tree based similarity search, but we have an additional array containing $F(W_i)$.
- This array is also represented as a wavelet tree, except this time viewed as a range tree.
- Extra constraint is just orthogonal range reporting.

▷ Highly scalable, very accurate results.

Libraries

- A number of good implementations of succinct data structures in C++ are available.
- Different platforms, coding styles:
  - `sdsl-lite` (Gog et al. U. Melbourne).
  - `succinct` (Grossi and Ottaviano, U. Pisa).
  - `Sux4J` (Vigna, U. Milan, Java).
  - `LIBCDS` (Claude and Navarro, Akori and U. Chile).
- All open-source and available as `Git` repositories.

sdsl-lite

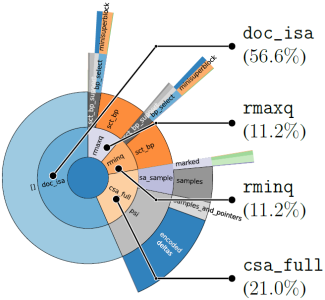
```
#include <sdsl/wavelet_trees.hpp>
#include <iostream>

using namespace sdsl;
using namespace std;

int main(int argc, char* argv[])
{
    wt_huff<rrr_vector<63>> wt;
    construct(wt, argv[1], 1);

    cout << "wt.size()="<< wt.size() << endl;
    cout << "wt.sigma ="<< wt.sigma << endl;
    if (wt.size() > 0) {
        cout << "wt[0]=" << wt[0] << endl;
        uint64_t r = wt.rank(wt.size(), wt[0]);
        cout << "wt.rank(wt.size(), wt[0])=" << r << endl;
        cout << "wt.select(r, wt[0]) = " << wt.select(r, wt[0]) << endl;
    }
}
```

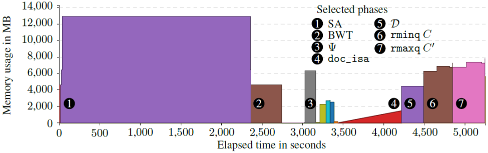
- Probably the most extensive, best-documented and maintained library.
- Easy to use, flexible, very efficient (may not be the absolute best in efficiency).

sdsl-lite (2)

Other sdsl-lite features:

- Structured to facilitate flexible prototyping of new high-level structures (building upon bases such as bit vectors).
- Robust in terms of scale, handling input sequences of arbitrary length over arbitrary alphabets.
- Serialization to disk and loading, memory usage visualization.





Conclusions

- Use of succinct data structures can allow scalable mining of big data *using existing algorithms*.
  - With machines with 100s of GB RAM, maybe even Big Data can be mined using compressed data structures.
- Succinct data structures need to be chosen and used appropriately: much room for application-specific tweaks and heuristics.
- Many of the basic theoretical foundations have been laid, and succinct data structures have never been easier to use.