MaxGeomHash: An Algorithm for Variable-Size Random Sampling of Distinct Elements

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Abstract. With the surge in sequencing data generated from an ever-expanding range of biological studies, designing scalable computational techniques has become essential. One effective strategy to enable large-scale computation is to split long DNA or protein sequences into k-mers, and summarize large k-mer sets into compact random samples (a.k.a. *sketches*). These random samples allow for rapid estimation of similarity metrics such as Jaccard or cosine, and thus facilitate scalable computations such as fast similarity search, classification, and clustering. Popular sketching tools in bioinformatics include Mash and sourmash. Mash uses the MinHash algorithm to generate fixed-size sketches; while sourmash employs FracMinHash, which produces sketches whose size scales linearly with the total number of k-mers.

Here, we introduce a novel algorithm, MaxGeomHash, which for a specified parameter $r > 1$, will produce, without prior knowledge of n (the number of k-mers) a random sample of size $r \lg(n/r) + \mathcal{O}(r)$. Notably, this is the first deterministic, permutation-invariant, and parallelizable sketching algorithm to date that can produce sub-linear sketches. We also introduce a variant, α-MaxGeomHash, that produces random samples of size $\Theta(n^\alpha)$ for a given $\alpha \in (0, 1)$. We study the algorithm's properties, analyze generated sample sizes, verify theoretical results empirically, provide a fast implementation, and investigate similarity estimate quality. With intermediate-sized samples between constant (MinHash) and linear (FracMinHash), MaxGeomHash balances efficiency (smaller samples need less storage and processing) with accuracy (larger samples yield better estimates). On genomic datasets, we demonstrate that MaxGeomHash computes common sketching tasks like database filtering, clustering, and similarity search, more efficiently than approaches like FracMinHash.

Keywords: Random sampling, sketching, k-mers, MinHash, FracMinHash, similarity estimation, dimensionality reduction

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1 Introduction

The exponential growth of genomic and metagenomic sequencing data has necessitated the development of scalable computational methods that can efficiently process and compare biological sequences. Central to many of these methods is the concept of k-mers: subsequences of length k extracted from longer sequences—which serve as the fundamental units for sequence comparison and analysis. However, the sheer number of distinct k-mers in modern sequencing datasets makes exact comparisons computationally prohibitive, driving the need for approximation techniques that trade perfect accuracy for dramatic improvements in speed and memory usage.

Sketching methods have emerged as a powerful solution to this challenge, creating compact representations or "fingerprints" of sequence data that preserve essential similarity information while dramatically reducing computational requirements. Among these, MinHash [1,16] has become ubiquitous in genomic applications, enabling rapid all-versus-all comparisons that would otherwise be intractable due to its fixed-size sketches. However, as we and others have shown [12,13], traditional MinHash exhibits significant limitations when comparing sets of very different sizes (due to its fixed-size sketch), a common scenario in metagenomic analyses where bacterial genomes must be compared against complex environmental samples.

FracMinHash was introduced to address these limitations by allowing sketch sizes to scale naturally with the underlying data [10,8]. Rather than maintaining a fixed number of hash values as in traditional MinHash, FracMinHash retains a fraction s of all k-mers, where $s \in [0, 1]$ is a user-defined scale factor. This seemingly simple modification enables accurate containment estimation between sets of arbitrary sizes due to the fact that sketch sizes scale linearly with the underlying data size.

While FracMinHash provides excellent accuracy, the price it pays is maintaining very large samples (linear in the number of distinct elements). In modern bioinformatics, genomic repositories and metagenomic studies often contain billions to trillions of sequences resulting in very large sketch sizes. This motivates the need for new sampling algorithms that can achieve a middle ground: maintaining the accuracy benefits of scaling samples while keeping sample sizes sub-linear.

In this work, we propose a new algorithm for random sampling, which we call MaxGeomHash (MGH for short), formulated as subsampling from a large finite dataset or data stream. Given a user-defined parameter r, our algorithm produces random samples of (expected) size $\Theta(r \log(n/r))$ from a data stream containing n distinct elements (where n is possibly unknown), providing a compelling balance between sample size and accuracy. We also present variants that render samples of expected size $\Theta(n^\alpha)$, $\alpha \in (0, 1)$, where α is a user-specified parameter.

Importantly, our algorithms are the first order-independent, parallelizable sub-linear sampling methods. Unlike existing sub-linear methods such as Affirmative Sampling [14], which depend on the order of data stream processing and cannot be reliably parallelized, our approach produces identical samples regardless of data partitioning or thread execution order.

As a first relevant application, we study the performance of these new algorithms in terms of time, space, and accuracy when used to estimate similarity measures among sequences in large genomic databases, for different similarity metrics including Jaccard, cosine, and others. We benefit from the results of [15,17] to obtain precise theoretical results describing the bias and variance (both asymptotically going to 0) of the similarity estimators.

We provide rigorous theoretical analysis establishing the expectation and variance of sample sizes and proving unbiased or asymptotically unbiased similarity estimation. Through empirical evaluation, we confirm our theoretical predictions and demonstrate practical utility on real genomic data, including efficient computation of pairwise similarities and phylogenetic tree construction from large genome collections. Lastly, we provide an efficient C++ implementation for computing and comparing MGH/α-MGH samples directly from FASTA/FASTQ files, making our methods readily accessible to the bioinformatics community.

2 Background: Random Sampling from Data Streams

Random sampling has a long history in algorithms and data systems, from early treatments and classic textbook expositions [11,5] to scalable streaming variants such as Reservoir Sampling [19] and its weighted forms [3]. In large-scale bioinformatics, sketching-based sampling is indispensable for scalable, diversity-aware analysis. Prominent families include MinHash and bottom-k [1,2], FracMinHash [9,7], and Affirmative

Sampling [14]; in biological contexts, FracMinHash-style sketches are particularly effective and can be used to estimate a variety of biologically relevant quantities [7,6].

Model and objective. We observe a long dataset or data stream $\mathcal{Z} = z_1, z_2, \ldots, z_N$ of items drawn from a large *universe* $\mathcal{D}$, with $z_i \in \mathcal{D}$. Let the multiset of distinct elements underlying $\mathcal{Z}$ be

$$\mathcal{M} = \{x_1^{f_1}, \ldots, x_n^{f_n}\},$$

with f_i the frequency of x_i in $\mathcal{Z}$, and let the set of distinct elements be

$$\mathcal{X} = \{x_1, \ldots, x_n\}.$$

The (unknown) number $n = |\mathcal{X}|$ is the *cardinality* of $\mathcal{Z}$. Our goal is to obtain a *random sample* $\mathcal{S}$ of distinct elements from $\mathcal{X}$ such that, for $s = |\mathcal{S}|$, every s-subset of $\mathcal{X}$ is equally likely to be drawn. We focus on methods that operate in one pass over $\mathcal{Z}$ without prior knowledge of n, and that are order-independent.

