The Power of Theory in the Practice of Hashing with Focus on Similarity Estimation

Mikkel Thorup

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Thanks for inviting me to talk here at AAML'24.

Talk surveys results from

- M. Patrascu and M. Thorup: The power of simple tabulation hashing. STOC 2011.
- M. Thorup: Bottom-k and priority sampling, set similarity and subset sums with minimal independence. STOC 2013.
- S. Dahlgaard, M.B.T. Knudsen and E. Rotenberg, and M. Thorup: Hashing for Statistics over K-Partitions. FOCS 2015.
- S. Dahlgaard, M.B.T. Knudsen, M. Thorup: Practical Hash Functions for Similarity Estimation and Dimensionality Reduction. NIPS 2017.
- S. Dahlgaard, M.B.T. Knudsen, M. Thorup: Fast Similarity Sketching. FOCS 2017.
- J.B.T. Houen, and M. Thorup: Understanding the Moments of Tabulation Hashing via Chaoses. ICALP 2022.
- J.B.T. Houen, and M. Thorup: A Sparse Johnson-Lindenstrauss Transform Using Fast Hashing. ICALP 2023.
- I.O. Bercea, L. Beretta, J. Klausen, J.B.T. Houen, and M. Thorup: Locally Uniform Hashing. FOCS 2023:

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- Bridging theory (assuming truly random hashing) with practice (needing something implementable).
- Many randomized algorithms are very simple and popular in practice, but often implemented with too simple hash functions, so guarantees only for sufficiently random input.
- Too simple hash functions may work deceptively well in random tests, but the real world is full of structured data on which they may fail miserably (as we shall see later).

Wegman & Carter [FOCS'77]

We do not have space for truly random hash functions, but

Family $\mathcal{H} = \{h : [u] \to [r]\}$ *k-independent* iff for rand om $h \in \mathcal{H}$:

- $(\forall) x \in [u]$, $h(x)$ is uniform in $[r]$;
- $(\forall) x_1, \ldots, x_k \in [u]$, $h(x_1), \ldots, h(x_k)$ are independent.

Prototypical example: degree $k-1$ polynomial

- $u = r = p$ prime;
- choose $a_0, a_1, \ldots, a_{k-1}$ uniformly and independently in $[p]$;
- $h(x) = \left(a_0 + a_1 x + \cdots + a_{k-1} x^{k-1}\right) \bmod p$.

For any algorithmic application, we can ask how much independence is needed (but we will do better).

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- Hashing used to create comparable sketches.
- Will study how hash function implementation impacts quality of estimates.

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k-Mins use k independent hash functions $h_1, ..., h_k$
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Expected relative error below $1/\sqrt{J(A, B) \cdot k}$.

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Bias ε not improved by k-mins no matter repetitions k.

Practice with k-mins

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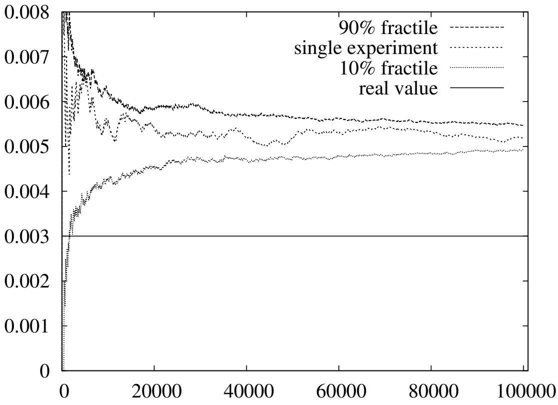

Measures dissimilarity between sets whose intersection are consecutive numbers and the rest is random numbers.

Bottom-k

With single hash function h, the bottom-k sketch of set X is

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Porat proved this for 8-independent hashing and $k \gg 1$.

