Conformalized Frequency Estimation from Sketched Data

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Abstract

A flexible conformal inference method is developed to construct confidence intervals for the frequencies of queried objects in a very large data set, based on the information contained in a much smaller sketch of those data. The approach is completely data-adaptive and makes no use of any knowledge of the population distribution or of the inner workings of the sketching algorithm; instead, it constructs provably valid frequentist confidence intervals under the sole assumption of data exchangeability. Although the proposed solution is much more broadly applicable, this paper explicitly demonstrates its use in combination with the famous count-min sketch algorithm and a non-linear variation thereof to facilitate the exposition. The performance is compared to that of existing frequentist and Bayesian alternatives through several experiments with synthetic data as well as with real data sets consisting of SARS-CoV-2 DNA sequences and classic English literature.

Keywords: Sketching, conformal inference, memory constraints, privacy, frequency estimation.

1. Introduction

1.1. Frequency queries from sketched data

Efficiently finding the frequency of an object from a sketch of a very large data set is an important problem in computer science (Misra and Gries, 1982; Charikar et al., 2002), which has applications in many scientific endeavors including machine learning (Shi et al., 2009), cybersecurity (Schechter et al., 2010), natural language processing (Goyal et al., 2012), genetics (Zhang et al., 2014), and data privacy (Cormode et al., 2018). The count-min sketch (CMS) of Cormode and Muthukrishnan (2005) is a renowned algorithm for compressing a data set of \( m \) objects \( Z_1, \ldots, Z_m \in \mathbb{Z} \), belonging to a discrete (and possibly infinite) space \( \mathbb{Z} \), into a representation with reduced memory footprint, while allowing simple approximate queries about the observed frequency of any possible \( z \in \mathbb{Z} \).

At the heart of the CMS lie \( d \geq 1 \) different \( w \)-wide hash functions \( h_j : \mathbb{Z} \to [w] := \{1, \ldots, w\} \), for all \( j \in [d] := \{1, \ldots, d\} \) and some integer \( w \geq 1 \). Each hash function maps the elements of \( \mathbb{Z} \) into one of \( w \) possible buckets, and it is designed to ensure that distinct values of \( z \) tend to populate the buckets uniformly. Hash functions are typically chosen at random from a pairwise independent family \( \mathcal{H} \), which ensures that the probability (over the randomness in the choice of hash functions) that two distinct objects \( z_1, z_2 \in \mathbb{Z} \) are mapped by two different hash functions into the same bucket is equal to \( 1/w^2 \). The data set \( Z_1, \ldots, Z_m \) is then compressed into a sketch matrix \( C \in \mathbb{N}^{d \times w} \) with row sums equal to \( m \). The element in the \( j \)-th row and \( k \)-th column of \( C \) counts the number of data points mapped by the \( j \)-th hash function into the \( k \)-th bucket:

\[
C_{j,k} = \sum_{i=1}^{m} \mathbb{1} \left[ h_j(Z_i) = k \right], \quad j \in [d].
\]
Because $d$ and $w$ are such that $d \cdot w \ll m$, the matrix $C$ loses information compared to the full data set, but it has the advantage of requiring much less space to store.

Given a sketch $C$ from (1), one may want to answer queries about the original data. A fundamental instance of this problem consists in estimating the empirical frequency of an object $z \in \mathcal{Z}$:

$$f_m(z) := \sum_{i=1}^{m} 1 \left[ Z_i = z \right].$$

(2)

One solution is to return the smallest count among the $d$ buckets into which $z$ is mapped:

$$\hat{f}_{CMS}^{up}(z) = \min_{j \in [d]} \{C_{j,h_j(z)}\} \geq f_m(z).$$

(3)

This is a valid deterministic upper bound for the true frequency $f_m(z)$ (Cormode and Muthukrishnan, 2005). Of course, $\hat{f}_{CMS}^{up}(z)$ generally tends to overestimate $f_m(z)$ because different objects are sometimes hashed into the same bucket. However, the independence of the hash functions ensures that collisions are not too common, leading to a probabilistic lower bound for the true $f_m(z)$.