A unifying hashed-sampling view. Most random sampling algorithms work by sequentially processing the dataset or data stream $\mathcal{Z}$, one element at a time, and keeping a current sample $\mathcal{S}$ (in all the cases that we study here $\mathcal{S}$ is a random sample from the subset of elements processed so far). For the current item z, if already present in $\mathcal{S}$, we can update frequency counts, and pass to the next. If z is not present, we compute its hash value $h = h(z)$ and use h to decide whether z is added to the sample or discarded. Moreover, and depending on our decision w.r.t. z, we might decide to make additional changes in $\mathcal{S}$, for example, removing some elements from $\mathcal{S}$. If the algorithm is dependable then those removed elements will never be sampled again, even if they occur again later in the data stream.

Examples of algorithms that fall into the general scheme outlined above include bottom-k and MinHash [1][4] FracMinHash [9,6,7], ModHash [1] [5], Adaptive Sampling [4], and Affirmative Sampling [14].

For example, for FracMinHash, an item z is sampled iff $h(z) \leq s$ for a given real value $s \in (0, 1)$, and interpret hash addresses h as real numbers in $(0, 1)$ too. In bottom-k, the size of the sample will be k (if $n \geq k$), where k is a parameter given in advance. At any given time, an item z is in the sample $\mathcal{S}$ iff it is among the k smallest hash values seen so far. If the current item z has a hash value smaller than the largest hash value in the sample then z is added to the sample; if $|\mathcal{S}| = k + 1$ then the item with the largest hash value in $\mathcal{S}$ is removed. MinHash actually applies k hash functions, and z is sampled if $h_i(z)$ is the minimum hash value among the h_i values observed so far, for some i.

In FracMinHash and ModHash the expected size of the sample $\mathcal{S}$ is linear in n. For FracMinHash, it will follow a binomial distribution of parameters n and s. Likewise, ModHash produces random samples with their size following a binomial distribution of parameters n and $1/m$. Last but not least, in Affirmative Sampling the expected size of $\mathcal{S}$ is $\sim r \ln(n/r)$, for a fixed parameter r, in the standard variant; in α-Affirmative Sampling, $0 < \alpha < 1$, the expected size of the sample is $\Theta(n^\alpha)$.

MinHash has the advantage of producing samples of fixed size and the samples/sketches are small and easy to obtain. However, inference based on those sketches is less accurate, specially when they are used to estimate containment and similarity indices between two sets. Conversely, FracMinHash and ModHash give excellent accuracy, but the price they pay is to keep very large samples (linear in the number of distinct elements). Midway, we have Affirmative Sampling, which guarantees very good accuracy and (asymptotically) unbiased estimation, while producing significantly smaller samples (of size $\Theta(\log n)$ or $\Theta(\sqrt{n})$, say).

All these algorithms return random samples of distinct elements. This is not hard to establish under pragmatic assumptions on the randomness and independence of the hash functions used.

A sampling algorithm is *dependable* [14] if it is order independent: membership of x_j in $\mathcal{S}$ is fixed at its first occurrence; items once removed are never reinserted. Reservoir sampling [19] is not dependable, whereas all algorithms we study are. This property allows exact frequency counts for sampled items.

[4] Both MinHash and bottom-k render samples of fixed size, say M. MinHash actually returns M hash values, not the elements themselves: it applies $h_1, \ldots, h_M$ hash functions to each item in the data set, and keeps the minimum values observed for each of the M hash functions. In bottom-M, we apply a hash function h to each item x in the data set, and we keep the M smallest observed hash values. Despite the two algorithms are different (specially in terms of practical efficiency) they render equivalent random samples of size M, and we will loosely use the terms MinHash and bottom-k interchangeably.

[5] This is not an standard name. It corresponds to the scheme proposed by Broder in [1], where we keep the subset of elements in $\mathcal{X}$ with hash address equal to 0 mod m, for some fixed m.

Parallel composition. Massive datasets must be processed in parallel by partitioning $\mathcal{Z}$ into p disjoint data subsets or substreams $\mathcal{Z}_1, \ldots, \mathcal{Z}_p$. For order-independent sketches there is a standard merge operation: compute a local sample $\mathcal{S}_i$ from each $\mathcal{Z}_i$ and then aggregate

$$\mathcal{S} = \phi\left(\bigcup_{1 \le i \le p} \mathcal{S}_i\right),$$

where ϕ is the algorithm-specific pruning rule (e.g., keep the k smallest hash values, or keep all items with $h(x) \le s$). This equivalence works both ways: running the algorithm on the concatenation $\mathcal{Z}$ or merging local sketches yields the same distribution. MinHash, bottom-k, FracMinHash, and ModHash satisfy this property; Reservoir Sampling does not (unless repetitions are filtered out), and Affirmative Sampling is not mergeable in the same sense.

Expected cost of random sampling. The expected cost $M(n, N)$ of the random sampling algorithms discussed here is of the form $\Theta(N + u(n) \cdot t(S))$, where N is the size of the dataset (or the length of the data stream), n the number of distinct elements ($n \le N$, in many applications $n \ll N$), $u(n)$ is the expected number of times there is an update of the sample (and of auxiliary data structures, if any), and $t(S)$ is the time to update a sample of size S. This cost is based on the assumption that we can test whether a given item z (or hash value $h = h(z)$) is already present in the sample or not in expected constant time. The expected number of updates $u(n)$ will be at least S, but it is often the case that $u(n) \gg S$, for example, in bottom-k we have $S = k$, but $u(n) = k \ln(n/k) + \mathcal{O}(k)$ [14]; using a min-heap to keep and efficiently update the sample we have $t(S) = \mathcal{O}(\log k)$. This gives a total expected cost for bottom-k of $\mathcal{O}(N + k \log k \log(n/k))$. On the other hand, the cost of producing a FracMinHash sketch is $\mathcal{O}(N + ns)$, as $u(n) = S = n \cdot s$ and $t(S) = \Theta(1)$. The expected cost of the new algorithms, MGH and α-MGH, will be investigated in Sections 3 and 4, respectively, where we describe and study their main properties.

At-a-glance comparison. We summarize the main properties that guide the choice of a sampler in practice. Order independence/dependability makes algorithms robust to stream ordering; mergeability enables distributed processing; the parameter controls the memory footprint; and the last column reports the expected sample size (asterisks indicate quantities that are either fixed or bounded by a constant).

Algorithm	Order-indep.?	Mergeable?	Parameter	Expected $\lvert\mathcal{S}\rvert$
MinHash [1]	yes	yes	$k \in \mathbb{N}$	k $(*)$
ModHash [1]	yes	yes	$m \in \mathbb{N}$	n/m
Adaptive Sampling [4]	yes	yes	$B \in \mathbb{N}$	$\frac{B}{2 \ln 2}$ $(*)$
Reservoir Sampling[6] [19]	no	no	$k \in \mathbb{N}$	$\le k$ $(*)$
FracMinHash [9]	yes	yes	$s \in (0, 1)$	$n \cdot s$
Affirmative Sampling [14]	yes	no	$r \in \mathbb{N}$	$r \ln(n/r) + \mathcal{O}(r)$
α-AS [14]	yes	no	$\alpha \in (0, 1)$	$\Theta(n^\alpha)$
MGH (this paper)	yes	yes	$r \in \mathbb{N}$	$r \log_2(n/r) + \mathcal{O}(r)$
α-MGH (this paper)	yes	yes	$\alpha \in (0, 1)$	$\left(\frac{3}{2} + \frac{1}{\alpha \ln 2} - \frac{1}{\ln 2}\right) \cdot n^\alpha + o(n^\alpha)$

In summary, the hashing approach we introduce fits neatly between the fixed-length samples of MinHash and the linearly-sized samples of FracMinHash, while retaining mergeability (which is absent from Affirmative Sampling).