Practice with bottom-k

We can use Dietzfelbinger's super fast 2-independent hashing

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random int64 a,b;
h(int32 x) return (a*x + b) >> 32;
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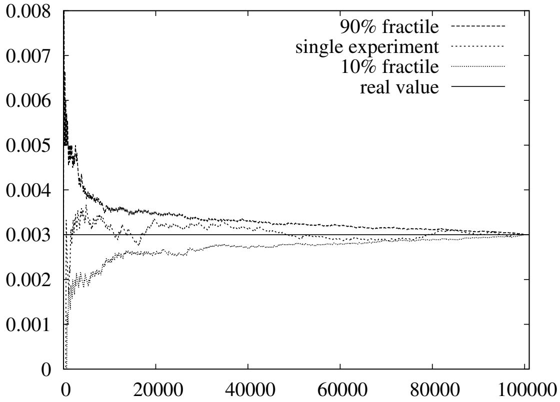

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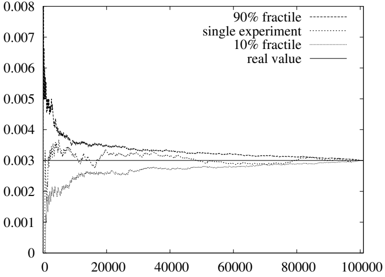

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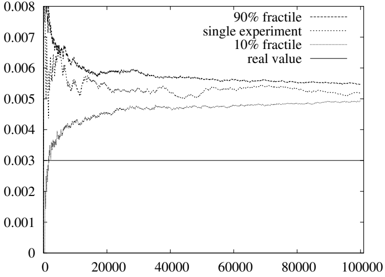

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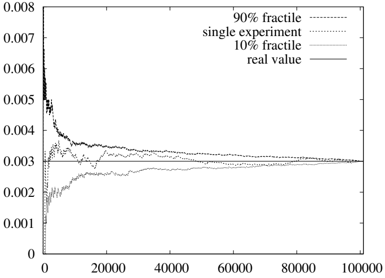

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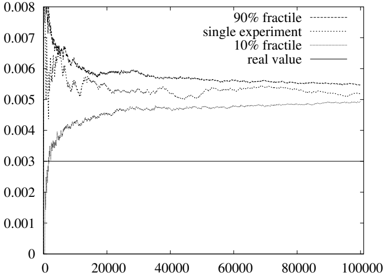

Besides diminishing bias with bottom-*k*, we have stronger convergence because it uses sampling without replacement, whereas *k*-mins is with replacement.

Analysis of Bottom-k

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Want same bound for bottom-k sample S with 2-independent hashing, but $x \in S$ depends on all hash values.

Analysis of Bottom-k by Simple Union Bound

With $n = |X|$, $S = S_k(X)$, $Y \subseteq X$, estimate $f = |Y|/|X|$ as

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Overestimate: For parameters $a < 1$, b, bound probability

$$(*) \qquad |Y \cap S| > \tfrac{1+b}{1-a} f\, k.$$

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$$p = \frac{k}{n\,(1-a)}.$$

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so $\Pr[(*)] \leq \Pr[(A)] + \Pr[(B)]$.

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Proof: ¬(A)∧¬(B) $\implies$ ¬($*$)

Suppose (A) is false, that is,

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Proof: $\neg$(A)$\wedge\neg$(B) $\implies \neg(*)$

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Then, since S contains k smallest,

$$\forall x \in S : h(x) < p.$$

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$$Y \cap S \subseteq \{x \in Y | h(x) < p\}$$

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With $p = k/(n\,(1 - a))$ and $|Y| = f\, n$, we get

$$|Y \cap S| \leq |\{x \in Y | h(x) < p\}| < (1 + b)\, p\, |Y| = \frac{1 + b}{1 - a} f\, k$$

so the overestimate $(*)$ did not happen.

2-independence

Proposition With $p = \frac{k}{n\,(1-a)}$, the overestimate

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so $\Pr[(*)] \leq \Pr[(\mathrm{A})] + \Pr[(\mathrm{B})]$.