**Theorem 1 (Cormode and Muthukrishnan (2005))** Fix any $\delta, \epsilon \in (0, 1)$. Suppose $d = \lceil -\log \delta \rceil$ and $w = \lceil e/e \rceil$. Then, $\Pr[H]\left[f_m(z) \geq \hat{f}_{CMS}^{up}(z) - \epsilon m\right] \geq 1 - \delta$ for any fixed $z \in \mathcal{Z}$, where $\hat{f}_{CMS}^{up}(z)$ is as in (1) and depends on $d, w$.

For example, if $d = 3$, a 95% lower bound on $f_m(z)$ is $\hat{f}_{CMS}^{up}(z) - \lceil e \cdot m/w \rceil$. The subscript $H$ in Theorem 1 clarifies that the randomness is with respect to the hash functions, while $Z_1, \ldots, Z_m$ and $z$ are fixed. Although this bound is useful, for example to choose $d$ and $w$ prior to sketching, it is not fully satisfactory. First, it is often very conservative if the data are randomly sampled from some distribution as opposed to adversarially fixed. Second, it is not flexible: $\delta$ is fixed by $d$ (as opposed to being determined by the user), while $\epsilon$ is fixed only by the hash width. To address these issues, a bootstrap method was developed by Ting (2018) to compute tighter and data-adaptive lower bounds for $f_m(z)$, under the additional assumptions that the data and the query are independent random samples from some underlying distribution. This approach is nearly exact and optimal for the CMS, up to a possible finite-sample discrepancy between the bootstrap and population distributions, but it relies on the specific linear structure of the CMS (the sketch matrix $C$ in (3) can be written as a linear combination of the true frequencies of all objects in the data set), and the idea is therefore not easily extendable to other sketching algorithms that may often be preferable in practice.

One limitation of the CMS is that it does not mitigate as well as possible the adverse effects of random hash collisions, which can result in an overly conservative deterministic upper bound with some data sets. Fortunately, a simple modification provides meaningful improvements: the CMS with conservative updates (CMS-CU). Whenever a new object $Z_i$ is sketched, the CMS-CU only updates the row of $C$ with the smallest value of $C_{j,h_j(z)}$, leaving the other counters unaltered. Then, the same CMS deterministic upper bound in (3) remains valid. The procedure is outlined in Algorithm 1, Appendix A. The CMS-CU can greatly improve query accuracy compared to the vanilla CMS (Estan and Varghese, 2002), but this practical advantage comes at some cost because the algorithm is non-linear. In particular, the theoretical analysis of the CMS-CU beyond a deterministic upper bound is more challenging, and it appears to be a relatively less explored topic.
1.2. Contributions
This paper will develop a novel method for constructing tight and provably valid frequentist confidence intervals for frequency queries based on sketched data, at any desired level. This method will work seamlessly with the CMS-CU as well as with any other possible sketching algorithm, regardless of whether it is linear or very complex. Our solution is a non-parametric statistical one, in the sense that it makes minimal exchangeability assumptions about the data generating process and then leverages the sampling randomization instead of the specific structure of the sketch or the randomness in its hash functions. Although this will require higher computational power and memory usage compared to traditional sketching, the difference in these requirements will be negligible compared to the size of the data sets involved. Given that our solution will make use of conformal inference, a brief review of the relevant ideas from that literature is provided in the next section.

1.3. Related work

Other types of lower bounds have been developed for the CMS (Cormode and Yi, 2020); however, most are similar to that of Theorem 1 in the sense that they make no assumptions about the data and only make use of the hashing randomness. A different Bayesian perspective is taken by Cai et al. (2018) and Dolera et al. (2021): they model the data distribution with a prior and then compute the posterior of the queried frequencies given the sketch. Our approach is closer to that of Ting (2018) in that we seek similar frequentist guarantees by leveraging the randomness in the data. However, the theoretical frameworks and methodologies are different: Ting (2018) exploits the specific linear structure of the CMS, while we view the sketch as a black box and rely on conformal inference.

Conformal inference was pioneered by Vovk and collaborators (Vovk et al., 2005) and was brought to the statistics spotlight by Lei et al. (2018). Although primarily conceived for supervised prediction (Vovk et al., 2009; Vovk, 2015; Lei and Wasserman, 2014; Romano et al., 2019; Izbicki et al., 2019), conformal inference has found many other applications including outlier detection (Bates et al., 2021), causal inference (Lei and Candès), and survival analysis (Candès et al., 2021). However, to the best of our knowledge its potential for sketching remained untapped.

