SET-MIN SKETCH: A PROBABILISTIC MAP FOR POWER-LAW DISTRIBUTIONS WITH APPLICATION TO k-MER ANNOTATION

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ABSTRACT

Motivation: In many bioinformatics pipelines, k-mer counting is often a required step, with existing methods focusing on optimizing time or memory usage. These methods usually produce very large count tables explicitly representing k-mers themselves. Solutions avoiding explicit representation of k-mers include Minimal Perfect Hash Functions (MPHFs) or Count-Min sketches. The former is only applicable to static maps not subject to updates, while the latter suffers from potentially very large point-query errors, making it unsuitable when counters are required to be highly accurate.

Results: We introduce Set-Min sketch, a sketching technique inspired by Count-Min sketch, for representing associative maps, more specifically, k-mer count tables. We show that Set-Min sketch provides a very low error rate, both in terms of the probability and the size of errors, much lower than a Count-Min sketch of similar dimensions. On the other hand, Set-Min sketches are shown to take up to an order of magnitude less space than MPHF-based solutions, especially for large values of k. Space-efficiency of Set-min takes advantage of the power-law distribution of k-mer counts in genomic datasets.

Availability: `https://github.com/yhhshb/fress`

***K*eywords** Sketching · k-mers · Counts

1 Introduction

Counting k-mer occurrences in genomic sequences is a rather common task in many bioinformatics pipelines. It is often the first step performed before a more complicated analysis, and its main applications go from read trimming [1] to alignment-free variant calling [2, 3]. In recent years, many k-mer counting algorithms have been proposed, such as Jellyfish[4], DSK[5] or KMC[6].

All these tools output a map associating k-mers to their counts. Such a map can require a fairly big amount of disk space, especially when large values of k are used. For example, the KMC output for a human genome with $k = 32$ weights in at around 28 GB, and even when compressed, memory efficiency remains an important issue. A way to tackle this problem is to only store counters, discarding k-mers information. This idea is supported by the fact that in many applications, queried k-mers come from partially assembled reads or succinct representations, such as SPSS [7, 8], or Colored de Bruijn graphs[9], that is, only k-mers present in the original data are queried for their frequencies.

The idea of storing only counter information and not k-mers is also supported by the observation that the number of distinct k-mer counts in genomic data is relatively small. It is known that k-mer counts in genomes obey a "heavy-tail" power-law distribution[1] with a relatively large absolute value of the exponent [10, 11]. For such distributions, the number of *distinct* k-mers makes a linear fraction of the data size, while the number of *distinct* k-mer counts is relatively

[1]Here we assume k to be sufficiently large, typically $k > \log_4 L$, where L is the data size.

small. For example, for the human genome and $k = 27$, there are about 2.5 billions distinct k-mers but only about 8,000 distinct frequency values. This is because the majority of k-mers have a very small count: in the above example, 97% of k-mers are unique and 99% of k-mers have a count of at most 5. Frequent k-mers often tend to have an identical count as well, due to transposable elements: for example, k-mers specific to Alu repeats in primate genomes will likely have the same count.

Our contribution. We propose a new probabilistic data structure that we call *Set-Min sketch* capable to represent k-mer count information in small space and with small errors. The sketch guarantees that the expected *cumulative error* obtained when querying all k-mers of the dataset can be bounded by εN where N is the number of *all* k-mers (i.e. essentially, the size of the dataset). We provide a theoretical analysis in order to dimension the sketch according to the desired error bound. We further present experimental results on a range of datasets illustrating the benefits of our approach, and compare it with alternative solutions: Count-Min sketch and Minimal Perfect Hashing. Note, finally, that Set-Min sketch is a general data structure in that it can be used to efficiently represent a mapping of k-mers to any type of labels, provided that the number of possible labels is relatively small.

Applications. Set-Min sketch can have different use cases. In this paper, we explore the probabilistic compression of genomic k-mer counter tables in case of large k values. Thanks to the characteristic skewed distribution of the frequencies for large ks, a Set-Min sketch is able to provide a more space-efficient map than other representations with low errors.

One application of Set-Min sketches, not explored here, is to act as a temporary representation while building more complex structures based on counters. Consider, for example, the exact computation of weighted pairwise distances between all pairs of genomes in a given set. Examples of such distances are the Bray-Curtis similarity measure, see e.g. [12], or Weighted Jaccard similarity estimation [13]. The most naive algorithm is to first produce count tables for each dataset and then compare them pair-wisely to produce the desired output. Instead of storing whole tables, one can store multiple Set-Min sketches together with a presence-absence data structure, such as a Bloom filter. By doing so, the weighted comparison computation is reduced to a single pass through the presence-absence data structure with the counters of a given k-mer retrieved on-demand from the Set-Min sketches of the datasets in which the k-mer is found.

Another possible application is sharing counter information between different computational units in a distributed setting. Consider, for example, a scenario where a server oversees multiple less powerful machines. All nodes have access to the same genomic representation (say, a set of contigs), but only the server can efficiently perform k-mer counting, while the smaller machines have the task of processing incoming data based on the counts. In this case, the server could send a Set-Min sketch to all its subordinates.

One further feature of Set-Min sketch is its mergeability from redundant maps. A large map can be split into m sub-maps without the restriction of having disjoint sets of keys. Even if some maps have redundant information, i.e. share common (key,value) pairs, the Set-Min sketch built by cell-wise union of the m sketches will be equivalent to the sketch built from the whole original map. Count-Min sketches do not have this property but instead they are mergeable when constituent maps should be "added up". In case of redundancy, Count-Min will simply count each repeated item multiple times. In this respect, Set-Min and Count-Min sketches may have complementary uses.

Outline of the paper. In Section 2, we start by formally introducing the relevant terminology and underlying methods. Section 3 presents the idea and algorithmic foundations of our method. Our results are presented in Section 4 while Section 5 discuss the limitations of our method and possible workarounds. We conclude in Section 6 with a summary of the work.

2 Background

2.1 k-mer spectrum

A k-mer spectrum is a distribution of k-mer frequencies across all k-mers occurring in the data, showing how many k-mers support each frequency value. For large values of k, k-mer spectra follow a power-law distribution [10, 11] characterized by a linear-like dependence when represented in the log-log scale. That is, the k-mer frequency distribution fits a dependence $f(t) \approx c \cdot t^{-a}$, where a is usually greater than 2. An example of the spectrum for the human reference genome with k equal to 32 is given in Figure 1.

According to this distribution, a very large fraction of k-mers have very low frequencies, while a few k-mers have "unexpectedly" large frequencies. Large value of a implies that there are relatively few distinct frequency values with non-zero support, whose number depends as the $\frac{1}{a}$-power of the number of k-mers.

2.2 Count-Min sketch

Count-Min sketch is a sketching technique for memory efficient representation of high-dimensional vectors. First introduced in [14], it is especially suitable for the streaming framework where vectors are dynamically updated. A Count-Min sketch is a matrix of $R \times B$ counters. Each row i of the matrix is associated with a hash function $h_i(\cdot)$. At construction time, each key is hashed using the hash functions to index one bucket in each row, and the counter for the key is added to each of these buckets. Because of the additive nature of the update, knowing the total counter of each key beforehand is not required and the construction can be maintained over a stream of keys. A query returns the minimum bucket value among the ones associated to the given key.

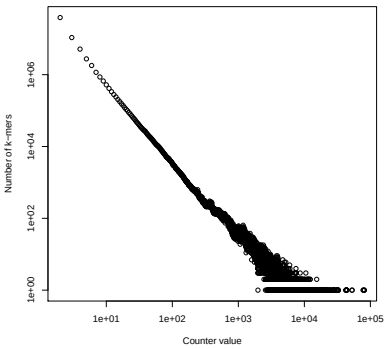


Figure 1: k-mer spectrum of the human genome for $k = 32$ in the log-log scale.

In general, given a Count-Min sketch built on a vector $\boldsymbol{a}$, with $R = \lceil \ln(\frac{1}{\delta}) \rceil$ and $B = \lceil \frac{e}{\varepsilon} \rceil$ for any given ε and δ, the over-estimate error of an individual counter is bounded by $\varepsilon \|\boldsymbol{a}\|_1$ with probability at least $1 - \delta$, where $\|\boldsymbol{a}\|_1$ is the L_1-norm of $\boldsymbol{a}$ [14]. If counts follow a power-low distribution with parameter $\alpha > 1$, B can be reduced to $O(\varepsilon^{-1/\alpha})$ to guarantee the same bounds [15].

However, when query accuracy is at a premium, these bounds may not be sufficient. For example, if $B = \Theta((\|\boldsymbol{a}\|_1)^{1/\alpha})$, then Count-Min sketches guarantees only $O(1)$ error for point queries, with high probability. In the experimental part of this work (Section 4), we show that when applied to the k-mer counting, the error of Count-Min may not be acceptable.

2.3 Minimal Perfect Hashing

Minimal Perfect Hash Functions (MPHFs) are hash functions associating an ordering to keys of an input set. More precisely, given a set S of keys, a minimal perfect hash function $h(\cdot)$ maps each key of S into a unique index of the interval $[0, |S| - 1]$. Therefore, MPFHs can represent k-mer counter tables when augmented with an accessory array A of size $|S|$ containing the counters.