Application If h is 2-independent, by Chebyshev,

$$\begin{aligned} \Pr[(A)] &\leq 1/(a^2 k) \\ \Pr[(B)] &\leq 1/(b^2 f\, k) \end{aligned}$$

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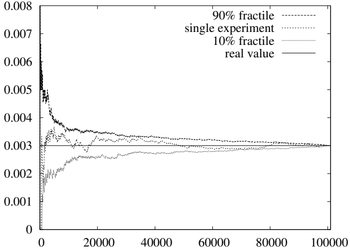

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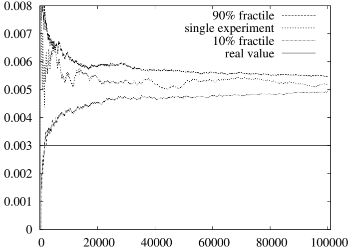

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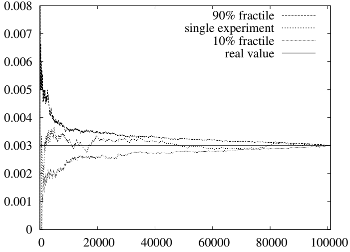

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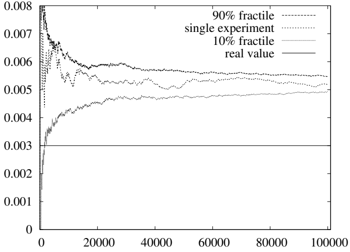

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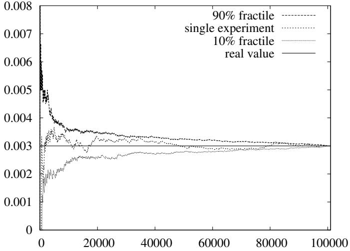

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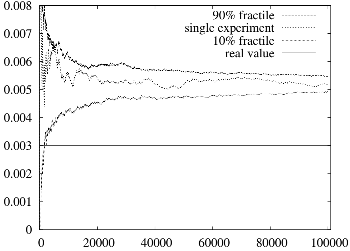

- Analysis: union bound over two simple Chebyshev bounds.
- Bottom-*k* also efficient in steaming: maintain *k* smallest elements in priority queue in $O(\log k)$ time per element.

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- With exponential concentration, suffices with $k = \Theta(\log n)$.

Consistency and uniformity

For each $i \in [t]$, we want

- *consistency*:

$$S(C)_i \in A \subseteq C \implies S(A)_i = S(C)_i.$$

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Each sample $S(A \cup B)_i$ uniform in $A \cup B$, so unbiased:

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- In black box manner (that also applies to other algorithms), argue that performance almost as good as with full randomness.
- Finally, with experiments, we demonstrate significance of using the right hash function.

Vector sample with k-mins of Broder et al.

For each $i \in [k]$ independently,

- we have hash function $h_i : U \to [0, 1)$,
- and define $S(A)_i = \text{argmin}_{x \in A} h_i(x)$.

Example

$k = 4$, $A = \{5, 27, 52, 73, 99\}$.

Ordered by h_i min on top

h_0	5	h_1	73	h_2	52	h_3	73
	99		27		99		5
	27		99		27		52
	52		5		5		99
	73		52		73		27

$S(A) = (5, 73, 52, 73)$.

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One-Permutation Sampling by Li et al. [NIPS'12]

- Two random hash function $h : U \rightarrow [0, 1)$ and $b : U \rightarrow [k]$.
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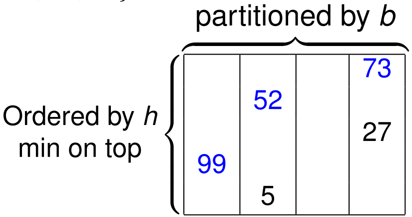

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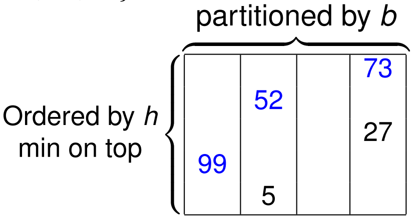

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But undefined samples pose problems.

Want sketching procedure with fixed k, not knowing set sizes.

One-permutation sampling with Densification [Shrivastava Li ICML'14,UAI'14,ICML'17]

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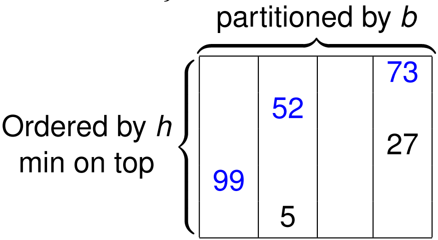

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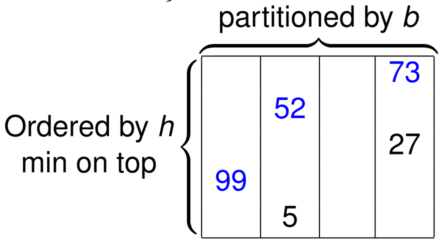

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but concentration no longer exponential in k.