There exist many algorithms for using a sketch of a large data set to compute approximate frequency queries; some are relatively similar to the CMS (Fan et al., 2000; Goyal and Daumé, 2011; Pitel and Fouquier, 2015; Cormode and Yi, 2020), while others are decidedly more complicated and may involve complex learning algorithms (Hsu et al., 2019; Jiang et al., 2019). Our methodology is applicable to all of them, since nothing that we do is specifically tied to the CMS. However, the CMS is a classic algorithm and it provides a familiar example that will facilitate the exposition.

2. Preliminaries on conformal prediction

As this paper will develop a novel approach for frequency estimation from sketched data that re-purposes and extends statistical techniques for conformal prediction, it will be helpful to begin with a brief review of the relevant concepts from that field. Conformal prediction is typically discussed in a supervised learning context, where the data consist of pairs of observations \((X_i, Y_i)\), with \(X_i\) indicating a vector of features for the \(i\)-th observation and \(Y_i\) denoting the corresponding continuous (or discrete) label. In supervised learning, the goal is to use the information contained in \((X_1, Y_1), \ldots, (X_m, Y_m)\) to learn a mapping between features and labels that can allow one to predict as accurately as possible the unseen label \(Y_{m+1}\) of a new sample with features \(X_{m+1}\). In
particular, conformal prediction assumes that \((X_1, Y_1), \ldots, (X_{m+1}, Y_{m+1})\) are exchangeable random samples from some unknown joint distribution over \((X, Y)\) and then constructs a prediction interval \([\hat{L}_{m,\alpha}(X_{m+1}), \hat{U}_{m,\alpha}(X_{m+1})]\) with guaranteed marginal coverage:

\[
P[\hat{L}_{m,\alpha}(X_{m+1}) \leq Y_{n+1} \leq \hat{U}_{m,\alpha}(X_{m+1})] \geq 1 - \alpha, \tag{4}
\]

for any fixed \(\alpha \in (0, 1)\). Conformal prediction is extremely flexible, as it can leverage any machine learning algorithm to approximate from the data the true relation between \(X\) and \(Y\), thus yielding relatively short intervals satisfying (4). Conformal inference can also be applied to construct more general prediction sets (Romano et al., 2020; Angelopoulos et al., 2020), which may be more useful than intervals for some applications, but it is appropriate to focus on intervals in this paper.

The most straightforward version of conformal prediction begins by randomly splitting the available observations into two disjoint subsets; these are assumed for simplicity to have equal size \(n = m/2\), although this is unnecessary. The first \(n\) samples are employed to fit a completely arbitrary black-box machine learning model for predicting \(Y\) given \(X\); think of a deep neural network or a random forest, for example. The remaining data are utilized to assess the out-of-sample predictive accuracy of this model, which is quantified in terms of individual conformity scores for all \(n\) hold-out samples. Combined with the model learnt from the first half of the data, the empirical distribution of these conformity scores is then translated into an explicit recipe for constructing prediction intervals for future test points as a function of \(X\); these intervals are guaranteed to cover \(Y_{n+1}\) with probability at least \(1 - \alpha\), treating all data as random. The details of this procedure will be clarified shortly. Importantly, the conformal coverage guarantee will hold exactly in finite samples, regardless of the accuracy of the machine learning model, under the sole assumption that \(X_{m+1}\) is exchangeable with the \(n\) hold-out data points. It is worth emphasizing that it is unnecessary for the exchangeability to involve also the data used to train the model, which in fact may even be considered as fixed, although it is sometimes easier to state that all data points are exchangeable.