3 MaxGeomHash

Here, we describe our algorithm,MGH which is dependable/order independent and parallelizable in the sense explained in the previous section. Like Affirmative Sampling, it has the nice property of returning samples

[6] Assuming repetitions are filtered out.

of variable size, growing with n. In particular, the standard variant of the algorithm, which we examine now, returns samples of expected size $\Theta(r \log(n/r))$.

Given a bit string $w \neq 000 \cdots 0$, let $\mathrm{zpl}(w)$ denote the length of the longest prefix of 0s in w (if $w = 0000 \cdots$ then $\mathrm{zpl}(w) = |w|$, by convention). In other words, if $\mathrm{zpl}(w) = j$ then the first j bits of w are 0 (bits 0 to $j-1$), and bit j is 1. We will also use $\mathrm{tail}(w, j)$ to denote the bit string that results from removing the first $j+1$ bits of w (that is, the longest prefix of zeros and the leftmost 1).

For each data stream item z, we compute its hash value $h := h(z)$, and determine the position $i = 1+\mathrm{zpl}(h)$ of the leftmost 1 in the binary representation of h. We also set h' as the suffix after the leftmost 1. We use i to index z into a bucket $\mathcal{S}_i$. If $\mathcal{S}_i$ already contains z or h' is not among the r largest hash values in $\mathcal{S}_i$ then we will discard[7] z. If $\mathcal{S}_i$ doesn't yet contain r elements or h' is among the r largest hashes in $\mathcal{S}_i$ then we add z to $\mathcal{S}_i$; in the later case, the element z^* with the smallest hash value h' is evicted, so that $\mathcal{S}_i$ will contain the $\leq r$ elements in the data stream such that their leftmost 1 is at position i of $h(z)$ and have largest $h' = \mathrm{tail}(h(z), i)$. MaxGeomHash is more formally given in Algorithm 1.

Algorithm 1 The basic MaxGeomSampling algorithm

```
procedure MaxGeomSampling(Z : data stream; S : sample)
  initialize S
  for all z in Z do
     h:= hash(z) // h = 0...0 1 h', h' = tail(h, 1+zpl(h))
     if h = 0 then break;
     i:= zpl(h)+1; // position of leftmost 1, 1 <= i <= |h|
     h':= tail(h, i);
     if S[i] does not exist then
       create S[i] and add z to S[i] with freq = 1 and hash h'
     elseif z in S[i]  then
       freq(z):= freq(z)+1
     elseif |S[i]| < r or h' is among the r largest hashes
       add z to S[i] with freq = 1 and hash h'
       if |S[i]| = r+1 then
         evict element with smallest hash from S[i]
       endif
     endif
  enfor
  return S
endprocedure
```

Let $x_1, \ldots, x_n$ denote the distinct elements in $\mathcal{Z}$. Let $\rho_i = 1 + \mathrm{zpl}(\mathrm{hash}(x_i))$. The ρ_i are i.i.d. geometric random variables with parameter $1/2$. Therefore, the probability that an item z has to be considered for bucket $\mathcal{S}_i$ is $1/2^i$. Using this, we can compute the expected sample size and variance,.

Theorem 1. *MaxGeomHash with parameter r will produce a random sample $\mathcal{S}$ of size $S = |\mathcal{S}| = \sum_{1 \leq i \leq R} |\mathcal{S}_i|$ such that*

$$\mathbb{E}[S] = \mathbb{E}\left[\sum_{i=1}^{R} |\mathcal{S}_i|\right] = r \lg(n/r) + r + \epsilon_{n,r}$$

where $R = \max\{\rho_j \mid 1 \leq j \leq n\}$ and $\epsilon_{n,r} \leq E_r + o(1)$ with $E_r = \sum_{m=0}^{r-1} (r-m) e^{-r} \frac{r^m}{m!}$.

Moreover, $\mathbb{V}[S] = r + V_r + o(1)$ for another explicitly computable constant V_r.

Proof (Sketch of the proof). We give here only an intuition of the proof. A fully detailed and rigorous proof can be found in Appendix A.

[7] If z is already in $\mathcal{S}_i$ we update an associated frequency counter, if such counters are needed by the application.

Each bucket $\mathcal{S}_i$ receives (but only keeps up to r) a certain number $X_i \sim \text{Binomial}(n, 1/2^i)$ of items from the data stream $\mathcal{Z}$, that is,

$$S_i = |\mathcal{S}_i| \sim \min(r, \text{Binomial}(n, 1/2^i))$$

and the indices of buckets run from 1 to R, with $R = \max\{\rho_1, \ldots, \rho_n\}$. We know $\mathbb{E}[R] = \lg n + \mathcal{O}(1)$ and $\mathbb{V}[R] = \Theta(1)$ [18]. For the size of the final sample $\mathcal{S}$ we have $S = |\mathcal{S}| = \sum_{i=1}^{R} S_i$, and because of linearity of expectations and the fast decay of the terms with $i \geq \lg n$, it is not difficult to prove that

$$\mathbb{E}[S] = \mathbb{E}\left[\sum_{i=1}^{R} \mathbb{E}[S_i]\right] = \sum_{i\geq 1} \mathbb{E}[S_i]\, \mathbb{P}\{R \geq i\} = \sum_{i=1}^{\mathbb{E}[R]} \mathbb{E}[S_i] + \mathcal{O}(1).$$

For $i = 1, \ldots, i^* = \lg(n/r)$ we will have $S_i = r$ with high probability; likewise, for $i > i^* = \lg(n/r)$, $S_i = \min\{X_i, r\} = X_i$ with high probability, hence $\mathbb{E}[S_i] = n/2^i$ and so $\sum_{i\geq \lg(n/r)+1} \mathbb{E}[S_i] = r + o(1)$. Summing up, we get the asymptotic estimate given in the statement of the theorem, after carefully considering the different errors in the approximation and bounding them. For the variance, the S_i's are not independent but are negatively associated. We can therefore approximate $\mathbb{V}[S] = \sum_{i\geq 1} \mathbb{V}[S_i]$: the sum of covariances between different indices is negligible because, for large n, $r \ll n$ and X_i, X_j are almost independent in the Poisson approximation. The contribution of indices $i < i^*$ is negligible because $Y_i = r$ almost surely. Likewise, the contribution of indices $i > i^*$ is dominated by the sum of small independent Poisson-like variables, giving roughly r. Finally, $i = i^*$ contributes the finite constant $V_r = \mathbb{V}[\min(r, \text{Poisson}(r)]$. □

The constant E_r in the error bound given in Theorem 1 depends only on r, and its value is very small, so we can easily dismiss the error from a practical standpoint. For example, $E_2 = 3e^{-2} \approx 0.406$ and $E_5 \approx 0.615$; for moderately large r we have $E_r \ll r$, and the error is much smaller than the main term $r \log_2(n/r) + r$.