Fast Similarity Sketch [Dahlgaard, Knudsen, T, FOCS'17]

We have

- k independent hash functions $h^j : U \to [0, 1)$, $j \in [k]$,
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- k independent hash functions $h^j : U \to [0,1)$, $j \in [k]$,
- k independent hash function $b^j : U \to [k]$, $j \in [k]$.
- k independent hash function $h_i : U \to [0,1)$, $i \in [k]$,

To compute $S(A)$:

- Initialize $S(A)$ with all empty entries $S(A)_i$.
- For $j = 0, \ldots, t-1$,
  - Make a one-permutation sketch $S^j(A)$ using h^j and b^j.
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  - If all entries of $S(A)_i$ full, return $S(A)$.
- If any empty entries, use last k hash functions for repeated min-wise sketch to fill remaining empty entries, that is, if $S(A)_i$ is empty, set $S(A)_i = \text{argmin}_{x \in A} h_i(x)$.

Example

$k = 4$, $A = \{5, 27, 52, 73, 99\}$.

				73
		52		
One-Permutation				27
	99			
		5		
		52		
			99	
One-Permutation			5	
		27		
				73
Another $k-2$ permutations	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	5	73	52	73
	99	27	99	5
k-Mins	27	99	27	52
	52	5	5	99
	73	52	73	27

$S(A) = (99, 52, 99, 73)$.

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	99			
		5		
		52		
			99	
One-Permutation			5	
All k samples found,		27		
so we can stop				73
Another $k-2$ permutations	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	5	73	52	73
	99	27	99	5
k-Mins	27	99	27	52
	52	5	5	99
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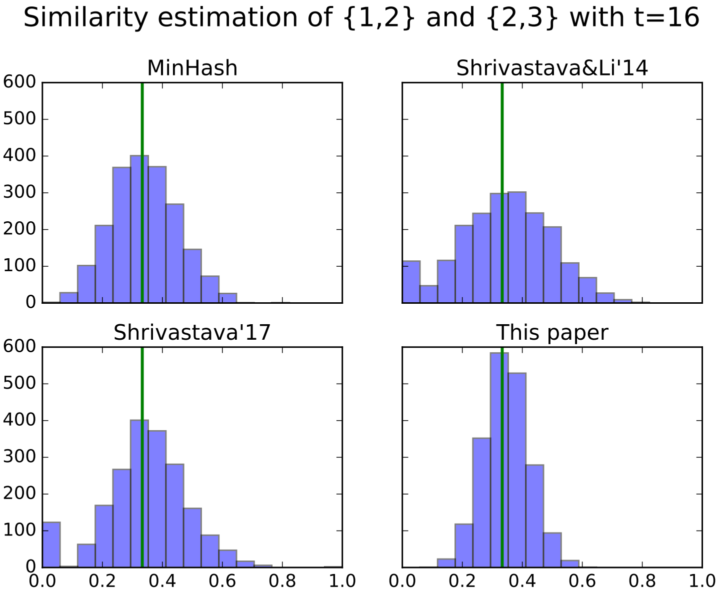
Experiments



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		52		
One-Permutation				27
	99			
		5		
		52		
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Another $k-2$ permutations	⋮	⋮	⋮	⋮
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Computed in $O(|A| + k \log k)$ w.h.p.

Efficiency

Lemma Our fast similarity sketch computed in $O(|A| + k \log k)$ time, w.h.p.

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- E.g., if $|A| = \omega(k \log k)$, w.h.p., all full after first one-permutation sketch.
- If we end up in the final k-Mins sketch, then this only doubles the total time.

With and without replacement

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  Takes $O(|A| + k \log k)$ time w.h.p.