The implementation of conformal inference depends on the choice of conformity scores. While several different options exist, an intuitive and general explanation is the following. Imagine that associated with the fitted machine learning model there exists a nested sequence (Gupta et al., 2019) of possible prediction intervals \([\hat{L}_{m,\alpha}(x; t), \hat{U}_{m,\alpha}(x; t)]\) for each possible \(x\). This sequence is indexed by the index \(t \in \mathcal{T} \subseteq \mathbb{R}\), which may be either discrete or continuous, and it is increasing, in the sense that \(\hat{L}_{m,\alpha}(x; t_2) \leq \hat{L}_{m,\alpha}(x; t_1)\) and \(\hat{U}_{m,\alpha}(x; t_2) \geq \hat{U}_{m,\alpha}(x; t_1)\) for all \(t_2 \geq t_1\). Further, assume this sequence to be such that there exists \(t_{\infty} \in \mathcal{T}\) such that \(\hat{L}_{m,\alpha}(x; t_{\infty}) \leq Y \leq \hat{U}_{m,\alpha}(x; t_{\infty})\) almost surely for all \(x\). For example, one may consider a sequence of intervals in the form of \(\hat{\psi}_m(x) \pm t\), where \(\hat{\psi}_m\) is a regression function for a bounded continuous label \(Y\) given \(X\) learnt by the black-box machine learning model and \(t\) plays the role of a predictive standard error. Then, the conformity score for a data point with features \(X = x\) and label \(Y = y\) can be defined as the smallest index \(t\) such that \(y\) is contained in the sequence of prediction intervals corresponding to \(x\):

\[
E(X, Y) := \min \left\{ t \in \mathcal{T} : Y \in [\hat{L}_{m,\alpha}(x; t), \hat{U}_{m,\alpha}(x; t)] \right\}. \tag{5}
\]

With this notation in place, the conformal prediction rule is then easily stated. Let \(\mathcal{T}^{\text{calib}} \subset \{1, \ldots, m\}\) indicate the subset of hold-out data points, which we have assumed without loss of generality to have size \(n = m/2\). Let \(\hat{Q}_{n,1-\alpha}\) denote the \([(1 - \alpha)(n + 1)]\) smallest value among the \(n\) conformity scores \(E(X_i, Y_i)\) evaluated for all \(i \in \mathcal{T}^{\text{calib}}\). Then, the output conformal prediction
intervals that are simultaneously valid for both rare and random queries, adapting related ideas from all but one specific query about $\phi$. The goal is to leverage the exchangeability and the information in $\phi$ regardless of whether it involves random hashing or any other specific data compression technique. That is, a sketching performed by the CMS or CMS-CU, in which case $C$ is some space with lower dimensions compared to $[Z]^m$. For example, $\phi$ may represent the sketching performed by the CMS or CMS-CU, in which case $C = \mathbb{N}^{d \times w}$ for some $d, w$ such that $d \cdot w \ll m$. In general, our framework will treat $\phi$ as a black box and allow it to be anything, regardless of whether it involves random hashing or any other specific data compression technique.

The goal is to leverage the exchangeability and the information in $\phi(Z_1, \ldots, Z_m)$ to estimate the unobserved true empirical frequency $f_m(z)$ of some object $z \in Z$, defined as in (2), while accounting for uncertainty. More precisely, although still informally speaking, we would like to construct a confidence interval in the form of $[L_{m,\alpha}(z), \hat{U}_{m,\alpha}(z)]$ that is guaranteed to contain $f_m(z)$ "with probability at least $1 - \alpha"$, where the randomness here is with respect to the random data sampling.

One way to address the above problem is to assume that the query point $z$ is also drawn exchangeably from the same distribution as $Z_1, \ldots, Z_m$. Taking this viewpoint, we will refer to $z$ as $Z_{m+1}$ and consider the goal of computing a confidence interval $[L_{m,\alpha}(Z_{m+1}), \hat{U}_{m,\alpha}(Z_{m+1})]$ depending on $\phi(Z_1, \ldots, Z_m)$ that is as short as possible and such that

$$\mathbb{P}[L_{m,\alpha}(Z_{m+1}) \leq f_m(Z_{m+1}) \leq \hat{U}_{m,\alpha}(Z_{m+1})] \geq 1 - \alpha,$$

where the probability is with respect to $Z_1, \ldots, Z_{m+1}$. The interpretation of (7) is as follows: the interval will cover the true frequency $f_m(z)$ for at least fraction $1 - \alpha$ of all future test points on average, if the queries are drawn exchangeably from the same distribution as the sketched data. Of course, this guarantee is not fully satisfactory because some random queries may be more likely to be observed than others, and therefore not all of our inferences will be equally reliable. In particular, the confidence intervals for rare queries may have lower coverage than expected, as illustrated by the following thought experiment. Imagine for example that $P_Z$ has support on $Z = \{0, 1, 2, \ldots, 10^{100}\}$, with $\mathbb{P}[Z_i = 0] = 0.95$ and $\mathbb{P}[Z_i = z] = 0.05/|Z| - 1$ for all $z \in Z \setminus \{0\}$ and $i \geq 1$. In that case, a 95% confidence interval such as that in (7) may be completely unreliable for all but one specific query about $f_m(0)$. Therefore, we will focus instead on constructing confidence intervals that are simultaneously valid for both rare and random queries, adapting related ideas from