The construction of a MPHF can be hyper-graph peeling-based [16, 17] or array-based [18]. The first family of algorithms leads to smaller MPHFs, close to the theoretical space lower-bound of 1.44 bits per key, while array-based MPHFs are more cache friendly and much easier conceptually despite being less memory efficient than their mainstream counterparts. First introduced in [18], array-based MPHFs have found their way to bioinformatics applications via a practical implementation called BBHash [19]. Albeit theoretically simpler than its inspiring method, BBHash achieves great time-memory trade-offs and was the first implementation capable of constructing a hash function for a set of cardinality of 10^{12}.

Array-based construction algorithms work by repeatedly resolving collisions when hashing the keys to arrays. Each cell of the arrays cannot contain more than one element. The index of a key is retrieved by a query to a rank/select data structure counting the number of cells occupied before the wanted element. During construction, it is thus necessary to save the sets of colliding keys or to re-run the construction algorithm over the entire stream of keys multiple times, generating a new array for each layer.

Given its simplicity and its reliance on simple arrays of elements, hereafter we focus on array-based MPHFs, with BBHash as the reference method.

3 Methods

3.1 Set-Min sketch in a nutshell

Assume we are given a set K of keys with associated values taken from a set L with $|L| \ll |K|$. In our case, K is a set of k-mers and L the set of their frequencies, although our method will hold for any set of labels L, not necessarily numerical. We want to compactly implement the associative map of (key,value) pairs. A Set-Min sketch is an $R \times B$ matrix M where each bucket is treated as a set, initially empty. Similar to Count-Min sketch, rows in the matrix correspond to hash functions h_i, $0 \leq i \leq R - 1$, that we assume pairwise independent.

At construction time, the key of each (key,value) pair (p, ℓ) is hashed by the hash functions to retrieve its buckets and the value ℓ is inserted into each set. Formally, we update $M(i, h_i(p)) = M(i, h_i(p)) \cup \{\ell\}$ for each row i. Figure 2 shows an example.

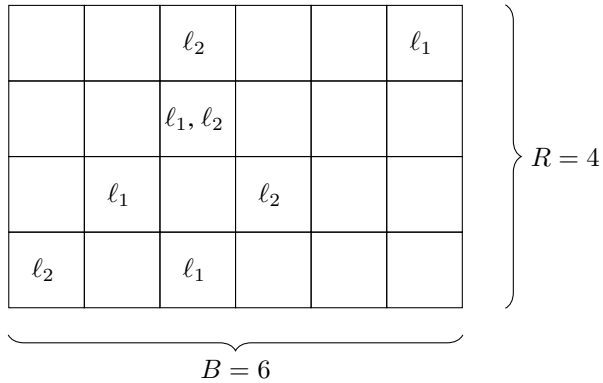


Figure 2: Example of a Set-Min sketch with $L = \{\ell_1, \ell_2\}$. Two pairs (e, ℓ_1) and (f, ℓ_2) with $e \neq f$ have been inserted into the sketch, with e, f hashed to the same bucket at line 2.

To retrieve the value associated with a key p, we compute the intersection of the corresponding sets, that is $\cap_{0 \leq i \leq R-1} h_i(p)$. If the intersection is a singleton, the value is returned. If the intersection is empty, p is not present in the map. If the intersection contains more than one value, we have a collision.

3.2 Dealing with collisions

When we have a collision, we have to decide which label to return to the query. The choice is guided by the number of k-mers supporting each label of the intersection: the label with the smallest support is returned. The rationale for this is that the label with the smallest support has the smallest probability to appear "by chance", as labels with larger support belong to more buckets in the sketch and are therefore more likely to occur in the intersection by chance. Thus, the algorithm compares spectrum values for all labels in the intersection, and returns the label with the smallest value (ties are broken randomly). If the spectrum is monotonically decreasing (as it is usually the case for large k, see Figure 1), then the label returned is simply the largest one among those in the intersection.

In this work we assume that only k-mers present in the dataset can be queried. In this case, a query can no longer result in an empty intersection. We further optimize by not storing in the sketch the label ℓ_1 with the largest support. For large k, ℓ_1 is usually 1, which is the frequency of the largest fraction of k-mers. ℓ_1 is retrieved implicitly: when the intersection is empty, ℓ_1 is returned. This optimization allows us to save space and will be further discussed later. Note that, with these modification, an error may occur even if the resulting intersection is a singleton but the right label is actually ℓ_1 and not the label obtained.

3.2.1 Bounding the total error

We now show that with Set-Min sketch, we can bound the *total* absolute error over all k-mers present in a dataset. Consider a sketch S built on a map assigning to each k-mer $p \in K$ a value (label) $\ell_p \in L$ which is the frequency of p in the dataset. We denote by c_ℓ the number of k-mers with frequency $\ell \in L$ (spectrum value).

Consider

$$D = \sum_{p \in K} |\hat{\ell}_p - \ell_p| \tag{1}$$

where $\hat{\ell}_p$ is the label of p returned by the sketch. Our goal is to dimension R and B such that $D \leq \varepsilon \|\boldsymbol{a}\|_1$, where $\|\boldsymbol{a}\|_1$ is the total number of k-mers in the dataset (roughly, the dataset size) and $0 < \epsilon \leq 1$.

Querying p returns an incorrect frequency $m \neq \ell_p$ iff m occurs in the intersection and $c_m < c_{\ell_p}$. The probability of this event is

$$\left(1 - \left(1 - \frac{1}{B}\right)^{c_m}\right)^R \approx \left(1 - e^{-\frac{c_m}{B}}\right)^R \tag{2}$$

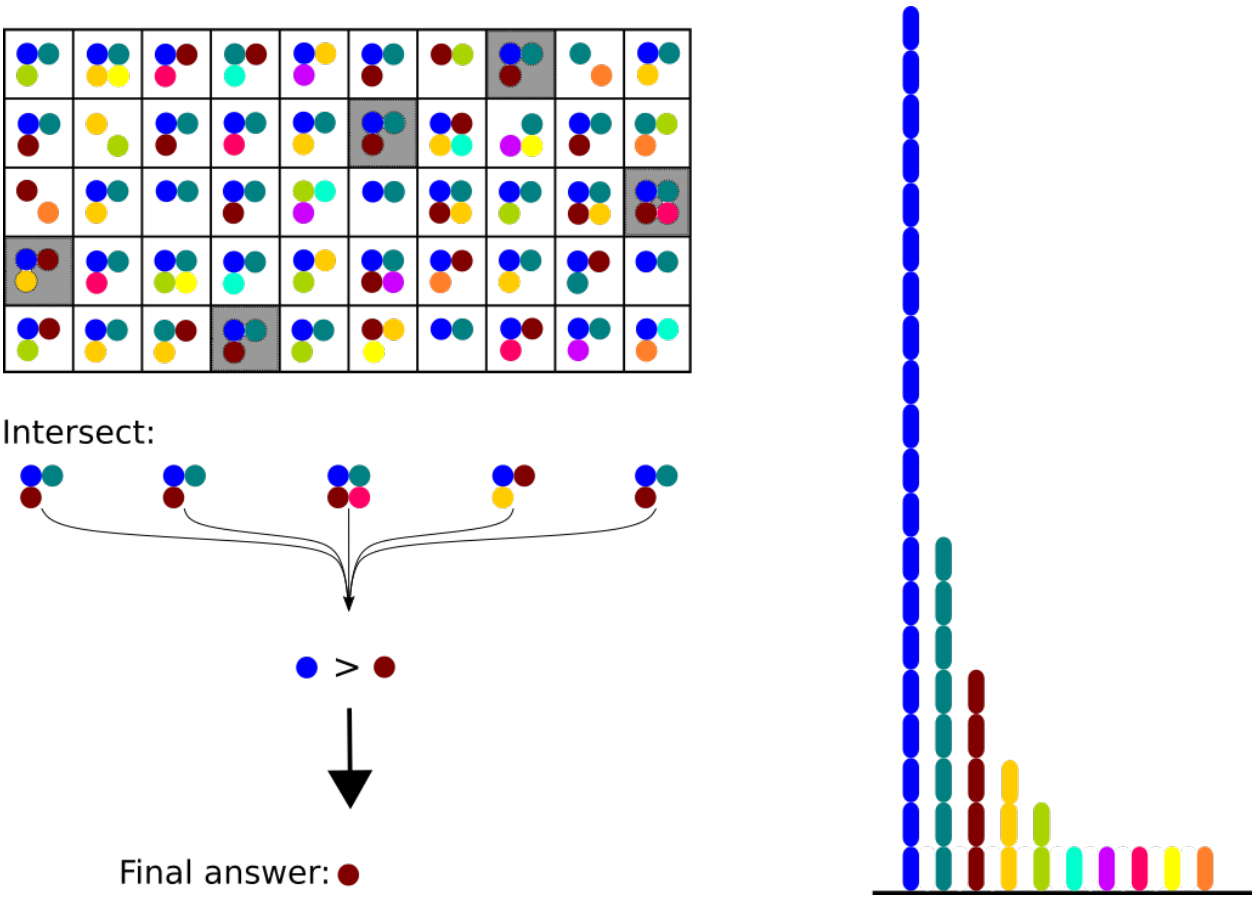


Figure 3: Example of collision resolution in case of multiple items occurring in the intersection. The brown label is returned because it is more rare compared to the blue one.

and the expectation of the error when querying p is then

$$\sum_{\substack{c_m < c_{\ell_p} \\ m \in L}} |m - \ell_p| \left(1 - e^{-\frac{c_m}{B}}\right)^R. \tag{3}$$