The numerical evaluation of V_r can be done using the Poisson distribution truncated at r:

$$V_r = \sum_{m=0}^{r} (m - \mathbb{E}[Y_{i^*}])^2 e^{-r} \frac{r^m}{m!} + (r - \mathbb{E}[Y_{i^*}])^2 \sum_{m=r+1}^{\infty} e^{-r} \frac{r^m}{m!}.$$

For example, for $r = 5$, $V_5 \approx 1.21$, thus $\mathbb{V}[S] \approx 6.21$. In general, $V_r \sim c \cdot r$ with $c = \frac{1}{2}\left(1 - \frac{2}{\pi}\right) \approx 0.2146\ldots$, when r gets large and $\mathbb{V}[S] \approx 1.215\ldots r + o(1)$.

The expected cost $M_r(n, N)$ of running MGH in a data stream of N items such that n of them are distinct is dominated by the cost of scanning the data stream $\mathcal{O}(N)$, plus the cost of updating the buckets i that contain r elements. We expect $N/2^i$ items to be directed to bucket i, but most will be discarded with cost $\Theta(1)$, as they are repetitions or because their hash h' is not among the r larger in $\mathcal{S}_i$. Like in a bottom-k approach, we expect $\sim r \ln(n/r2^i)$ updates in bucket $\mathcal{S}_i$, and the cost of each of these updates is $\mathcal{O}(\log r)$. Summing over all possible i, we get the expected cost

$$M_r(n, N) \in \mathcal{O}(N + r \log r \log^2(n/r)).$$

4 α-MaxGeomHash

We now discuss a variant of MGH, called α-MGH, that renders samples of expected size $\Theta(n^\alpha)$ for a fixed parameter $\alpha \in (0, 1)$ of our choice. The algorithm is exactly as Algorithm 1, but instead of keeping at most r distinct elements on each $\mathcal{S}_i$, we will keep up to $\lceil 2^{\beta i} \rceil$ in bucket i, with $\beta := \frac{\alpha}{1-\alpha}$. Additional fine tuning can be introduced by setting the maximum capacity of each bucket to $\gamma \cdot 2^{\beta i}$, for a given constant $\gamma > 0$, but for the rest of the section we will stick to $\gamma = 1$.

The intuition is that bucket i, for small i, namely, $i < i^* = (1 - \alpha) \lg n$, will "receive" a lot of elements ($\sim n/2^i$) but only will keep very few ($2^{\beta i} \ll n/2^i$), whereas for "large" i, $i > i^*$, there are very few items going to bucket i but all of them will be kept ($n/2^i \ll 2^{\beta i}$). For $i^* = (1 - \alpha) \lg n$, and since $\alpha = \beta/(1 + \beta)$ and $2^{i^*} = n^{1-\alpha}$, it follows that $\mathcal{S}_{i^*}$ will contain at most $2^{\beta \cdot i^*} = n^{\beta/(1+\beta)} = n^\alpha$ elements, but on the other hand we expect that $n/n^{1-\alpha} = n^\alpha$ distinct elements are directed to bucket i^* and kept since $n/2^{i^*} = 2^{\beta i^*}$. Hence $\mathbb{E}[S_{i^*}] \sim n^\alpha$. The accumulated contribution of the other buckets with values of $i \neq i^*$ can be shown to be $\mathcal{O}(n^\alpha)$. Actually, a more delicate analysis yields the following theorem.

Theorem 2. *The variant α-MGH of* MaxGeomHash *with parameter $\alpha \in (0,1)$ will produce a random sample $\mathcal{S}$ of size S such that*

$$\mathbb{E}[S] = \left(\frac{2^{1/(1-\alpha)}-1}{2^{\alpha/(1-\alpha)}-1}\right)\cdot n^\alpha + o(n^\alpha) \sim \left(\frac{1}{\alpha \ln 2} + \frac{3}{2} - \frac{1}{\ln 2}\right)\cdot n^\alpha.$$

Moreover $\mathbb{V}[S] = n^\alpha + o(n^\alpha)$.

The proof can be found in Appendix B and runs along similar lines as that of Theorem 1.

In α-MGH the expected cost $M_\alpha(n,N)$ of the algorithm is of the form, as we have discussed for the other algorithms, $\mathcal{O}(N + u(n)t(S))$; the expected total number of updates $u(n)$ is $\mathcal{O}(n^\alpha)$ and we can bound the cost of updating any bucket by $\mathcal{O}(\log(n^\alpha)) = \mathcal{O}(\log n)$, one therefore has

$$M_\alpha(n,N) \in \mathcal{O}(N + n^\alpha \log n).$$

5 Similarity estimation of MGH and α-MGH

Given two sets A and B and random samples $\mathcal{S} = \{\mathcal{S}_i\}_{1\le i\le R_A}$ and $\mathcal{T} = \{\mathcal{T}_i\}_{1\le i\le R_B}$, we will use them to estimate Jaccard(A,B). We use A_i and B_i to denote the subsets of A and B of elements x with $\mathrm{zpl}(x)+1 = i$. If we use the same hash function to sample from A and from B, then if an item $x \in A$ is considered for bucket $\mathcal{S}_i$ then it will be also considered for bucket $\mathcal{T}_i$ if x also appears in B (and likewise, exchanging the roles of A and B. and of $\mathcal{S}_i$ and $\mathcal{T}_i$). By definition, we have $A_i \cap A_j = \emptyset$ whenever $i \ne j$, and $\bigcup_{i\ge 1} A_i = A$; likewise, $\{B_i\}_{i\ge 1}$ gives a partition of B. One important result [15] establishes that if $A \cap B = \emptyset$ then $\mathcal{S} + \mathcal{T}$ is a random sample of $A + B$ (this also holds for $\mathcal{S}_i + \mathcal{T}_i$). But $\mathcal{S}_i \cup \mathcal{T}_i$ is not a random sample of $A_i \cup B_i$, nor $\mathcal{S} \cup \mathcal{T}$ a random sample of $A \cup B$. We need therefore to apply some "filtering" or "refining". In particular, we will keep only the r elements with larger hash values (à la bottom-k). So for each i, we will compute $\mathcal{S}_i \cup \mathcal{T}_i$ but keep the r elements with larger hash values h' (or only $|\mathcal{S}_i \cup \mathcal{T}_i|$ elements if that cardinality is smaller than r). Let us call this new sample $\mathcal{U}_i$. This is indeed a random sample of $A_i \cup B_i$. Moreover, we will compute $\mathcal{V}_i = \mathcal{S}_i \cap \mathcal{T}_i$. Notice that $|\mathcal{V}_i| \le r$, since both $\mathcal{S}_i$ and $\mathcal{T}_i$ contain at most r elements each.