3. Conformalized sketching

3.1. Problem statement

Assume the $m$ data points to be sketched, $Z_1, \ldots, Z_m \in Z$, are exchangeable random samples from some distribution $P_Z$ on $Z$. Although $P_Z$ may be arbitrary and unknown, the statistical framework assumed here is more restrictive compared to the classical deterministic setting reviewed in Section 1.1, which treats the observations as fixed and therefore can in principle also handle non-stationary data streams as well as completely adversarial data sets. Yet, there are interesting applications in which the assumption of exchangeable random samples can be justified; this will be discussed in more detail in Sections 4 and 5. Consider an arbitrary sketching function $\phi : [Z]^m \rightarrow C$, where $C$ is some space with lower dimensions compared to $[Z]^m$. For example, $\phi$ may represent the sketching performed by the CMS or CMS-CU, in which case $C = \mathbb{N}^{d \times w}$ for some $d, w$ such that $d \cdot w \ll m$. In general, our framework will treat $\phi$ as a black box and allow it to be anything, regardless of whether it involves random hashing or any other specific data compression technique. The goal is to leverage the exchangeability and the information in $\phi(Z_1, \ldots, Z_m)$ to estimate the unobserved true empirical frequency $f_m(z)$ of some object $z \in Z$, defined as in (2), while accounting for uncertainty. More precisely, although still informally speaking, we would like to construct a confidence interval in the form of $[L_{m,\alpha}(z), \hat{U}_{m,\alpha}(z)]$ that is guaranteed to contain $f_m(z)$ "with probability at least $1 - \alpha"$, where the randomness here is with respect to the random data sampling.

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the conformalized multi-class classification (Vovk et al., 2005; Sadinle et al., 2019; Romano et al., 2020). Precisely, fix any partition \( B = (B_1, \ldots, B_L) \) of \( \{1, \ldots, m\} \) into \( L \) bins, such that each \( B_i \) is a sub-interval of \( \{1, \ldots, m\} \), and construct a confidence interval \([\hat{L}_{m,\alpha}(Z_{m+1}), \hat{U}_{m,\alpha}(Z_{m+1})]\) depending on \( \phi(Z_1, \ldots, Z_m) \) and \( B \) that is as short as possible and such that:

\[
P\left[ \hat{L}_{m,\alpha}(Z_{m+1}) \leq f_m(Z_{m+1}) \leq \hat{U}_{m,\alpha}(Z_{m+1}) \mid f_m(Z_{m+1}) \in B \right] \geq 1 - \alpha, \quad \forall B \in B. \tag{8}
\]

The choice of \( B \) will involve some trade-offs: finer partitions yield more reliable theoretical guarantees but possibly wider confidence intervals; in particular, intervals associated with a bin \( B \) may tend to be wider if \( P\{Z \in B\} \) is small. In practice, we will adopt \(|B| = 5\) later in this paper, but much larger \(|B|\) can be utilized when working with very big data, as it will become clear below.

### 3.2. Conformalization

In the attempt of adapting conformal inference to address the sketching problem, the first difficulty is that the latter is a data recovery problem, not a supervised prediction task. We propose to overcome this challenge by storing in memory the true frequencies for all objects in the first \( m_0 \) observations, with \( m_0 \ll m \); but sufficiently large subject to memory constraints. Without loss of generality, assume \( m_0 \ll m \); otherwise, the problem would be trivial. Let \( n \leq m_0 \) indicate the number of distinct objects among the first \( m_0 \) observations. The memory required to store these frequencies is \( O(n) \), which will typically be negligible as long as \( m_0 \) is also small compared to the size of the sketch, \(|C|\). This approach turns our problem into a supervised prediction one, as detailed below.