Summing up over all k-mers, we obtain

$$\mathrm{E}[D] = \sum_{\ell \in L} c_\ell \sum_{\substack{c_m < c_\ell \\ m \in L}} |m - \ell| \left(1 - e^{-\frac{c_m}{B}}\right)^R. \tag{4}$$

The total number of k-mers is $\|\boldsymbol{a}\|_1 = \sum_{\ell \in L} \ell c_\ell$. Given $0 < \varepsilon \leq 1$, our goal is to choose B and R in order to ensure

$$\sum_{\ell \in L} c_\ell \sum_{\substack{c_m < c_\ell \\ m \in L}} |m - \ell| \left(1 - e^{-\frac{c_m}{B}}\right)^R < \varepsilon \sum_{\ell \in L} \ell c_\ell. \tag{5}$$

For sufficiently large k, the spectrum is monotonically decreasing, i.e. $c_m < c_\ell$ iff $m > \ell$. (5) then rewrites to

$$\sum_{\ell \in L} c_\ell \sum_{\substack{m > \ell \\ m \in L}} (m - \ell) \left(1 - e^{-\frac{c_m}{B}}\right)^R < \varepsilon \sum_{\ell \geq 1} \ell c_\ell. \tag{6}$$

Assume now that the spectrum follows a power-law with large exponent, that is, $c_\ell = C \cdot \ell^{-a}$ for some $a > 2$. Note that under this assumption, the number of unique k-mers is $c_1 = C$, and the number of all k-mers is

$$\sum_{\ell \geq 1} \ell c_\ell = C \cdot \sum_{\ell \geq 1} \frac{1}{\ell^{a-1}} \leq C \cdot \frac{a-1}{a-2},$$

since $\zeta(s) = \sum_{i \geq 1} \frac{1}{i^s} \leq \frac{s}{s-1}$ for $s > 1$.

We then have the following result.

Theorem 1. *Given $0 < \varepsilon \leq 1$, if $B > C$ and R, B satisfy*

$$R \cdot \log \frac{B}{C} > \log \frac{1}{\varepsilon}, \tag{7}$$

then (6) holds.

The proof of Theorem 1 is given in the Appendix. The theorem allows us to dimension the Set-Min sketch. For example, one can set $B = \alpha C$ for some constant $\alpha > 1$ and $R = \log_\alpha \frac{1}{\varepsilon}$.

3.3 Computing tighter sketch dimensions

Theorem 1 provides a way to dimension a Set-Min sketch, provided that the spectrum follows a power-law distribution with a sufficiently large parameter a. In order to validate these estimates experimentally, and, at the same time, obtain a tool for computing tighter values B and R for arbitrary spectra, we implemented a simple heuristic hill climbing algorithm to compute those values by directly solving equation 5.

The algorithm, given below, starts with $R = 1$ and some initial value of B and then iteratively increments R and recomputes (4) until equation (5) holds true. In the implementation, B is initially set to $1.44 \times c_{max}$, where c_{max} is the largest spectrum value. After such a value of R is found, the algorithm starts decrementing R while incrementing B to maintain the total space RB constant as long as (5) holds. The rationale for this step is to have as small R as possible in order to reduce the query time, while maintaining the total space.

Algorithm 1 Heuristic to compute R and B

Input: $\{c_\ell\}_{\ell \in L}$, $\|\boldsymbol{a}\|_1 = \sum_{\ell \in L} \ell c_\ell$, ε
Output: R and B
$R \leftarrow 1$
$B \leftarrow 1.44 \times c_{max}$
$T \leftarrow \varepsilon \|\boldsymbol{a}\|_1$
$E \leftarrow \mathrm{E}(D)$ (computed by (4))
while $E > T$ **do**
    $R \leftarrow R + 1$
    $E \leftarrow \mathrm{E}(D)$
end while
$M \leftarrow R \times B$
while $E < T$ **do**
    $R \leftarrow R - 1$
    $B \leftarrow \lceil \frac{M}{R} \rceil$
    $E \leftarrow \mathrm{E}(D)$
end while
$R \leftarrow R + 1$
$B \leftarrow \lceil \frac{M}{R} \rceil$

4 Results

4.1 Implementation

We implemented Set-Min in a software tool named `fress`, available at https://github.com/yhhshb/fress. The `fress` pipeline compares Set-Min with Count-Min and MPHF implementations. `BBHash` [19] (`https://github.com/rizkg/BBHash`) is the only external library required for comparison as Count-Min is implemented within `fress`.

Type	Name	Total k-mers [M]	k	Distinct k-mers [M]	Distinct counts
assembled	Sakai	5.50	11	2.38	69
			15	5.23	42
			21	5.30	28
	melanogaster	143	15	101	883
			21	122	710
			27	124	605
			32	125	522
	raimondii	727	15	251	1944
			21	546	1019
			27	604	699
			32	632	540
	GRCh38	2935	15	547	12718
			21	2327	10038
			27	2483	7946
			32	2567	6651
unassembled	USakai	25	11	3.06	239
			15	9.74	143
			21	10.0	97
	SRR622461_1	7500	15	676	22323
			21	3635	17211
			27	3734	13157
			32	3703	10643

Table 1: Data-sheet for the datasets used in our study. Columns Total and Distinct k-mers report the number of all and distinct k-mers respectively. The Distinct counts column reports the number of distinct k-mer frequencies.

Rather than storing a set in each bucket of the sketch, `fress` only stores an index to an array of involved sets. Note that its purpose is to only validate the approach, and it does not include any complex optimisation, such as multi-threading or bit-packing of the final matrix. Sorted spectra and lists of involved sets are explicitly stored in text format in order to be human-readable and allow for an easier analysis of the results.

4.2 Data

We tested Set-Min on six data sets of different size and complexity. Four of them are fully assembled genomes:

- "Sakai" strain of *Escherichia Coli*, downloadable from AFproject[20],
- genome of *Drosophila melanogaster* from FlyBase[2],
- genome of *Gossypium Raimondii* from AFproject,
- human reference genome assembly GRCh38[3].

The other two contain unassembled reads:

- Sakai strain at 5x coverage from AFproject,
- low-coverage human data SRR622461 from the 1000 Genomes Project[4].

Table 1 summarizes the characteristics of each data set for each value of k in our analysis. Observe that, while the number of distinct k-mers is comparable to the total number of k-mers (data size), the number of distinct k-mer counts is small. This is in accordance with the power-low distribution discussed in Section 2.1.

4.3 Set-Min vs Count-Min sketch

Table 2 compares Set-Min sketch to Count-Min sketch. Sketch dimensions R and B have been calculated using Algorithm 1 from Section 3 to insure bound (5) to hold for $\varepsilon = 0.01$. Dimensions of Count-Min sketch were set to be

[2] http://flybase.org

[3] ftp://ftp.ncbi.nlm.nih.gov/genomes/all/GCA/000/001/405/GCA_000001405.15_GRCh38/seqs_for_alignment_pipelines.ucsc_ids/GCA_000001405.1

[4] ftp://ftp.sra.ebi.ac.uk/vol1/fastq/SRR622/SRR622461/SRR622461_1.fastq.gz . Only the file SRR622461_1 is used in this study and we then omit the underscored nomenclature to simplify the notation.

the same. To make the comparison fair, the count with the greatest number of k-mers was not inserted into Count-Min sketch, similarly to Set-Min. Zero values are thus interpreted as the non-inserted count.

For ease of comparison, column T reports the threshold $\varepsilon\|\boldsymbol{a}\|_1$ given to Algorithm 1. Columns E_s and E_c report the actual total sum of errors for Set-Min and Count-Min, respectively. In all reported cases $E_s < T$, as expected. The total error of Count-Min, E_c is, most of the time, one order of magnitude larger than E_s. For SRR622461 with k = 15, it even exceeds the total number of k-mers $\|\boldsymbol{a}\|_1$ in the dataset.

The average error of Set-Min is, in most cases, very close to 1, which suggests that the overwhelming majority of collisions occur between successive counts. Most of them occur between counts 1 and 2, the most abundant ones in the spectra considered here. The average error of Count-Min is bigger but of the same order of magnitude, except for small k and unassembled datasets.

On the other hand, the fraction of k-mers producing an error is in striking contrast: in case of Set-Min, about only 1-3% of distinct k-mers produce an error, while for Count-Min, this fraction is much larger. This shows that Count-Min cannot be used when most of k-mer counts are expected to be retrieved precisely, for comparable sketch sizes.