All $\mathcal{U}_i$ are mutually disjoint ($\mathcal{U}_i \cap \mathcal{U}_j = \emptyset$ if $i \ne j$) which entails that $\mathcal{U} = \bigcup_{1\le i\le R_{A\cup B}} \mathcal{U}_i$ is a random sample of $A \cup B$. Likewise $\mathcal{V} = \bigcup_i \mathcal{V}_i = A \cap B \cap \mathcal{U}$, hence (see [15] for a detailed proof) $|\mathcal{V}|/|\mathcal{U}|$ is an unbiased estimator of Jaccard(A,B). In fact, we can use $\mathcal{U}$ and $\mathcal{V}$ to estimate many other set similarity and set containment measures [15].

The arguments also work *verbatim* if instead of buckets with maximum capacity equal to r, their capacity is given by f_i, e.g.,$f_i = \lceil 2^{\beta i}\rceil$, as in α-MGH. When computing $\mathcal{U}_i$ we would just need to do the unions $\mathcal{S}_i \cup \mathcal{T}_i$, then retain the elements with the f_i larger h' values (or less if there are not f_i elements in $\mathcal{S}_i \cup \mathcal{T}_i$).

In order to merge two samples $\mathcal{S}$ and $\mathcal{T}$ we should proceed as described above, taking advantage that the two samples are already classified into buckets, and computing the unions/intersections of the buckets $\mathcal{S}_i$ and $\mathcal{T}_i$ while only keeping the k (or $f_i = \lceil 2^{\beta i}\rceil$) elements with larger h' hash values, doing it in one single pass. But from the point of view of the result, the process is equivalent to applying MGH (or α-MGH) to $\mathcal{S} \cup \mathcal{T}$, or $\mathcal{S} \cap \mathcal{T}$, to get the union or the intersection of the two samples; indeed, we have the following important property[8]:

$$\mathrm{MGH}(A \cup B) = \mathrm{MGH}(\mathrm{MGH}(A) \cup \mathrm{MGH}(B)),$$
$$\mathrm{MGH}(A \cap B) = \mathrm{MGH}(\mathrm{MGH}(A) \cap \mathrm{MGH}(B)).$$

Notice that MinHash and FracMinHash satisfy the analogous equalities.

From there, the results of [7,15,17] apply, showing that we can use MGH or α-MGH samples to get (asymptotically) unbiased estimates of the Jaccard similarity of A and B, of their cosine similarity, of the containment index, and many other similarity measures, like Kulczinsky 1, Kulczinsky 2, or Sørensen-Dice.

For some similarity measures like Jaccard, containment index or Kulczinsky 2, the estimates are unbiased; for others, like cosine or Kulczinsky 1, the bias is $\mathcal{O}(\mathbb{E}[1/S])$, with S the size of the sample—which is a random

[8] It holds for any variant of the algorithm, whether the capacity of the buckets is r, $\lceil 2^{\beta i}\rceil$ or any function f_i.

variable for MGH and α-MGH. Also, the variance for all the different similarity measures mentioned above is $\mathcal{O}(\mathbb{E}[1/S])$.

Hence the bias, if any, the variance, and the mean square error (MSE) of all our estimates based on MGH or α-MGH samples will all go to 0 because $\mathbb{E}[1/S] = 1/\mathbb{E}[S] + o(1/\mathbb{E}[S])$ and $\mathbb{E}[S] \to \infty$ if $n \to \infty$. Details of the proof that $\mathbb{E}[1/S] \sim 1/\mathbb{E}[S]$ can be found in Appendix C. In general, it is not true, but because $\mathbb{E}[S] \to \infty$, plus $\mathbb{V}[S] = \mathcal{O}(\mathbb{E}[S])$, it is not difficult to obtain such remarkable result.

Irrespective of how we produce the random samples to be used in similarity estimation, the cost of computing such estimates will be linear in the sizes of the samples (plus the time needed to sort the samples, but this is only paid once, or can be omitted if we use hash-join to compute intersections and unions). Therefore, when we have smaller sketches (like in bottom-k) the computation of similarity estimates is lightning fast, but can be too inaccurate. On the contrary, when the sketches are very large (like in FracMinHash) the estimates are very accurate, but the computation of the estimate is very time-consuming (see, for example, Table 1 in subsection **??**). MGH and α-MGH offer appealing compromises of good accuracy and moderate computational resources.

6 Experiments

In this section, we present our experiments. - simulation experiments verifying theoretical expectations and asymptotically unbiased estimators - one real data experiment highlighting the balance provided by our algorithms

6.1 Empirical evaluation of the growth of samples

Here we present a set of simulation experiments to validate the theoretical expectation of MGH and α-MGH sample sizes. In these experiments, we generated random sets of 10K to 1M elements, where the sets comprise of randomly generated alphanumeric strings of length 10. We generated MGH samples with parameters $r \in \{70, 80, 90, 100\}$, and α-MGH samples with parameters $\alpha \in \{0.4, 0.45, 0.5\}$. For each choice of r and α, we ran 50 independent trials using different hash seeds, and recorded the resulting sample size. The averages of these 50 trials are shown in Figure 1. The theoretical expectations outlined in Theorems 1 and 2 are also shown in Figure 1 using dashed black line. When plotting these expected sizes, we excluded the smaller order terms (specifically, $\epsilon_{n,r}$ for the case of MGH, and $o(n^\alpha)$ for the case of α-MGH) from calculation.

The plots clearly show that the growth of the MGH and α-MGH samples aligns closely with the theoretically derived expectation. As the size of the original set grows, the sample size scales sub-linearly, as we expect them to. Figure 1 also shows one standard deviation for each point. Interestingly, the variance we observe for MGH and α-MGH samples is quite small – which highlights the stability of MaxGeomHash despite its probabilistic design.

6.2 Estimating similarity

6.3 Real data experiment

	Computing sketches		Storing sketches	Computing all-pair Jaccard	
Algorithm name	CPU Time (s)	Peak Memory Usage (GB)	Disk space	CPU Time (s)	Memory (MB)
bottom-k MinHash ($k = 1000$)	5021.74	1.397	160 KB	0.05	4.203
FracMinHash (s=0.001)	3970.84	1.421	360 MB	20.64	977.621
MaxGeomHash (r=80)	4501.39	1.397	0.797 MB	0.03	5.504
α-MaxGeomHash (α=0.4)	5023.92	1.398	6.7 MB	0.34	19.563

Table 1: Computational resources used by four sketching algorithms in estimating phylogeny of ten mammals.