During an initial **warm-up** phase, the frequencies of the \( n \) distinct objects among the first \( m_0 \) observations from the data stream, \( Z_1, \ldots, Z_{m_0} \), are stored exactly into:

\[
f_{m_0}^{wu}(z) := \sum_{i=0}^{m_0} 1_{[Z_i = z]}. \tag{9}
\]

Next, the remaining \( m - m_0 \) data points are streamed and sketched, storing also the true frequencies for all instances of objects already seen during the warm-up phase. In other words, the following counters are computed and stored along with the data sketch \( \phi(Z_{m_0+1}, \ldots, Z_m) \):

\[
f_{m-m_0}^{sv}(z) := \begin{cases} 
\sum_{i=m_0+1}^{m} 1_{[Z_i = z]} , & \text{if } f_{m_0}^{wu}(z) > 0, \\
0 , & \text{otherwise}.
\end{cases} \tag{10}
\]

Again, this requires only \( O(n) \) memory. Now, let us define the variable \( Y_i \) for all \( i \in \{1, \ldots, m_0\} \cup \{m + 1\} \) as the true frequency of \( Z_i \) among \( Z_{m_0+1}, \ldots, Z_m \):

\[
Y_i := \sum_{i'=m_0+1}^{m} 1_{[Z_{i'} = Z_i]}. \tag{11}
\]

Note that \( Y_i \) is observable for \( i \in \{1, \ldots, m_0\} \), in which case \( Y_i = f_{m-m_0}^{sv}(Z_i) \). For a new query, \( Z_{m+1} \) is the target of inference—in truth, the target is \( f_m(Z_i) = Y_i + f_{m_0}^{wu}(Z_i) \), but the second term is already known exactly. To complete the connection between sketching and supervised conformal prediction, one still needs to define meaningful features \( X \), and this is where the sketch
\(\phi(Z_{m+1}, \ldots, Z_m)\) comes into play. For each \(i \in \{1, \ldots, m_0\} \cup \{m+1, \ldots\}\), define \(X_i\) as the vector containing the object of the query as well as all the information in the sketch:

\[
X_i := (Z_i, \phi(Z_{m_0+1}, \ldots, Z_m)).
\]

The following result establishes that the pairs \((X_1, Y_1), \ldots, (X_{m_0}, Y_{m_0}), (X_{m+1}, Y_{m+1})\) are exchangeable with one another. This anticipates that conformal prediction techniques can be applied to the supervised observations \((X_1, Y_1), \ldots, (X_{m_0}, Y_{m_0})\) to predict \(Y_{m+1}\) given \(X_{m+1}\), guaranteeing the marginal coverage property in (7). All mathematical proofs are in Appendix B.

**Proposition 1** If the data \(Z_1, \ldots, Z_{m+1}\) are exchangeable, then the pairs of random variables \((X_1, Y_1), \ldots, (X_{m_0}, Y_{m_0}), (X_{m+1}, Y_{m+1})\) defined in (11)–(12) are exchangeable with one another.

Further, confidence sets satisfying the stronger conditional coverage property defined in (8) can be obtained by modifying the standard conformal inference procedure as follows. First, each data point \((X_i, Y_i)\) in the calibration set \(I_{\text{calib}} = \{1, \ldots, m_0\}\) is assigned to the appropriate frequency bin based on \(Y_i\). Define \(n_l\) as the number of calibration data points assigned to bin \(B_l\), for all \(l \in \{1, \ldots, L\}\). Then, \(\hat{Q}_{n_l,1-\alpha}(B_l)\) is defined as the \(\lceil (1 - \alpha)(n_l + 1) \rceil\) smallest value among the \(n_l\) conformity scores assigned to bin \(B_l\). Finally, the confidence interval for a new random query \(X_{m+1}\) is given by

\[
[\hat{L}_{m,\alpha}(X_{m+1}; \hat{Q}_{n,1-\alpha}^*), \hat{U}_{m,\alpha}(X_{m+1}; \hat{Q}_{n,1-\alpha}^*)],
\]

where

\[
\hat{Q}_{n,1-\alpha}^* := \max_{l \in \{1, \ldots, L\}} \hat{Q}_{n_l,1-\alpha}(B_l),
\]

and \([\hat{L}_{m,\alpha}(\cdot; t), \hat{U}_{m,\alpha}(\cdot; t)]\) is a rule for computing a nested sequence of intervals depending on \(Z_{m+1}\) and \(\phi(Z_{m_0+1}, \ldots, Z_m)\). Examples of such rules are in the next section. Importantly, these rules may involve parameters to be fitted on a subset of \(m_0^{\text{train}}\) supervised data points \((X_i, Y_i)\) for \(i \in \{1, \ldots, m_0^{\text{train}}\}\), as long as the scores are only evaluated on the remaining \(m_0 - m_0^{\text{train}}\) points. This procedure is outlined in Algorithm 2, Appendix A. The following result states that the confidence interval output by Algorithm 2 has the desired frequency-range conditional coverage.