Name	k	R	B	T	E_s	E_c	N_s	N_c	A_s	A_c
Sakai	11	4	$1.04 \cdot 10^6$	$5.50 \cdot 10^4$	$5.00 \cdot 10^4$	$1.39 \cdot 10^6$	1.8	26	1.15	2.24
Sakai	15	5	$2.13 \cdot 10^5$	$5.50 \cdot 10^4$	$4.66 \cdot 10^4$	$2.38 \cdot 10^5$	0.9	4	1.01	1.1
Sakai	21	5	$1.20 \cdot 10^5$	$5.50 \cdot 10^4$	$5.29 \cdot 10^4$	$4.57 \cdot 10^5$	0.9	7	1.05	1.18
melanogaster	15	5	$1.79 \cdot 10^7$	$1.43 \cdot 10^6$	$1.39 \cdot 10^6$	$8.35 \cdot 10^6$	1.4	7	1	1.25
melanogaster	21	4	$4.69 \cdot 10^6$	$1.43 \cdot 10^6$	$1.41 \cdot 10^6$	$2.26 \cdot 10^7$	1.1	12	1.03	1.61
melanogaster	27	5	$3.72 \cdot 10^6$	$1.43 \cdot 10^6$	$1.11 \cdot 10^6$	$2.28 \cdot 10^7$	0.9	12	1.01	1.48
melanogaster	32	5	$3.81 \cdot 10^6$	$1.42 \cdot 10^6$	$1.11 \cdot 10^6$	$2.10 \cdot 10^7$	0.9	12	1.01	1.44
raimondii	15	4	$8.36 \cdot 10^7$	$7.27 \cdot 10^6$	$5.65 \cdot 10^6$	$1.50 \cdot 10^8$	2.1	27	1.08	2.25
raimondii	21	4	$8.47 \cdot 10^7$	$7.27 \cdot 10^6$	$5.73 \cdot 10^6$	$4.09 \cdot 10^7$	1	6	1.01	1.3
raimondii	27	4	$7.14 \cdot 10^7$	$7.27 \cdot 10^6$	$6.49 \cdot 10^6$	$3.56 \cdot 10^7$	1.1	5	1.01	1.22
raimondii	32	4	$6.38 \cdot 10^7$	$7.27 \cdot 10^6$	$6.87 \cdot 10^6$	$3.15 \cdot 10^7$	1.1	4	1.01	1.17
GRCh38	15	3	$2.26 \cdot 10^8$	$2.93 \cdot 10^7$	$2.78 \cdot 10^7$	$1.36 \cdot 10^9$	2.9	52	1.78	4.74
GRCh38	21	4	$1.42 \cdot 10^8$	$2.93 \cdot 10^7$	$2.60 \cdot 10^7$	$1.65 \cdot 10^8$	1.1	6	1.01	1.23
GRCh38	27	4	$1.07 \cdot 10^8$	$2.93 \cdot 10^7$	$2.82 \cdot 10^7$	$1.91 \cdot 10^8$	1.1	6	1.01	1.25
GRCh38	32	4	$9.84 \cdot 10^7$	$2.93 \cdot 10^7$	$2.92 \cdot 10^7$	$1.85 \cdot 10^8$	1.1	6	1.01	1.22
USakai	11	5	$4.58 \cdot 10^5$	$2.57 \cdot 10^5$	$1.99 \cdot 10^5$	$7.44 \cdot 10^7$	2.6	99	2.46	24.6
USakai	15	4	$4.79 \cdot 10^6$	$2.49 \cdot 10^5$	$2.45 \cdot 10^5$	$8.01 \cdot 10^6$	1.9	33	1.31	2.53
USakai	21	5	$3.99 \cdot 10^6$	$2.38 \cdot 10^5$	$2.00 \cdot 10^5$	$7.91 \cdot 10^6$	1.6	34	1.21	2.35
SRR622461	15	4	$1.17 \cdot 10^8$	$7.90 \cdot 10^7$	$4.93 \cdot 10^7$	$1.34 \cdot 10^{10}$	3.3	96	2.2	20.68
SRR622461	21	3	$2.39 \cdot 10^9$	$7.35 \cdot 10^7$	$7.09 \cdot 10^7$	$5.63 \cdot 10^8$	1.8	9	1.11	1.68
SRR622461	27	4	$1.78 \cdot 10^9$	$6.80 \cdot 10^7$	$4.92 \cdot 10^7$	$4.58 \cdot 10^8$	1.3	8	1.04	1.53
SRR622461	32	4	$1.72 \cdot 10^9$	$6.34 \cdot 10^7$	$4.95 \cdot 10^7$	$4.01 \cdot 10^8$	1.3	7	1.03	1.48

Table 2: Set-Min compared to Count-Min. R and B are dimensions of Set-Min and Count-Min matrices. T is the reference upper bound on the sum of errors equal to $\varepsilon\|\boldsymbol{a}\|_1$ (right-hand side of (5)). E_s and E_c are the sum of errors for Set-Min and Count-Min respectively. N_s and N_c are the percentages (rounded to integers) of the fractions of distinct k-mers producing an error, for Set-Min and Count-Min respectively. A_s and A_c are respective average errors, with average taken over the number of distinct k-mers resulting in an error in the respective sketch.

4.4 Set-Min sketch vs KMC output

Not surprisingly, Set-Min achieves better memory consumptions than KMC in all our tests (columns M_{kmc} and M_s of Table 3). Values of R and B do not change from Table 2. The compression ratio is variable: from a small factor to two orders of magnitude. The best compression is achieved for larger values of k and assembled genomes. The former is primarily explained by the decreasing number of distinct counts, due to the power-law behaviour. As for the difference between assembled genomes and sequencing data, we will discuss it in more details in Section 5.

Name	k	M_{kmc}	M_s	C_s	M_{bbhash}	M_{bball}	C_{bball}
Sakai	11	$1.21 \cdot 10^7$	$5.75 \cdot 10^6$	$3.41 \cdot 10^6$	$9.13 \cdot 10^5$	$3.00 \cdot 10^6$	$2.01 \cdot 10^6$
Sakai	15	$3.80 \cdot 10^7$	$1.20 \cdot 10^6$	$5.55 \cdot 10^5$	$2.06 \cdot 10^6$	$5.99 \cdot 10^6$	$2.18 \cdot 10^6$
Sakai	21	$4.77 \cdot 10^7$	$6.77 \cdot 10^5$	$3.57 \cdot 10^5$	$2.03 \cdot 10^6$	$6.00 \cdot 10^6$	$2.09 \cdot 10^6$
melanogaster	15	$7.08 \cdot 10^8$	$1.68 \cdot 10^8$	$5.74 \cdot 10^7$	$3.87 \cdot 10^7$	$2.15 \cdot 10^8$	$5.76 \cdot 10^7$
melanogaster	21	$9.80 \cdot 10^8$	$3.55 \cdot 10^7$	$1.62 \cdot 10^7$	$4.66 \cdot 10^7$	$2.45 \cdot 10^8$	$5.22 \cdot 10^7$
melanogaster	27	$1.24 \cdot 10^9$	$3.75 \cdot 10^7$	$1.77 \cdot 10^7$	$4.73 \cdot 10^7$	$2.48 \cdot 10^8$	$5.26 \cdot 10^7$
melanogaster	32	$1.37 \cdot 10^9$	$3.84 \cdot 10^7$	$1.78 \cdot 10^7$	$4.90 \cdot 10^7$	$2.36 \cdot 10^8$	$5.38 \cdot 10^7$
raimondii	15	$1.76 \cdot 10^9$	$7.54 \cdot 10^8$	$3.34 \cdot 10^8$	$9.59 \cdot 10^7$	$5.98 \cdot 10^8$	$2.11 \cdot 10^8$
raimondii	21	$4.37 \cdot 10^9$	$6.78 \cdot 10^8$	$2.08 \cdot 10^8$	$2.16 \cdot 10^8$	$1.24 \cdot 10^9$	$2.90 \cdot 10^8$
raimondii	27	$6.04 \cdot 10^9$	$5.36 \cdot 10^8$	$1.62 \cdot 10^8$	$2.37 \cdot 10^8$	$1.29 \cdot 10^9$	$2.94 \cdot 10^8$
raimondii	32	$6.96 \cdot 10^9$	$4.79 \cdot 10^8$	$1.36 \cdot 10^8$	$2.70 \cdot 10^8$	$1.38 \cdot 10^9$	$3.10 \cdot 10^8$
GRCh38	15	$3.83 \cdot 10^9$	$1.70 \cdot 10^9$	$9.32 \cdot 10^8$	$2.09 \cdot 10^8$	$1.65 \cdot 10^9$	$5.67 \cdot 10^8$
GRCh38	21	$1.86 \cdot 10^{10}$	$1.28 \cdot 10^9$	$3.58 \cdot 10^8$	$9.32 \cdot 10^8$	$6.46 \cdot 10^9$	$1.03 \cdot 10^9$
GRCh38	27	$2.48 \cdot 10^{10}$	$9.66 \cdot 10^8$	$2.79 \cdot 10^8$	$9.86 \cdot 10^8$	$6.57 \cdot 10^9$	$1.05 \cdot 10^9$
GRCh38	32	$2.82 \cdot 10^{10}$	$8.38 \cdot 10^8$	$2.50 \cdot 10^8$	$1.08 \cdot 10^9$	$6.54 \cdot 10^9$	$1.12 \cdot 10^9$
USakai	11	$1.54 \cdot 10^7$	$1.49 \cdot 10^7$	$7.99 \cdot 10^6$	$1.17 \cdot 10^6$	$4.61 \cdot 10^6$	$3.68 \cdot 10^6$
USakai	15	$6.95 \cdot 10^7$	$2.87 \cdot 10^7$	$1.54 \cdot 10^7$	$3.72 \cdot 10^6$	$1.35 \cdot 10^7$	$8.34 \cdot 10^6$
USakai	21	$8.53 \cdot 10^7$	$3.00 \cdot 10^7$	$1.61 \cdot 10^7$	$3.91 \cdot 10^6$	$1.39 \cdot 10^7$	$8.40 \cdot 10^6$
SRR622461	15	$4.73 \cdot 10^9$	$2.00 \cdot 10^9$	$1.51 \cdot 10^9$	$2.59 \cdot 10^8$	$2.12 \cdot 10^9$	$8.38 \cdot 10^8$
SRR622461	21	$2.91 \cdot 10^{10}$	$1.61 \cdot 10^{10}$	$3.66 \cdot 10^9$	$1.48 \cdot 10^9$	$1.10 \cdot 10^{10}$	$2.71 \cdot 10^9$
SRR622461	27	$3.73 \cdot 10^{10}$	$1.60 \cdot 10^{10}$	$3.88 \cdot 10^9$	$1.48 \cdot 10^9$	$1.08 \cdot 10^{10}$	$2.66 \cdot 10^9$
SRR622461	32	$4.07 \cdot 10^{10}$	$1.46 \cdot 10^{10}$	$3.59 \cdot 10^9$	$1.57 \cdot 10^9$	$1.04 \cdot 10^{10}$	$2.65 \cdot 10^9$

Table 3: Set-Min ($\epsilon = 0.01$) compared to KMC and BBHash ($\gamma = 1$). All memory is reported in bytes. Column M_{kmc}, M_s, M_{bball} are the memory requirements to have a fully functional map between k-mers and their frequencies when applying KMC, Set-Min sketch and BBHash. M_{bbhash} is the memory of the hash function produced by BBHash without the external array of frequencies, C_s and C_{bball} are the compressed versions of M_s and M_{bball} using `gzip`.