Chernoff Bound

- Similarity estimator $J_S(A, B)$ unbiased and concentrated around its mean $J = J(A, B)$. For $\delta > 0$,

$$\Pr[J_S(A, B) \geq J(1 + \delta)] \leq \left(\frac{e^{\delta}}{(1 + \delta)^{1+\delta}} \right)^{J\,k},$$

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Proof idea Negative correlation from without replacement can only decrease the moments in standard proof based on Taylor expansion.

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Example $k = 4$, $A = \{5, 27, 52, 73, 99, 63, 96\}$.

	96			73
		52		
One-Permutation			63	27
All k samples found,	99			
so we can stop		5		
		52		96
			99	
One-Permutation	63		5	
		27		
				73
Another $k-2$ permutations	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	5	73	52	73

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- Want number of red samples $|R \cap S|$ concentrated around expectation $k|R|/|R \cup B|$.

Implementing one-permuation hashing

Generic implementation of one-permutation sampling uses single hash function $H : U \to [2^\ell]$

$$H(x) = \overbrace{0010101110010101001}^{\substack{\text{bucket} \\ b(x) = \text{first } \log_2 k \text{ bits}}}\overbrace{00011001010001110010011100}^{\substack{\text{local hash} \\ h(x) = \text{remaining } \ell - \log_2 k \text{ bits}}}$$

$$S(A)_i = \text{argmin}_{x \in A, b(x) = i} h(x).$$

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partitioned by b

Ordered by h
min on top

96			73
	52		
		63	27
99			
	5		

$S(A) = (96, 52, 63, 73)$.

Too simple implementation of one-permuation hashing

Classic $H(x) = (ax + b) \bmod p$, Mersenne prime $p = 2^\ell - 1$.

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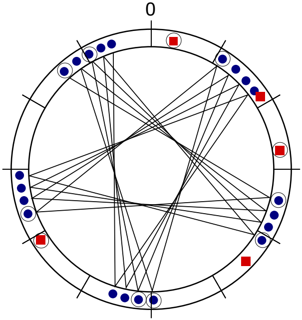
$B = \{1, \ldots, 25\}$ (consecutive) and
$R = \{926, 53, 478, 734, 263\}$ (random outliers)



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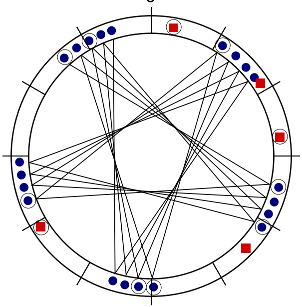

$S(R \cap B) = (■, •, ■, •, •, •, •, ■, •, \div, •)$.
Then $|S \cap R|/|S| = 3/11$ far from $|R|/|R \cup B| = 5/30 = 1/6$.

Need more independence between buckets

- one-permutation sampling throws elements into k buckets, and pick a random element from each bucket.
- k samples without replacement if all buckets non-empty,
- Sampling from $R \cup B$.
- With full randomness, fraction of samples from R concentrated around $|R|/|R \cup B|$ with Chernoff bounds —without replacement only decreases the moments.

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- Requires high indpendence between bucket contents —not clear if k independence suffices.
- This is a very generic issue: using hashing to distribute elements in buckets, and aggregating statistics over the buckets to get well-concentrated estimates.
- Idea also used for counting distinct elements [Flajolet et al. FOCS'83], count sketches, and feature hashing.

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  - Finally, we show experiments.

Simple Tabulation Hashing [Zobrist'70 chess]

- Key x divided into $c = O(1)$ characters $x_1, ..., x_c \in \Sigma$, e.g., 32-bit key as $4 \times$ 8-bit characters.

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- ... and it has a lot of power..

How much independence needed?

Chaining $\mathbf{E}[t] = O(1)$ $\mathbf{E}[t^k] = O(1)$ $\max t = O(\lg n / \lg\lg n)$	2 $2k+1$ $\Theta(\lg n / \lg\lg n)$	
Linear probing	≤ 5 [Pagh², Ružić'07]	≥ 5 **[PT ICALP'10]**
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Still many applications missing, e.g., for statistics, if we toss n coins, we want number of tails to be concentrated around $n/2$. Also, above, the O-notation hides large constant factors depending exponentially in c.