**Theorem 2** If the data \(Z_1, \ldots, Z_{m+1}\) are exchangeable, the confidence interval output by Algorithm 2 satisfies the frequency-range conditional coverage property defined in (8).

### 3.3. Conformity scores

Algorithm 2 can accommodate virtually any data-adaptive rule, depending on \(Z_{m+1}\) and on the sketch \(\phi := \phi(Z_{m_0+1}, \ldots, Z_m)\), for computing nested confidence intervals. Two concrete options are presented here. For simplicity, we focus on one-sided confidence intervals; that is, we seek a \(1 - \alpha\) lower bound for \(f_m(X_{m+1})\). This is of particular interest when a deterministic upper bound \(\hat{f}_{\text{up}}(Z_{m+1}) \geq f_m(Z_{m+1})\) is already available, as it is the case with the CMS or CMS-CU. Then, one can simply set \(\hat{U}_{m,\alpha}(\cdot; t) := \hat{f}_{\text{up}}(z)\) and focus on computing \(\hat{L}_{m,\alpha}(\cdot; t)\).

The first option for \(\hat{L}_{m,\alpha}(\cdot; t)\) is to use the following fixed rule:

\[
\hat{L}_{m,\alpha}^\text{fixed}(\langle z, \phi \rangle; t) := \max\{0, \hat{f}_{\text{up}}(Z_{m+1}) - t\}, \quad t \in \{0, 1, \ldots, m\}.
\]
In words, the lower bound for $f_m(Z_{m+1})$ in (14) is defined by shifting the deterministic upper bound downward by $t$. The appropriate value of $t$ guaranteeing the desired coverage for future random queries is calculated by the conformal inference procedure outlined in Algorithm 2. This approach has the advantage of being simple and intuitive, and it is very similar to the optimal solution of Ting (2018) for the special case of the CMS. Further, it does not need training data, so all $m_0$ observations with tracked frequencies can be utilized for computing conformity scores.

The second option involves training but has the advantage of being more flexible; this is inspired by the approaches of Chernozhukov et al. (2021) and Sesia and Romano (2021) for conformalized regression. Concretely, consider a machine learning model that takes as input the known upper bound $\hat{f}_{up}(Z_i)$ and estimates the conditional distribution of $\hat{f}_{up}(Z_i) - f_m(Z_i)$ given $\hat{f}_{up}(Z_i)$. For example, think of a multiple quantile neural network (Taylor, 2000) or a quantile random forest (Meinshausen, 2006). After fitting this model on the $m_0^{\text{train}}$ supervised data points $(X_i, Y_i)$ allocated for training, let $\hat{q}_t$ be the estimated $\alpha_t$ lower quantile of the of $\hat{f}_{up}(Z_i) - f_m(Z_i)$, for all $t \in \{1, \ldots, T\}$ and some fixed sequence $1 = \alpha_1 < \ldots < \alpha_T = 0$. Without loss of generality, assume the machine learning model is that $\hat{q}_0 = 0$ and $\hat{q}_T = m$. Then, define $\hat{L}_{m,\alpha}(\cdot; t)$ as:

$$\hat{L}_{m,\alpha}^{\text{adaptive}}((z, \phi); t) := \max \left\{ 0, \hat{f}_{up}(X_{m+1}) - \hat{q}_t \left( \hat{f}_{up}(X_{m+1}) \right) \right\}, \quad t \in \{0, 1, \ldots, m\}. \quad (14)$$

The advantage of this second approach is that it can lead to an adaptive lower bound whose distance from the upper bound is data adaptive. For example, it may be the case that the sketching algorithm introduces higher uncertainty about the frequencies of more common items compared to rarer ones, or vice versa, and this pattern can be learnt given a sufficient number of supervised samples.