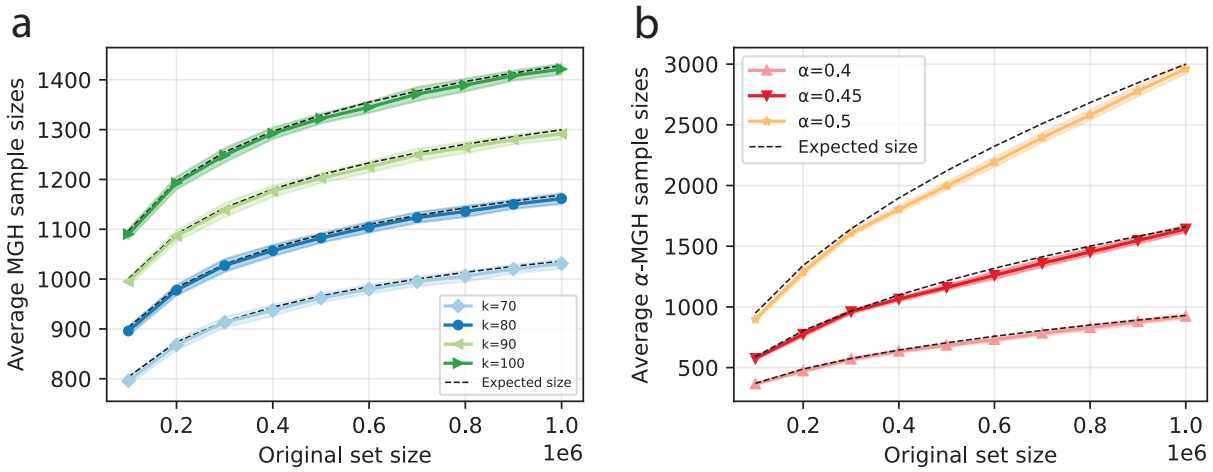

Fig. 1: Average MGH and α-MGH sample sizes consistently track the expected value closely. For the expected size of MGH samples, we showed $\mathbb{E}[S] = r\lg(n/r) + r$ (excluding $\epsilon_{n,r}$), and for the expected size of α-MGH samples, we showed $\left(\frac{1}{\alpha \ln 2} + \frac{3}{2} - \frac{1}{\ln 2}\right) \cdot n^{\alpha}$ (excluding $o(n^{\alpha})$). The solid lines show the average from 50 independent trials, and the shaded regions around the solid lines highlight one standard deviation. The shaded regions are very small, owing to the low variance of sample sizes observed in the simulations.