Zero sets and linear independence

Key set $Z \neq \emptyset$ is a zero set if in each position every character occurs an even number of times, i.e.,

$$\forall i, a \in [c] \times \Sigma : |\{x \in Z | x_i = a\}| \text{ is even.}$$

E.g., $\{a_1 a_2, a_1 b_2, b_1 a_2, b_1 b_2)\} \subset \Sigma^2$.

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Key set X linearly indepedent if it does not contain a zero set.

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Key set X linearly indepedent if it does not contain a zero set.

Lemma Key set $X \subseteq \Sigma^c$ is linearly independent if and only if simple tabulation hashing is fully random on X.

Zero sets and linear independence

Key set $Z \neq \emptyset$ is zero set if

$$\forall i, a \in [c] \times \Sigma : |\{x \in Z | x_i = a\}| \text{ is even.}$$

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C-code for Tornado Tabulation Hashing

```
#include <stdint.h>
uint32_t Tornado(uint32_t x, uint64_t[8][256] H) {
  uint32_t i; uint64_t h=0; uint8_t a;
  for (i=0;i<3;i++) {
    a=x;
    x>>=8;
    h^=H[i][a];}
  h^=x;
  for (i=3;i<8;i++) {
    a=h;
    h>>=8;
    h^=H[i][a];}
  h=&((1<<24)-1);
  return ((uint32_t) h);}
```

Local Uniformity

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- For vector k-sample based on one-permutation, w.h.p

$$1 - 7|X|^3(3/|\Sigma|)^{d+1} - 1/2^{|\Sigma|/2} .$$

we get almost as good as fully random if $|\Sigma| \geq \max\{7k \lg(dk|\Sigma|), d2^{16}\}$.

Local Uniformity: Under the Hood

Technical Theorem

- Let $h : \Sigma^c \to \{0,1\}^\ell$ be a tornado tabulation hash function with d derived characters.
- Let $D \subseteq [\ell]$ be set of output bit positions, called select bits.
- Let $h^{|D}$ be h outputting only hash bits from positions in D.
- Let M be a vector of $|D|$ bits
- For a given key set $X \subseteq \Sigma^c$, h selects a subset $S = \{x \in X | s(h^{|D}(x)) = M\}$.
- If $|\Sigma| \geq \max\{2^8, \mathbf{E}[|S|]\}$, then with probability

$$1 - 7|X|^3(3/|\Sigma|)^{d+1} - 1/2^{|\Sigma|/2} \ (= \text{w.h.p}),$$

all non-select hash bits from S are fully random.

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all non-select hash bits from S are fully random.

Note: If $D = \emptyset$ then $S = X$ and then h fully random on X.

- If moreover $|\Sigma| > d\,2^{16}$ and $\mu = \mathbf{E}[|S|]$, then, w.h.p.,

$$\Pr[||S| - \mu|] \geq \delta\mu] \leq 4\exp(-\mu\delta^2/7)$$

Fast Vector *k*-Sampling with Tornado Tabulation

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- If $|R \cup B| > |\Sigma|/2 = 7k \ln \sigma$, then, w.h.p, fast vector k-sampling uses single one-permutation sampling:

One-Permutation All k samples found, so we can stop	96 99	52 5	63	73 27
One-Permutation	63	52 27	99 5	96 73
Another $k-2$ permutations	⋮	⋮	⋮	⋮
	5 99	73 27	52 99	73 5

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- If $|R \cup B| > |\Sigma|/2 = 7k \ln \sigma$, then, w.h.p, fast vector k-sampling uses single one-permutation sampling.
- Henceforth focus on this one-permutation case.

One-Permutation k-Sample using Tornado Tabulation

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- With probability $1 - k/\sigma > 1/|\Sigma|^{d-1}$, every bucket has a small key, so all samples $S(R \cup B)_i$ are small.

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- Assume $|R| = |B|$ (will be removed later).
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- Then $\mathbf{E}[|R_z|] = p_z|R| = 3.5k(\ln \sigma) \ll |\Sigma|/2$, so by Tornado Chernoff, w.h.p,

$$|R_z| = \left(1 \pm \sqrt{\frac{7 \ln \sigma}{\mathbf{E}[|R_z|]}}\right)\mathbf{E}[|R_z|] = (1 \pm \sqrt{2/k})p_z|R|.$$

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One-Permutation k-Sample using Tornado Tabulation

Tornado table size $|\Sigma| \geq 14k \ln \sigma$ where $\sigma = |\Sigma|^d$.