4.5 Set-Min sketch vs MPHFs

Table 3 also reports the space usage for `BBHash` with parameter $\gamma = 1$ to obtain the best memory-optimized hash functions. Column M_{bbhash} is the space (in bytes) required by the hash function only, while M_{bball} is the space required by the hash function plus the external array of frequencies.

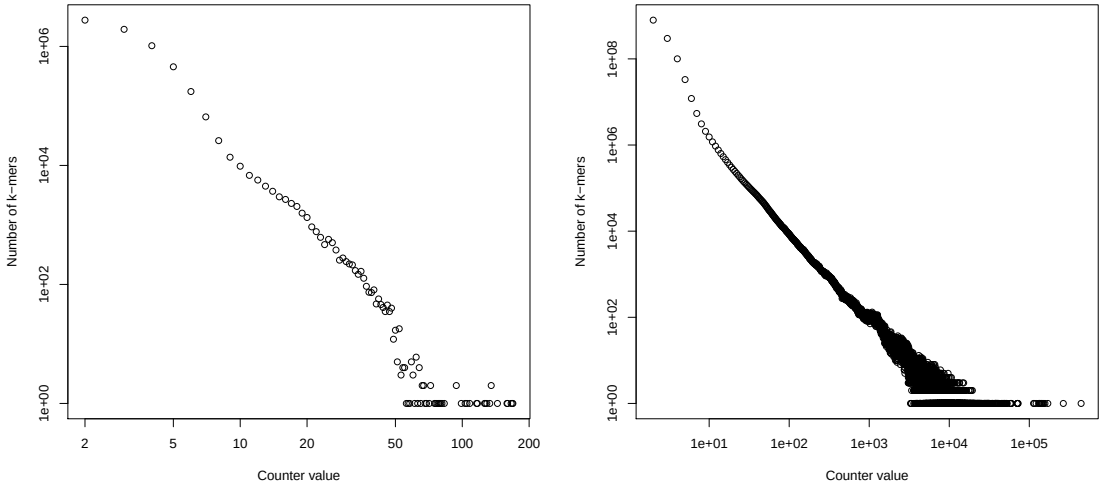
As in the previous case, Set-Min sketch is more memory-efficient when k is large, where it takes about an order of magnitude less memory than a MPHF. For small values of k, MPHF takes slightly less space and, being exact, may therefore be preferable to use. However, one should keep in mind that MPHF does not support any updates of the k-mer counter map, while a Set-Min sketch is updatable to a certain extent with new (k-mer,count) pairs, and also mergeable with another possibly redundant map. For long-term storage through gzip compression of the sketches (columns C_s and C_{bball}) Set-Min and MPHFs give equivalent results.

The behaviour of the unassembled datasets is of particular interest. Even for large k's, MPHF appears to be a better choice for this type of data. The causes of this phenomenon and possible solutions are discussed in Section 5.

5 Discussion

5.1 Unassembled datasets

As seen in Table 3, for the unassembled datasets, Set-Min sketch does not seem to have an advantage in memory usage, even for large k's. We found that this is due to low-count k-mers, specifically to k-mers whose count does not exceed the sequencing coverage. It is known that for Illumina sequencing, sequencing errors produce a linear growth of the number of new distinct k-mers (for large k) depending on the coverage (see e.g. Figure 2(b) of [21]). Frequencies of these "erroneous" k-mers do not have the same statistical behaviour as *bona fide* k-mers, in particular first spectrum values do not decay at the same rate as the rest of the spectrum.



(a) USakai

(b) SRR622461

Figure 4: Spectra for the unassembled data sets. Both plots are in log-log scale. $k = 21$ for USakai, $k = 32$ for SRR622461.

Figure 4 shows spectra of the unassembled USakai and SRR622461 datasets. One can observe a slower decay behaviour for a first few spectrum values. In this situation, Algorithm 1 generates a lot of rows just to make the sketch able to distinguish, with required precision, between small frequency values.

Note that in practice, distinguishing between small frequencies is often irrelevant. For example, many read assemblers simply discard low-frequency reads as a way to de-noise the data. In the case of Set-Min, it is possible to collapse together the first m columns of the spectrum by assigning to all k-mers in this subset the same frequency. This would considerably reduce the sketch size. Formally, the error guarantee (5) would not hold anymore but most of newly introduced errors would be small (typically, equal to 1) and occur for low counts only.

To check the above, we constructed a Set-Min sketch for SRR622461 with dimensions $(R, B) = (4, 3310557)$, merging together the first five columns of the sorted spectrum and assigning count 5 to all merged k-mers. While the final sum of errors was well above the theoretical limit (10^9 against $7 \cdot 10^6$), the maximum and average error were respectively 55 and 2.8. In many applications this error level could be acceptable.

5.2 Presence-absence information

As introduced in Section 3.2, in this work we assumed that only k-mers present in the dataset can be queried. This assumption allowed us to discard the largest value of the spectrum corresponding to unique k-mers, thereby saving more space than a complete sketch.

Set-Min sketches can seamlessly work without this assumption, but the space required for storing k-mer counters may not be competitive to other solutions. An alternative is to build an additional data structure, specifically optimized to answer presence/absence queries (such as a Bloom filter), as a complement to Set-Min sketches.

Another scenario occurs when working with multiple datasets of very high similarity, such as a large collection of bacterial strains or a collection of RNA-seq data [22, 23]. In this case, it might be beneficial to build a Bloom filter for the k-mers present in the union of the datasets, and maintain multiple Set-Min sketches to represent k-mer counts in each dataset.

Note that Set-Min sketches can be also used for long-term storage and transmission of the k-mer composition of a dataset augmented with count information. The k-mers of the dataset can be reassembled into simplitigs [7] with a Set-Min sketch storing the (approximated) frequencies. The full count table can be restored from the simplitigs and the sketch.

6 Conclusions

We presented Set-Min sketch – a novel sketching method inspired by the Count-Min sketch. Its primary use is to associate keys to labels without explicitly storing the former. In this paper, we demonstrated the performance of Set-Min sketch for storing k-mer counts information, where the distribution of labels (k-mer counts) follows a power-law. Under this assumption, we proposed simple bounds for a Set-Min sketch that guarantee the total error sum to be within an ε fraction of the total number of k-mers in the dataset.

We showed that Set-Min sketch allows us to save space compared to the raw output of the popular KMC k-mer counting tool when applied to labels following a skewed distribution, at the price of a very modest error rate. Memory efficiency is particularly significant in case of whole-genome data and large values of k, where it can reach reductions of two orders of magnitude. Set-Min has been shown to be more space efficient than the MPHF-based soluton for large values of k. For smaller k's, however, MPHFs provide an implementation with comparable memory consumption. Finally, when compared to Count-Min sketches of comparable dimensions, our sketch achieves better point-query errors thanks to the distribution-aware dimensioning performed on the k-mer spectrum, and the reliance on already computed count tables as input.

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Supplemental Material: Set-Min sketch

Proof of Theorem 1

Our goal is to estimate

$$\sum_{\ell \in L} c_\ell \sum_{\substack{m>\ell \\ m \in L}} (m-\ell) \left(1 - e^{-\frac{c_m}{B}}\right)^R, \tag{1}$$

where $c_\ell = C \cdot \ell^{-a}$. We assume $B > C$ and approximate $1 - e^{-\frac{c_m}{B}} \approx \frac{c_m}{B} = \frac{C}{B} m^{-a}$. We further lower-approximate (1) by replacing sums by integrals, thus obtaining

$$\int_1^\infty C \cdot \ell^{-a} \int_\ell^\infty (m-\ell) \left(\frac{C}{B} m^{-a}\right)^R dm\, d\ell. \tag{2}$$

Routine computation of the integral yields

$$C \left(\frac{C}{B}\right)^R \frac{1}{(aR-2)(aR-1)(aR+a+3)}. \tag{3}$$

The inequality of the Theorem becomes

$$\left(\frac{C}{B}\right)^R \frac{1}{(aR-2)(aR-1)(aR+a+3)} < \varepsilon \frac{a-1}{a-2}. \tag{4}$$

The Theorem follows.