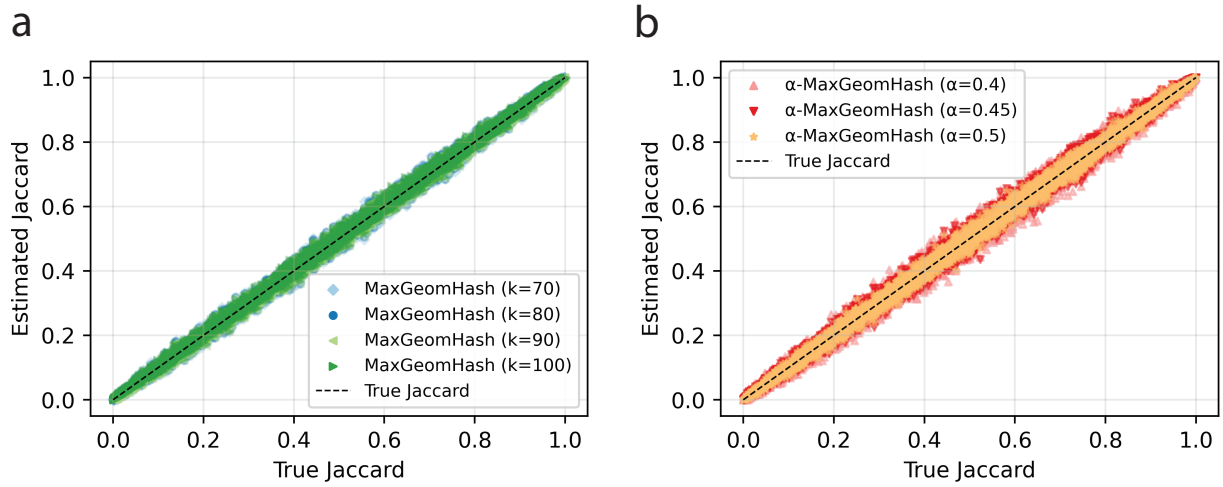

Fig. 2: How accurately we estimate Jaccard

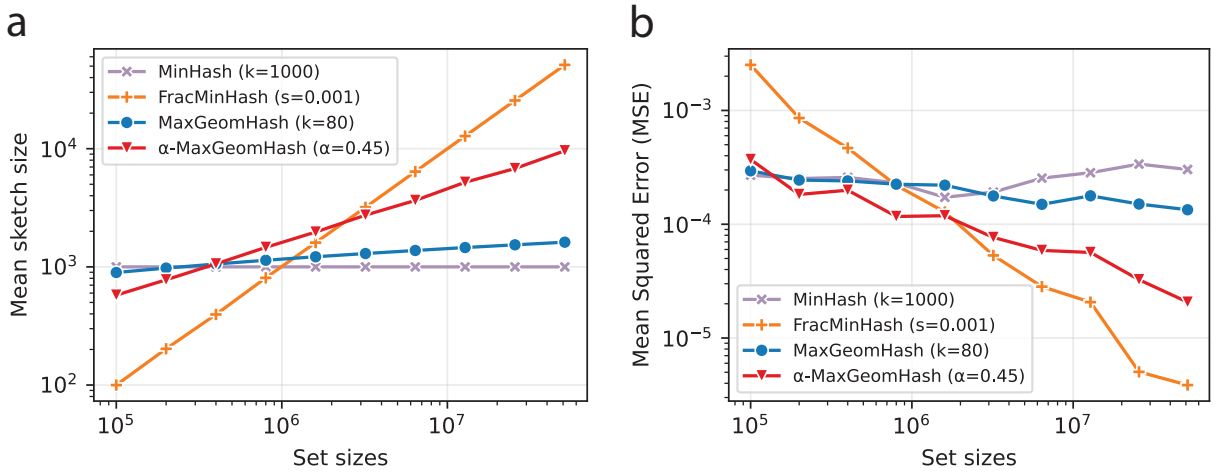

Fig. 3: How accurately we estimate, against other algorithms

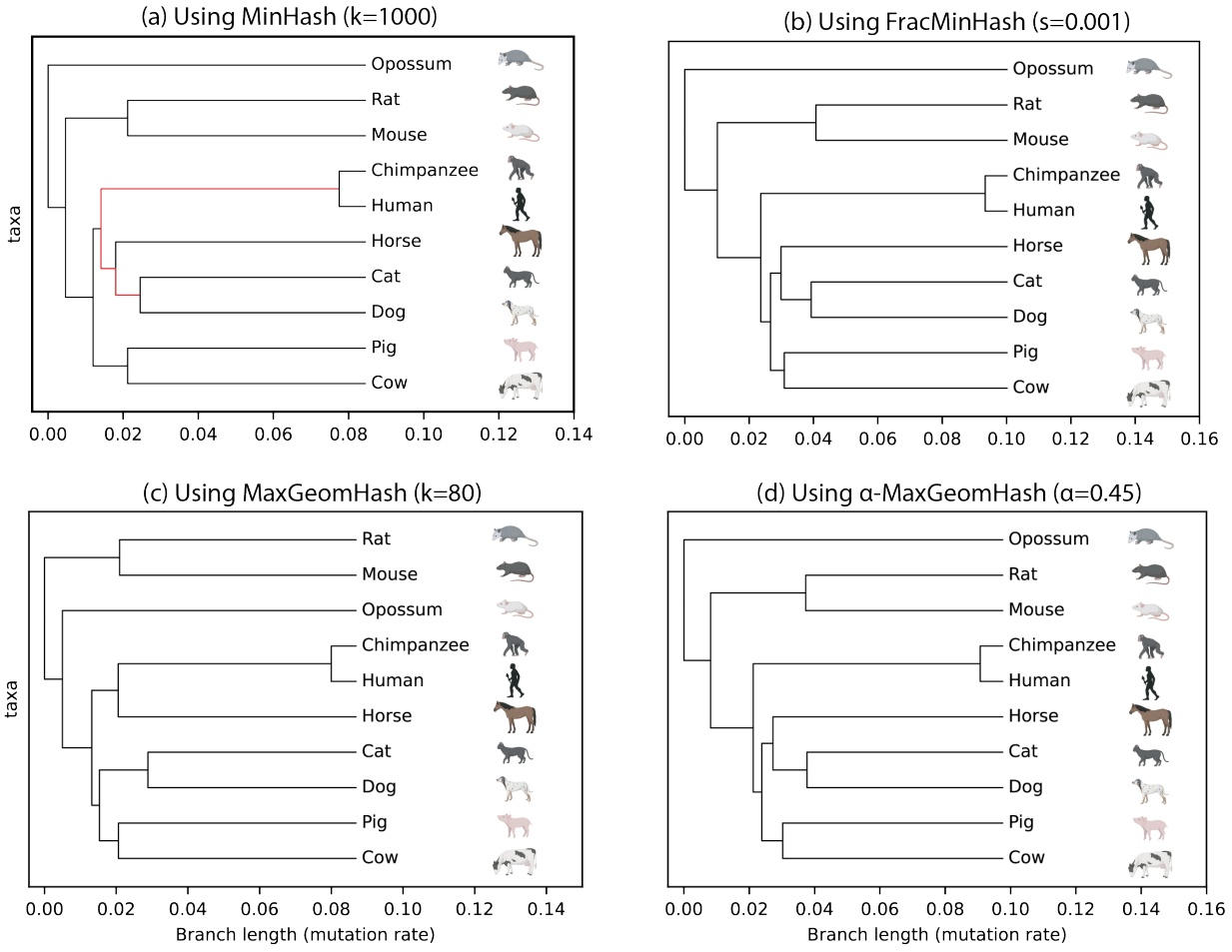

Fig. 4: Estimating similarity tree of real mammal genomes.

7 Conclusion

We introduced MGH and α-MGH, both sketching algorithms that are one-pass, order-independent, and mergeable. Without knowing the number of distinct elements n, MGH yields an expected distinct element sample size of $\Theta(r \log(n/r))$ while α-MGH yields $\Theta(n^\alpha)$. We analyzed sample-size expectation/variance and obtained (asymptotically) unbiased estimators for the Jaccard index, and leveraged recent theory results that automatically extend these estimators to a variety of other metrics (containment, cosine, Kulczinsky 1, etc.) as well as provide explicit error bounds and concentration inequalities.

Sketching in computational biology. Sketches are a core substrate for sequence search, clustering, assembly-scale quality assessment, phylogeny, and metagenomic surveillance. Both MGH and α-MGH are situated between two of the most popular bioinformatics sketching approaches: MinHash (constant sketch size) and FracMinHash (linear sketch size). Hence, we obtain the more accurate scaling feature of FracMinHash, but with the advantage of having smaller sketch sizes. As such, the kinds of biological applications that MinHash and FracMinHash are used for (similarity search, clustering, metagenomic taxonomic and functional profiling, etc.) can all benefit from utilizing MGH. Indeed, workflows that use FracMinHash or MinHash (such as YACHT [**?**], sourmash gather [9], Mash screen [**?**], Skani [**?**], etc. etc.) could be retooled to use MGH to shrink memory/IO budgets whithout altering sacrificing accuracy guarantees.

Similarly, recent work relating sketching based metrics to biologically informative metrics like ANI [8], AAI [**?**], and dN/dS [**?**] translate directly to MGH: one merely replaces a FracMinHash estimate of these metrics with the MGH counterpart.

Recent large-scale computational biology projects, like the Logan effort [**?**] prioritize storage efficiency. Utilizing MGH in such infrastructures and projects can substantially reduce persistent index size with only modest (and exactly quantifiable) accuracy changes, while retaining compatibility with downstream operations on such sketches.

Future improvements include refining our C++ implementation which is not yet fully optimized. There remains headroom from cache-aware bucket layouts, succinct per-bucket priority structures, SIMD-friendly hash partitioning, and task-parallel refinement. These engineering improvements should further reduce runtime and memory while preserving the theoretical guarantees established for MGH and α-MGH.

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A Proof of Theorem 1

Recall that for each item x_j we compute the position of the leftmost 1 in $h(x_j)$. These follow a geometric distribution $\rho_j \sim \mathrm{Geom}(1/2)$ with $p_i := \mathbb{P}\{\rho_j = i\} = 2^{-i}$. Denote $X_i := \#\{j : \rho_j = i\}$, the number of items that would be eventually kept in bucket i. Marginally, each $X_i \sim \mathrm{Binomial}(n, 2^{-i})$ with mean $\mu_i = n2^{-i}$, and the vector $(X_1, X_2, \dots)$ is multinomial $\mathrm{Mult}(n, (p_i)_{i\geq 1})$. But we only keep at most r items on each bucket—those with the r largest hash values—and thus the final size of bucket i is given by $S_i = \min(r, X_i)$, and that of the returned sample is $S = \sum_{i\geq 1} S_i$.

Let $i^* = \lg(n/r)$. If i^* is not integer we may replace it by $\lfloor i^* \rfloor$ (or $\lceil i^* \rceil$) without affecting the nature of the bounds.