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- Key x small if $z = \log_2(|R \cup B|/(7k \ln \sigma))$ leading zeros in $h(x)$. W.h.p, all samples $S(R \cup B)_i$ are small.
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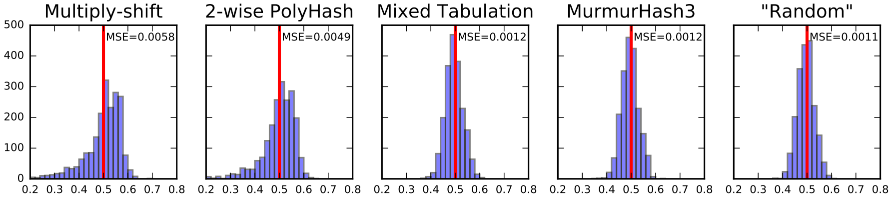
- As before, we get
  $|S \cap R| = |S \cap R_z| = (1 \pm \sqrt{(3 \ln \sigma + 9)/k})\, kf$.

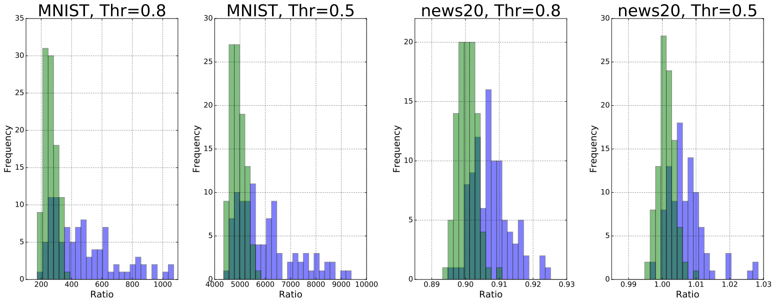
Experiments [Dahlgaard, Knudsen, T, NIPS'17] using Mixed Tabulation, a predecessor of Tornado

Hash function	time ($1..10^7$)	time (News20)
Multiply-shift	7.72 ms	55.78 ms
2-wise PolyHash	17.55 ms	82.47 ms
3-wise PolyHash	42.42 ms	120.19 ms
MurmurHash3	59.70 ms	159.44 ms
CityHash	59.06 ms	162.04 ms
Blake2	3476.31 ms	6408.40 ms
Mixed tabulation	42.98 ms	90.55 ms



Real-World Data inside Locality Sensitive Hashing

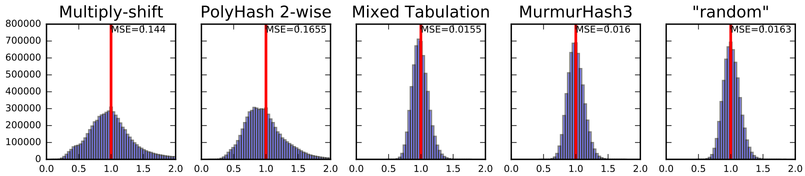
- **MNIST** Standard collection of handwritten digits.
- **News20** Collection of newsgroup documents.



Mixed tabulation smaller (=better) than Multiply-Shift.

Real-World Data inside Feature Hashing

MNIST Standard collection of handwritten digits.



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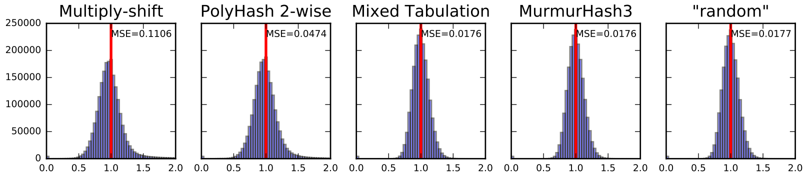
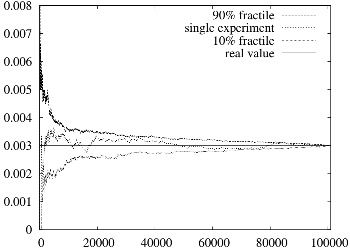