Performance comparison for epsilon = 0.01

Name	k	R	B	T	E_s	N_s	A_s	D_s^{Max}	E_c	N_c	A_c	D_c^{Max}
Sakai	8	7	1,020	$5.50 \cdot 10^4$	42,059	$3.00 \cdot 10^0$	21.56	122	$2.80 \cdot 10^8$	$1.00 \cdot 10^2$	4,284.98	6,129
Sakai	11	4	1,042,202	$5.50 \cdot 10^4$	49,953	$1.80 \cdot 10^0$	1.15	7	$1.39 \cdot 10^6$	$2.60 \cdot 10^1$	2.24	15
Sakai	15	5	212,522	$5.50 \cdot 10^4$	46,619	$9.00 \cdot 10^{-1}$	1.01	2	$2.38 \cdot 10^5$	$4.00 \cdot 10^0$	1.1	7
Sakai	21	5	120,006	$5.50 \cdot 10^4$	52,852	$9.00 \cdot 10^{-1}$	1.05	4	$4.57 \cdot 10^5$	$7.00 \cdot 10^0$	1.18	7
melanogaster	15	5	17,850,639	$1.43 \cdot 10^6$	$1.39 \cdot 10^6$	$1.40 \cdot 10^0$	1	4	$8.35 \cdot 10^6$	$7.00 \cdot 10^0$	1.25	18
melanogaster	21	4	4,694,088	$1.43 \cdot 10^6$	$1.41 \cdot 10^6$	$1.10 \cdot 10^0$	1.03	13	$2.26 \cdot 10^7$	$1.20 \cdot 10^1$	1.61	55
melanogaster	27	5	3,717,540	$1.43 \cdot 10^6$	$1.11 \cdot 10^6$	$9.00 \cdot 10^{-1}$	1.01	7	$2.28 \cdot 10^7$	$1.20 \cdot 10^1$	1.48	34
melanogaster	32	5	3,814,440	$1.42 \cdot 10^6$	$1.11 \cdot 10^6$	$9.00 \cdot 10^{-1}$	1.01	8	$2.10 \cdot 10^7$	$1.20 \cdot 10^1$	1.44	30
raimondii	15	4	83,575,168	$7.27 \cdot 10^6$	$5.65 \cdot 10^6$	$2.10 \cdot 10^0$	1.08	11	$1.50 \cdot 10^8$	$2.70 \cdot 10^1$	2.25	65
raimondii	21	4	84,742,080	$7.27 \cdot 10^6$	$5.73 \cdot 10^6$	$1.00 \cdot 10^0$	1.01	9	$4.09 \cdot 10^7$	$6.00 \cdot 10^0$	1.3	36
raimondii	27	4	71,403,946	$7.27 \cdot 10^6$	$6.49 \cdot 10^6$	$1.10 \cdot 10^0$	1.01	7	$3.56 \cdot 10^7$	$5.00 \cdot 10^0$	1.22	32
raimondii	32	4	63,793,114	$7.27 \cdot 10^6$	$6.87 \cdot 10^6$	$1.10 \cdot 10^0$	1.01	7	$3.15 \cdot 10^7$	$4.00 \cdot 10^0$	1.17	22
GRCh38	15	3	225,505,316	$2.93 \cdot 10^7$	$2.78 \cdot 10^7$	$2.90 \cdot 10^0$	1.78	33	$1.36 \cdot 10^9$	$5.20 \cdot 10^1$	4.74	335
GRCh38	21	4	141,645,448	$2.93 \cdot 10^7$	$2.60 \cdot 10^7$	$1.10 \cdot 10^0$	1.01	12	$1.65 \cdot 10^8$	$6.00 \cdot 10^0$	1.23	108
GRCh38	27	4	107,171,949	$2.93 \cdot 10^7$	$2.82 \cdot 10^7$	$1.10 \cdot 10^0$	1.01	12	$1.91 \cdot 10^8$	$6.00 \cdot 10^0$	1.25	66
GRCh38	32	4	98,414,723	$2.93 \cdot 10^7$	$2.92 \cdot 10^7$	$1.10 \cdot 10^0$	1.01	8	$1.85 \cdot 10^8$	$6.00 \cdot 10^0$	1.22	70
USakai	8	7	276	$2.62 \cdot 10^5$	$2.30 \cdot 10^5$	$3.50 \cdot 10^0$	101.03	623	$5.55 \cdot 10^9$	$1.00 \cdot 10^2$	84,769.1	$1.00 \cdot 10^5$
USakai	11	5	458,224	$2.57 \cdot 10^5$	$1.99 \cdot 10^5$	$2.60 \cdot 10^0$	2.46	23	$7.44 \cdot 10^7$	$9.90 \cdot 10^1$	24.6	121
USakai	15	4	4,786,091	$2.49 \cdot 10^5$	$2.45 \cdot 10^5$	$1.90 \cdot 10^0$	1.31	5	$8.01 \cdot 10^6$	$3.30 \cdot 10^1$	2.53	16
USakai	21	5	3,992,620	$2.38 \cdot 10^5$	$2.00 \cdot 10^5$	$1.60 \cdot 10^0$	1.21	4	$7.91 \cdot 10^6$	$3.40 \cdot 10^1$	2.35	13
SRR622461	15	4	117,393,511	$7.90 \cdot 10^7$	$4.93 \cdot 10^7$	$3.30 \cdot 10^0$	2.2	55	$1.34 \cdot 10^{10}$	$9.60 \cdot 10^1$	20.68	398
SRR622461	21	3	2,385,949,540	$7.35 \cdot 10^7$	$7.09 \cdot 10^7$	$1.80 \cdot 10^0$	1.11	13	$5.63 \cdot 10^8$	$9.00 \cdot 10^0$	1.68	74
SRR622461	27	4	1,782,384,901	$6.80 \cdot 10^7$	$4.92 \cdot 10^7$	$1.30 \cdot 10^0$	1.04	6	$4.58 \cdot 10^8$	$8.00 \cdot 10^0$	1.53	21
SRR622461	32	4	1,719,165,525	$6.34 \cdot 10^7$	$4.95 \cdot 10^7$	$1.30 \cdot 10^0$	1.03	5	$4.01 \cdot 10^8$	$7.00 \cdot 10^0$	1.48	18

Table 1: Full table comparing the performance of Set-Min sketch constructed for $\epsilon = 0.01$ to all other variables for all possible ks. R = number of rows, B = number of columns, T = theoretical maximum error bound, E_s = sum of errors for Set-Min, N_s = total number of collisions for Set-Min, A_s = average point-query error (E_s/N_s), D_s^{Max} = Maximum point-query error for Set-Min, E_c = sum of errors for Count-Min, N_c = total number of collisions for Count-Min, A_c = average point-query error (E_c/N_c), D_c^{Max} = Maximum point-query error for Count-Min