We aim to make precise the heuristic argument that we gave in the main body of the paper: if $i \leq i^*$ then typically $\mu_i \gtrsim r$ and therefore $Y_i = r$ with high probability; if $i > i^*$ then typically $\mu_i \ll r$ and therefore $Y_i = X_i$ with high probability. From that heuristic one expects (crudely)

$$\mathbb{E}[S] \approx \sum_{i\leq i^*} r + \sum_{i>i^*} \mu_i = r\lfloor i^* \rfloor + \sum_{i>i^*} n2^{-i} = r\lfloor i^* \rfloor + r.$$

Observe the exact identity

$$\mathbb{E}[Y_i] = r - \mathbb{E}[(r - X_i)_+] = \mu_i - \mathbb{E}[(X_i - r)_+],$$

where $(u)_+ := \max(u, 0)$. Hence

$$\mathbb{E}[S] = \sum_{i\geq 1} \mathbb{E}[Y_i] = \sum_{i\leq i^*} \Big(r - \mathbb{E}[(r - X_i)_+]\Big) + \sum_{i>i^*} \Big(\mu_i - \mathbb{E}[(X_i - r)_+]\Big).$$

Define the approximation

$$A := \sum_{i\leq i^*} r + \sum_{i>i^*} \mu_i = r\lfloor i^* \rfloor + \sum_{i>i^*} n2^{-i} = r\lfloor i^* \rfloor + r.$$

The exact error is then

$$\mathrm{err} := \mathbb{E}[S] - A = -\sum_{i\leq i^*} \mathbb{E}[(r - X_i)_+] - \sum_{i>i^*} \mathbb{E}[(X_i - r)_+].$$

Now, for indices below the cutoff $i < i^*$, we can use standard Chernoff bounds to show

$$\mathbb{E}[(r - X_i)_+] \leq r\mathbb{P}\{X_i < r\} \leq r\exp\Big(-\frac{(\mu_i - r)^2}{2\mu_i}\Big),$$

and summing over all $i < i^*$ gives a negligible contribution $\epsilon_n \to 0$. When we are above the cutoff $i > i^*$ we have $\mu_i < r$ by definition, and we can using the upper-tail bound:

$$\mathbb{E}[(X_i - r)_+] \leq \mu_i \mathbb{P}\{X_i \geq r\} \leq \mu_i \left(\frac{e\mu_i}{r}\right)^r,$$

which also goes to 0 exponentially fast in n; thus summing over $i > i^*$ gives another negligible contribution. We have therefore only left the critical index $i = i^*$, when $\mu_{i^*} = r$. Because we assume r is constant, for n large enough the binomial X_{i^*} converges to a Poisson distribution

$$X_{i^*} \sim \mathrm{Binomial}(n, r/n) \xrightarrow[n\to\infty]{d} \mathrm{Poisson}(r).$$

and thus

$$\mathbb{E}[(r - X_{i^*})_+] \longrightarrow E_r := \sum_{m=0}^{r-1} (r - m)e^{-r}\frac{r^m}{m!}.$$

Combining all three contributions:

$$|\mathrm{err}| \leq E_r + \epsilon_n,$$

where $\epsilon_n \to 0$ as $n \to \infty$.

STILL MISSING: The detailed computation of $\mathbb{V}[S]$ along the lines sketched in the main body of the text. The explicit formula for V_r must be given here and discussed. The approximation of the truncated Poisson by a Gaussian gives us the nice expression $V_r \sim cr$, and $c = \mathbb{V}[\min 0, \mathcal{N}(0, 1)]$.

B Proof of Theorem 2

STILL MISSING: the detailed and rigorous calculation of $\mathbb{E}[S]$ and $\mathbb{V}[S]$. I will try to keep it shorter as it follows the same idea as the previous proof.

C Analysis of $\mathbb{E}[1/S_n]$

The variance of the similarity estimators discussed in 5 is in all cases $\Theta(\mathbb{E}[1/S_n])$, where we write S_n for the size of the samples, stressing the fact that the random variable depends on n. Moreover, for similarity measures such as cosine or Kulczinsky 1, we have asymptotically unbiased estimation, with the bias of order $\Theta(\mathbb{E}[1/S_n])$.

It is therefore important to know the behavior of $\mathbb{E}[1/S_n]$ as $n \to \infty$; we show that for the two variants of MGH in this paper we have

$$\mathbb{E}\left[\frac{1}{S_n}\right] = \frac{1}{\mathbb{E}[S_n]} + o\left(\frac{1}{\mathbb{E}[S_n]}\right), \tag{1}$$

and since $\mathbb{E}[S_n] \to \infty$ as $n \to \infty$, we conclude that the variance tends to 0 for large n, and likewise the bias, if any, also tends to 0.

To show (1) we will use the following: 1) S_n is a positive integer value, $0 < S_n \leq n$, whenever $n > 0$; 2) $\mu_n = \mathbb{E}[S_n]$ is a non-decreasing function of n and tends to $+\infty$ when $n \to \infty$; 3) $\sigma_n^2 = \mathbb{V}[S_n] = \mathcal{O}(\mu_n)$ for both variants of MGS: it is $\mathbb{V}[S_n] = \Theta(r)$ for standard MGH, and $\mathbb{V}[S_n] = \Theta(n^\alpha)$ for α-MGH.

Applying Chevbyshev's inequality, we immediately get that S_n has concentration around its mean—we write $S_n = \mu_n + \mathcal{O}_{\mathrm{P}}(\sigma_n)$, that is, for any $\epsilon > 0$, there exists $\delta := \delta(\epsilon)$ such that

$$\mathbb{P}\left\{|S_n - \mu_n| \geq \delta \cdot \sqrt{\mathbb{V}[S_n]}\right\} \leq \frac{\mathbb{V}[S_n]}{\delta^2 \cdot (\sqrt{\mathbb{V}[S_n]})^2} = \frac{1}{\delta^2} = \epsilon,$$

using $\delta = 1/\sqrt{\epsilon}$. Because of (2) and (3) above, we have that $\sqrt{\mathbb{V}[S_n]}/\mathbb{E}[S_n] \to 0$ as $n \to \infty$ and $S_n = \mu_n + \mathcal{O}_{\mathrm{P}}(\sigma_n)$ are equivalent.

Define now $X_n := S_n - \mu_n$, so that $\mathbb{E}[X_n] = 0$ and $\mathbb{V}[X_n] = \mathbb{E}\left[X_n^2\right] = \mathbb{V}[S_n] = \sigma_n^2$. Note that $-n \leq X_n \leq n$ for all $n > 0$. Using a Taylor expansion of $1/S_n$ around μ_n:

$$\frac{1}{S_n} = \frac{1}{\mu_n + X_n} = \frac{1}{\mu_n}\left(1 - \frac{X_n}{\mu_n} + \frac{X_n^2}{\mu_n^2} - \frac{X_n^3}{\mu_n^3} + \dots\right),$$

and taking expectations, we obtain

$$\mathbb{E}\left[\frac{1}{S_n}\right] = \frac{1}{\mu_n} + \frac{\sigma_n^2}{\mu_n^3} - \frac{\mathbb{E}\left[X_n^3\right]}{\mu_n^4} + \dots$$

The second-order term $\sigma_n^2/\mu_n^3 = \mathcal{O}(1/\mu_n^2)$ and higher-order terms are negligible, because the concentration $S_n = \mu_n + \mathcal{O}_{\mathrm{P}}(\sigma_n)$ and $-n \leq X_n \leq n$ guarantee $\mathbb{E}\left[X_n^k\right] = \mathcal{O}(\sigma_n^k)$ for all $k \geq 2$.