Concluding remarks

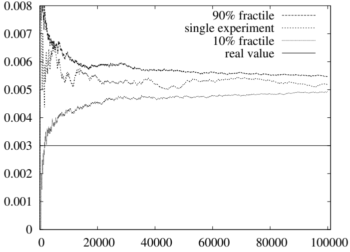
Conclusion on k-mins versus bottom-k

- Both k-mins and bottom-k generalize the idea of storing the smallest hash value.
- With limited independence
  k-mins has major problems with bias whereas bottom-k works perfectly even with 2-independence.

bottom-k



k-mins



- Analysis: union bound over two simple Chebyshev bounds.
- Bottom-k also efficient in steaming: maintain k smallest elements in priority queue in $O(\log k)$ time per element.

Similarity Vector Sample

- Sketch S maps any set A to vector of k samples from A.
- Want S to preserve similarity between sets A and B:
- For each coordinate $i \in [k]$, unbiased estimator

$$\Pr[S(A)_i = S(B)_i] = J(A, B) = |A \cap B| / |A \cup B|.$$

- Let

$$J_S(A, B) = \sum_{i \in [k]} [S(A)_i = S(B)_i] / k.$$

- Want strong concentration of $J_S(A, B)$ around $J(A, B)$.
- The alignment property, that $S(A)_i$ only compared with $S(B)_i$ important, e.g., for Support Vector Machines (SVMs).
- To code similarity as inner product, hash each $S(A)_i$ to b bits with single 1 [Li König CACM'11], e.g, $k = 2$, $b = 4$,

$$\{5, 27, 52, 73, 99\} \rightarrow (72, 5) \rightarrow (0, 0, 0, 1 \textbf{,} 0, 1, 0, 0)$$

- Alignment not satisfied by bottom-k sketch.

Fast vector k-sampling $k = 4$, $A = \{5, 27, 52, 73, 99\}$.

				73
		52		
One-Permutation				27
	99			
		5		
		52		
			99	
One-Permutation			5	
		27		
				73
Another $k-2$ permutations	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	5	73	52	73
	99	27	99	5
k-Mins	27	99	27	52
	52	5	5	99
	73	52	73	27

$S(A) = (99, 52, 99, 73)$.

Fast vector k-sampling $k = 4$, $A = \{5, 27, 52, 73, 99\}$.

One-Permutation	99	52 5		73 27
One-Permutation All k samples found, so we can stop		52 27	99 5	73
Another $k-2$ permutations	⋮	⋮	⋮	⋮
k-Mins	5 99 27 52 73	73 27 99 5 52	52 99 27 5 73	73 5 52 99 27

$S(A) = (99, 52, 99, 73)$.

- $O(|A| + k \log k)$ time and Chernoff concentration bounds.

Concentration needs independence between buckets

- Fast Vector Sampling and One-Permutation sampling throws elements into k buckets, and pick a random element from each bucket.
- With full randomness, fraction of samples from R concentrated around $|R|/|R \cup B|$ with Chernoff bounds
- Requires high indpendence between bucket contents.
- Not clear if k independent hashing suffices.
- Generic issue: using hashing to distribute elements in buckets, and aggregating statistics over the buckets to get well-concentrated estimates.
- Idea also used for counting distinct elements [Flajolet et al. FOCS'83], count sketches, and feature hashing.
- Mixed Tabulation Hashing solves the problem quite generically.

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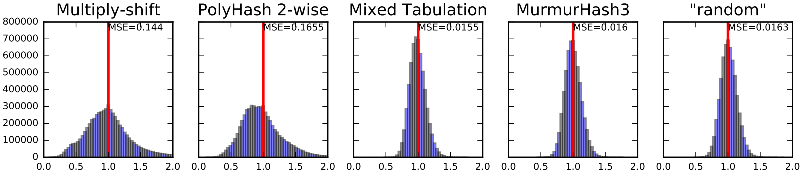

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- The bad thing is that analysis is non-trivial.
- The good thing is that the tabulation hashing is simple and efficient, ready for use in applications.
- This contrast the use of too simple hash functions relying on randomness in input.

Thanks for your attention