Memory comparison for epsilon = 0.01

Name	k	R	B	M_{kmc}	M_s	C_s	M_c	C_c	M_{bbhash}	M_{bball}	C_{bball}
Sakai	8	7	1,020	$3.29 \cdot 10^5$	$1.27 \cdot 10^6$	$3.32 \cdot 10^5$	$1.25 \cdot 10^4$	$1.57 \cdot 10^4$	$2.61 \cdot 10^4$	$1.08 \cdot 10^5$	$1.21 \cdot 10^5$
Sakai	11	4	1,042,202	$1.21 \cdot 10^7$	$5.75 \cdot 10^6$	$3.41 \cdot 10^6$	$3.65 \cdot 10^6$	$2.96 \cdot 10^6$	$9.13 \cdot 10^5$	$3.00 \cdot 10^6$	$2.01 \cdot 10^6$
Sakai	15	5	212,522	$3.80 \cdot 10^7$	$1.20 \cdot 10^6$	$5.55 \cdot 10^5$	$7.97 \cdot 10^5$	$5.63 \cdot 10^5$	$2.06 \cdot 10^6$	$5.99 \cdot 10^6$	$2.18 \cdot 10^6$
Sakai	21	5	120,006	$4.77 \cdot 10^7$	$6.77 \cdot 10^5$	$3.57 \cdot 10^5$	$4.50 \cdot 10^5$	$3.53 \cdot 10^5$	$2.03 \cdot 10^6$	$6.00 \cdot 10^6$	$2.09 \cdot 10^6$
melanogaster	15	5	17,850,639	$7.08 \cdot 10^8$	$1.68 \cdot 10^8$	$5.74 \cdot 10^7$	$1.56 \cdot 10^8$	$5.48 \cdot 10^7$	$3.87 \cdot 10^7$	$2.15 \cdot 10^8$	$5.76 \cdot 10^7$
melanogaster	21	4	4,694,088	$9.80 \cdot 10^8$	$3.55 \cdot 10^7$	$1.62 \cdot 10^7$	$3.05 \cdot 10^7$	$1.35 \cdot 10^7$	$4.66 \cdot 10^7$	$2.45 \cdot 10^8$	$5.22 \cdot 10^7$
melanogaster	27	5	3,717,540	$1.24 \cdot 10^9$	$3.75 \cdot 10^7$	$1.77 \cdot 10^7$	$3.02 \cdot 10^7$	$1.44 \cdot 10^7$	$4.73 \cdot 10^7$	$2.48 \cdot 10^8$	$5.26 \cdot 10^7$
melanogaster	32	5	3,814,440	$1.37 \cdot 10^9$	$3.84 \cdot 10^7$	$1.78 \cdot 10^7$	$2.86 \cdot 10^7$	$1.45 \cdot 10^7$	$4.90 \cdot 10^7$	$2.36 \cdot 10^8$	$5.38 \cdot 10^7$
raimondii	15	4	83,575,168	$1.76 \cdot 10^9$	$7.54 \cdot 10^8$	$3.34 \cdot 10^8$	$6.69 \cdot 10^8$	$2.70 \cdot 10^8$	$9.59 \cdot 10^7$	$5.98 \cdot 10^8$	$2.11 \cdot 10^8$
raimondii	21	4	84,742,080	$4.37 \cdot 10^9$	$6.78 \cdot 10^8$	$2.08 \cdot 10^8$	$6.36 \cdot 10^8$	$1.94 \cdot 10^8$	$2.16 \cdot 10^8$	$1.24 \cdot 10^9$	$2.90 \cdot 10^8$
raimondii	27	4	71,403,946	$6.04 \cdot 10^9$	$5.36 \cdot 10^8$	$1.62 \cdot 10^8$	$5.00 \cdot 10^8$	$1.54 \cdot 10^8$	$2.37 \cdot 10^8$	$1.29 \cdot 10^9$	$2.94 \cdot 10^8$
raimondii	32	4	63,793,114	$6.96 \cdot 10^9$	$4.79 \cdot 10^8$	$1.36 \cdot 10^8$	$4.47 \cdot 10^8$	$1.32 \cdot 10^8$	$2.70 \cdot 10^8$	$1.38 \cdot 10^9$	$3.10 \cdot 10^8$
GRCh38	15	3	225,505,316	$3.83 \cdot 10^9$	$1.70 \cdot 10^9$	$9.32 \cdot 10^8$	$1.78 \cdot 10^9$	$6.30 \cdot 10^8$	$2.09 \cdot 10^8$	$1.65 \cdot 10^9$	$5.67 \cdot 10^8$
GRCh38	21	4	141,645,448	$1.86 \cdot 10^{10}$	$1.28 \cdot 10^9$	$3.58 \cdot 10^8$	$1.35 \cdot 10^9$	$3.32 \cdot 10^8$	$9.32 \cdot 10^8$	$6.46 \cdot 10^9$	$1.03 \cdot 10^9$
GRCh38	27	4	107,171,949	$2.48 \cdot 10^{10}$	$9.66 \cdot 10^8$	$2.79 \cdot 10^8$	$9.65 \cdot 10^8$	$2.56 \cdot 10^8$	$9.86 \cdot 10^8$	$6.57 \cdot 10^9$	$1.05 \cdot 10^9$
GRCh38	32	4	98,414,723	$2.82 \cdot 10^{10}$	$8.38 \cdot 10^8$	$2.50 \cdot 10^8$	$8.37 \cdot 10^8$	$2.30 \cdot 10^8$	$1.08 \cdot 10^9$	$6.54 \cdot 10^9$	$1.12 \cdot 10^9$
USakai	8	7	276	$3.30 \cdot 10^5$	$1.59 \cdot 10^6$	$4.60 \cdot 10^5$	$4.35 \cdot 10^3$	$5.24 \cdot 10^3$	$2.62 \cdot 10^4$	$1.24 \cdot 10^5$	$1.42 \cdot 10^5$
USakai	11	5	458,224	$1.54 \cdot 10^7$	$1.49 \cdot 10^7$	$7.99 \cdot 10^6$	$2.86 \cdot 10^6$	$3.05 \cdot 10^6$	$1.17 \cdot 10^6$	$4.61 \cdot 10^6$	$3.68 \cdot 10^6$
USakai	15	4	4,786,091	$6.95 \cdot 10^7$	$2.87 \cdot 10^7$	$1.54 \cdot 10^7$	$1.91 \cdot 10^7$	$1.39 \cdot 10^7$	$3.72 \cdot 10^6$	$1.35 \cdot 10^7$	$8.34 \cdot 10^6$
USakai	21	5	3,992,620	$8.53 \cdot 10^7$	$3.00 \cdot 10^7$	$1.61 \cdot 10^7$	$2.00 \cdot 10^7$	$1.48 \cdot 10^7$	$3.91 \cdot 10^6$	$1.39 \cdot 10^7$	$8.40 \cdot 10^6$
SRR622461	15	4	117,393,511	$4.73 \cdot 10^9$	$2.00 \cdot 10^9$	$1.51 \cdot 10^9$	$1.29 \cdot 10^9$	$6.55 \cdot 10^8$	$2.59 \cdot 10^8$	$2.12 \cdot 10^9$	$8.38 \cdot 10^8$
SRR622461	21	3	2,385,949,540	$2.91 \cdot 10^{10}$	$1.61 \cdot 10^{10}$	$3.66 \cdot 10^9$	$1.88 \cdot 10^{10}$	$3.59 \cdot 10^9$	$1.48 \cdot 10^9$	$1.10 \cdot 10^{10}$	$2.71 \cdot 10^9$
SRR622461	27	4	1,782,384,901	$3.73 \cdot 10^{10}$	$1.60 \cdot 10^{10}$	$3.88 \cdot 10^9$	$1.78 \cdot 10^{10}$	$3.89 \cdot 10^9$	$1.48 \cdot 10^9$	$1.08 \cdot 10^{10}$	$2.66 \cdot 10^9$
SRR622461	32	4	1,719,165,525	$4.07 \cdot 10^{10}$	$1.46 \cdot 10^{10}$	$3.59 \cdot 10^9$	$1.63 \cdot 10^{10}$	$3.65 \cdot 10^9$	$1.57 \cdot 10^9$	$1.04 \cdot 10^{10}$	$2.65 \cdot 10^9$

Table 2: Full table comparing the memory of Set-Min sketch constructed for $\epsilon = 0.01$ to all other variables for all possible ks. R = number of rows, B = number of columns, M_{kmc}, M_s = size of Set-Min sketch in bytes, C_s = compressed Set-Min sketch size, M_c = size of Count-Min sketch in bytes, C_c = compressed size of Count-Min sketch, M_{bbhash} = size of the MPHF generated by BBHash without the external array, M_{bball} = total memory for BBHash taking into account the external array, C_{bball} = compressed size of M_{bball}

Performance comparison for epsilon = 0.001

Name	k	R	B	T	E_s	N_s	A_s	D_s^{Max}	E_c	N_c	A_c	D_c^{Max}
Sakai	8	8	1,227	$5.50 \cdot 10^3$	4,921	$4.00 \cdot 10^{-1}$	21.03	76	$2.24 \cdot 10^8$	$1.00 \cdot 10^2$	3,429.11	4,933
Sakai	11	6	1,111,682	$5.50 \cdot 10^3$	5,332	$2.00 \cdot 10^{-1}$	1.05	3	$4.78 \cdot 10^5$	$1.10 \cdot 10^1$	1.85	13
Sakai	15	8	189,752	$5.50 \cdot 10^3$	5,405	$1.00 \cdot 10^{-1}$	1	1	60,364	$1.00 \cdot 10^0$	1.05	4
Sakai	21	9	95,243	$5.50 \cdot 10^3$	5,142	$1.00 \cdot 10^{-1}$	1.01	2	$1.69 \cdot 10^5$	$3.00 \cdot 10^0$	1.07	5
melanogaster	15	6	24,792,555	$1.43 \cdot 10^5$	$1.32 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	2	$1.20 \cdot 10^6$	$1.00 \cdot 10^0$	1.18	10
melanogaster	21	8	3,352,920	$1.43 \cdot 10^5$	$1.27 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	4	$9.23 \cdot 10^6$	$6.00 \cdot 10^0$	1.23	19
melanogaster	27	8	3,319,232	$1.43 \cdot 10^5$	$1.29 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	3	$8.68 \cdot 10^6$	$6.00 \cdot 10^0$	1.21	19
melanogaster	32	8	3,405,750	$1.42 \cdot 10^5$	$1.30 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	3	$7.83 \cdot 10^6$	$5.00 \cdot 10^0$	1.19	17
raimondii	15	6	89,146,846	$7.27 \cdot 10^5$	$6.71 \cdot 10^5$	$3.00 \cdot 10^{-1}$	1.02	5	$4.99 \cdot 10^7$	$1.10 \cdot 10^1$	1.77	24
raimondii	21	7	69,177,208	$7.27 \cdot 10^5$	$6.07 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	3	$1.12 \cdot 10^7$	$2.00 \cdot 10^0$	1.15	11
raimondii	27	7	58,288,935	$7.27 \cdot 10^5$	$6.94 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	3	$8.89 \cdot 10^6$	$1.00 \cdot 10^0$	1.11	9
raimondii	32	8	45,566,510	$7.27 \cdot 10^5$	$6.41 \cdot 10^5$	$1.00 \cdot 10^{-1}$	1	2	$7.73 \cdot 10^6$	$1.00 \cdot 10^0$	1.08	7
GRCh38	15	6	157,853,721	$2.93 \cdot 10^6$	$2.45 \cdot 10^6$	$4.00 \cdot 10^{-1}$	1.24	9	$1.18 \cdot 10^9$	$5.50 \cdot 10^1$	3.95	58
GRCh38	21	7	115,628,937	$2.93 \cdot 10^6$	$2.77 \cdot 10^6$	$1.00 \cdot 10^{-1}$	1	3	$4.42 \cdot 10^7$	$2.00 \cdot 10^0$	1.09	14
GRCh38	27	8	76,551,392	$2.93 \cdot 10^6$	$2.59 \cdot 10^6$	$1.00 \cdot 10^{-1}$	1	2	$5.81 \cdot 10^7$	$2.00 \cdot 10^0$	1.08	13
GRCh38	32	8	70,296,231	$2.93 \cdot 10^6$	$2.69 \cdot 10^6$	$1.00 \cdot 10^{-1}$	1	2	$5.46 \cdot 10^7$	$2.00 \cdot 10^0$	1.07	10
USakai	8	10	236	$2.62 \cdot 10^4$	28,302	$5.00 \cdot 10^{-1}$	88.72	325	$6.48 \cdot 10^9$	$1.00 \cdot 10^2$	98,860.29	$1.17 \cdot 10^5$
USakai	11	6	610,965	$2.57 \cdot 10^4$	18,949	$3.00 \cdot 10^{-1}$	2.12	14	$4.18 \cdot 10^7$	$9.40 \cdot 10^1$	14.58	81
USakai	15	6	5,105,164	$2.49 \cdot 10^4$	23,817	$2.00 \cdot 10^{-1}$	1.19	4	$3.15 \cdot 10^6$	$1.50 \cdot 10^1$	2.1	11
USakai	21	7	4,562,994	$2.38 \cdot 10^4$	19,817	$2.00 \cdot 10^{-1}$	1.12	3	$2.88 \cdot 10^6$	$1.50 \cdot 10^1$	1.96	11
SRR622461	15	5	140,872,213	$7.90 \cdot 10^6$	$7.38 \cdot 10^6$	$6.00 \cdot 10^{-1}$	1.69	28	$8.27 \cdot 10^9$	$9.00 \cdot 10^1$	13.66	231

Table 3: Full table comparing the performance of Set-Min sketch constructed for $\epsilon = 0.001$ to all other variables for all possible ks. R = number of rows, B = number of columns, T = theoretical maximum error bound, E_s = sum of errors for Set-Min, N_s = total number of collisions for Set-Min, A_s = average point-query error (E_s/N_s), D_s^{Max} = Maximum point-query error for Set-Min, E_c = sum of errors for Count-Min, N_c = total number of collisions for Count-Min, A_c = average point-query error (E_c/N_c), D_c^{Max} = Maximum point-query error for Count-Min

Memory comparison for epsilon = 0.01

Name	k	R	B	M_{kmc}	M_s	C_s	M_c	C_c	M_{bbhash}	M_{bball}	C_{bball}
Sakai	8	8	1,227	$3.29 \cdot 10^5$	$1.49 \cdot 10^6$	$4.08 \cdot 10^5$	$1.72 \cdot 10^4$	$2.11 \cdot 10^4$	$2.61 \cdot 10^4$	$1.08 \cdot 10^5$	$1.21 \cdot 10^5$
Sakai	11	6	1,111,682	$1.21 \cdot 10^7$	$1.00 \cdot 10^7$	$5.44 \cdot 10^6$	$5.84 \cdot 10^6$	$4.63 \cdot 10^6$	$9.13 \cdot 10^5$	$3.00 \cdot 10^6$	$2.01 \cdot 10^6$
Sakai	15	8	189,752	$3.80 \cdot 10^7$	$1.71 \cdot 10^6$	$8.23 \cdot 10^5$	$1.14 \cdot 10^6$	$8.41 \cdot 10^5$	$2.06 \cdot 10^6$	$5.99 \cdot 10^6$	$2.18 \cdot 10^6$
Sakai	21	9	95,243	$4.77 \cdot 10^7$	$9.67 \cdot 10^5$	$5.65 \cdot 10^5$	$6.43 \cdot 10^5$	$5.49 \cdot 10^5$	$2.03 \cdot 10^6$	$6.00 \cdot 10^6$	$2.09 \cdot 10^6$
melanogaster	15	6	24,792,555	$7.08 \cdot 10^8$	$2.79 \cdot 10^8$	$8.14 \cdot 10^7$	$2.60 \cdot 10^8$	$7.88 \cdot 10^7$	$3.87 \cdot 10^7$	$2.15 \cdot 10^8$	$5.76 \cdot 10^7$
melanogaster	21	8	3,352,920	$9.80 \cdot 10^8$	$5.42 \cdot 10^7$	$2.77 \cdot 10^7$	$4.36 \cdot 10^7$	$2.21 \cdot 10^7$	$4.66 \cdot 10^7$	$2.45 \cdot 10^8$	$5.22 \cdot 10^7$
melanogaster	27	8	3,319,232	$1.24 \cdot 10^9$	$5.36 \cdot 10^7$	$2.67 \cdot 10^7$	$4.32 \cdot 10^7$	$2.15 \cdot 10^7$	$4.73 \cdot 10^7$	$2.48 \cdot 10^8$	$5.26 \cdot 10^7$
melanogaster	32	8	3,405,750	$1.37 \cdot 10^9$	$5.49 \cdot 10^7$	$2.66 \cdot 10^7$	$4.09 \cdot 10^7$	$2.16 \cdot 10^7$	$4.90 \cdot 10^7$	$2.36 \cdot 10^8$	$5.38 \cdot 10^7$
raimondii	15	6	89,146,846	$1.76 \cdot 10^9$	$1.27 \cdot 10^9$	$5.18 \cdot 10^8$	$1.07 \cdot 10^9$	$4.22 \cdot 10^8$	$9.59 \cdot 10^7$	$5.98 \cdot 10^8$	$2.11 \cdot 10^8$
raimondii	21	7	69,177,208	$4.37 \cdot 10^9$	$1.03 \cdot 10^9$	$3.30 \cdot 10^8$	$9.08 \cdot 10^8$	$3.04 \cdot 10^8$	$2.16 \cdot 10^8$	$1.24 \cdot 10^9$	$2.90 \cdot 10^8$
raimondii	27	7	58,288,935	$6.04 \cdot 10^9$	$8.16 \cdot 10^8$	$2.55 \cdot 10^8$	$7.14 \cdot 10^8$	$2.42 \cdot 10^8$	$2.37 \cdot 10^8$	$1.29 \cdot 10^9$	$2.94 \cdot 10^8$
raimondii	32	8	45,566,510	$6.96 \cdot 10^9$	$6.84 \cdot 10^8$	$2.28 \cdot 10^8$	$6.38 \cdot 10^8$	$2.19 \cdot 10^8$	$2.70 \cdot 10^8$	$1.38 \cdot 10^9$	$3.10 \cdot 10^8$
GRCh38	15	6	157,853,721	$3.83 \cdot 10^9$	$2.51 \cdot 10^9$	$1.59 \cdot 10^9$	$2.49 \cdot 10^9$	$9.64 \cdot 10^8$	$2.09 \cdot 10^8$	$1.65 \cdot 10^9$	$5.67 \cdot 10^8$
GRCh38	21	7	115,628,937	$1.86 \cdot 10^{10}$	$1.82 \cdot 10^9$	$5.74 \cdot 10^8$	$1.92 \cdot 10^9$	$5.21 \cdot 10^8$	$9.32 \cdot 10^8$	$6.46 \cdot 10^9$	$1.03 \cdot 10^9$
GRCh38	27	8	76,551,392	$2.48 \cdot 10^{10}$	$1.46 \cdot 10^9$	$4.75 \cdot 10^8$	$1.38 \cdot 10^9$	$4.25 \cdot 10^8$	$9.86 \cdot 10^8$	$6.57 \cdot 10^9$	$1.05 \cdot 10^9$
GRCh38	32	8	70,296,231	$2.82 \cdot 10^{10}$	$1.27 \cdot 10^9$	$4.25 \cdot 10^8$	$1.20 \cdot 10^9$	$3.83 \cdot 10^8$	$1.08 \cdot 10^9$	$6.54 \cdot 10^9$	$1.12 \cdot 10^9$
USakai	8	10	236	$3.30 \cdot 10^5$	$2.21 \cdot 10^6$	$6.17 \cdot 10^5$	$5.31 \cdot 10^3$	$6.38 \cdot 10^3$	$2.62 \cdot 10^4$	$1.24 \cdot 10^5$	$1.42 \cdot 10^5$
USakai	11	6	610,965	$1.54 \cdot 10^7$	$1.59 \cdot 10^7$	$1.07 \cdot 10^7$	$4.12 \cdot 10^6$	$4.66 \cdot 10^6$	$1.17 \cdot 10^6$	$4.61 \cdot 10^6$	$3.68 \cdot 10^6$
USakai	15	6	5,105,164	$6.95 \cdot 10^7$	$4.98 \cdot 10^7$	$2.41 \cdot 10^7$	$3.06 \cdot 10^7$	$2.18 \cdot 10^7$	$3.72 \cdot 10^6$	$1.35 \cdot 10^7$	$8.34 \cdot 10^6$
USakai	21	7	4,562,994	$8.53 \cdot 10^7$	$4.79 \cdot 10^7$	$2.48 \cdot 10^7$	$3.19 \cdot 10^7$	$2.29 \cdot 10^7$	$3.91 \cdot 10^6$	$1.39 \cdot 10^7$	$8.40 \cdot 10^6$
SRR622461	15	5	140,872,213	$4.73 \cdot 10^9$	$2.65 \cdot 10^9$	$2.08 \cdot 10^9$	$1.94 \cdot 10^9$	$9.50 \cdot 10^8$	$2.59 \cdot 10^8$	$2.12 \cdot 10^9$	$8.38 \cdot 10^8$

Table 4: Full table comparing the memory of Set-Min sketch constructed for $\epsilon = 0.001$ to all other variables for all possible ks. R = number of rows, B = number of columns, M_{kmc}, M_s = size of Set-Min sketch in bytes, C_s = compressed Set-Min sketch size, M_c = size of Count-Min sketch in bytes, C_c = compressed size of Count-Min sketch, M_{bbhash} = size of the MPHF generated by BBHash without the external array, M_{bball} = total memory for BBHash taking into account the external array, C_{bball} = compressed size of M_{bball}