Of course, the two above examples of $\hat{L}_{m,\alpha}(\cdot; t)$ are not the only possible ones. Algorithm 2 can be applied in combination with any rule for computing nested sequences of lower bounds, and it could potentially leverage all high-dimensional information contained in $\phi(Z_{m_0+1}, \ldots, Z_m)$, not just the deterministic upper bound for the CMS and CMS-CU. However, the applications in this paper focus on the CMS and CMS-CU, so other families of lower bounds are not discussed here.

4. Applications

4.1. Experiments with synthetic data sets

Conformalized sketching is applied with the two types of conformity scores described in Section 3.3. The adaptive scores are based on an isotonic distributional regression model (Henzi et al., 2021). The goal is to compute lower frequency bounds for random queries based on simulated data compressed by the CMS-CU, implemented with $d = 3$ hash functions of width $w = 1000$. In particular, $m = 100,000$ observations are sampled independently and identically distributed, from some distribution that will be specified below. The first $m_0 = 5000$ observations are stored without loss during the warm-up phase, as outlined in Algorithm 2, while the remaining 95,000 are compressed through the CMS-CU. The conformity scores are evaluated separately within $L = 5$ frequency bins, seeking the frequency-range conditional coverage property defined in (8). The bins are determined in a data-driven fashion so that each contains approximately the same probability mass; in practice, this is achieved by partitioning the range of frequencies for the objects tracked exactly by Algorithm 2 according to the observed empirical quantiles. Lower bounds for new frequency queries are computed for 10,000 new query points sampled exchangeably from the same distribution, adopting the significance level $1 - \alpha$. The quality of these lower bounds is quantified with two metrics: the
mean length of the resulting confidence intervals and the coverage the proportion of queried objects for which the true frequency is correctly covered, or empirical coverage. The average performance over 10 independent realizations of each experiment is reported.

Experiments are performed using synthetic data sampled from two families of distributions. First, we consider a Zipf distribution with probability mass \( P[Z_i = z] = \frac{z^{-a}}{\zeta(a)} \) for all \( z \in \{1, 2, \ldots\} \), where \( \zeta \) is the Riemann Zeta function and \( a > 1 \) is a parameter that controls the power-law behavior of the tails and will be varied. Second, synthetic data will be generated from a random probability measure distributed as the Pitman-Yor prior (Pitman and Yor, 1997) with a standard Gaussian base distribution and parameters \( \lambda > 0 \) and \( \sigma \in [0, 1) \), as explained in Appendix A.3. The parameter \( \lambda \) is set to \( \lambda = 5000 \), while \( \sigma \) is varied. For \( \sigma = 0 \) the Pitman-Yor prior reduces to the Dirichlet prior (Ferguson, 1973), while \( \sigma > 0 \) results in heavier tails.

Three alternative methods are considered as benchmarks. The first benchmark is the classical 95% lower bound reviewed in Theorem 1. The second benchmark is the Bayesian method of Cai et al. (2018), which assumes a non-parametric Dirichlet process prior for the distribution of the data stream, estimates its scaling parameter by maximizing the marginal likelihood of the observed sketch, and then computes the posterior distribution of the queried frequencies conditional on the observed sketch. The performance of the lower 5% posterior quantile is compared to the lower bounds obtained with the other methods according to the frequentist metrics defined above. The third benchmark is the bootstrap method of Ting (2018), which is nearly exact and optimal for the vanilla CMS (up to some possible finite-sample discrepancy between the bootstrap and population distributions) but is not theoretically valid for other sketching techniques.

Figure 1 compares the average performance of the proposed conformal method to those of the three benchmarks on the Zipf data. All methods achieve the desired marginal coverage (4), with the exception of the Bayesian approach which is based on a misspecified prior family in this case. The length of the confidence intervals indicates the classical bound is extremely conservative, while the bootstrap and conformal methods can provide relative informative bounds, particularly when \( a \) is larger and hash collisions become rarer. However, the conformal confidence intervals can be shorter, especially when implemented with the adaptive conformity scores. This result should not be surprising because the bootstrap approach is not guaranteed to be optimal for the non-linear compression induced by the CMS-CU. Indeed, as shown in Figure 2, the machine learning model deployed by our adaptive conformity scores is able to detect and take advantage of the fact that this non-linear sketch allows increased precision in the queries for more common objects.

Supplementary results reported in Appendix C demonstrate empirically that the CMS-CU leads to more precise queries with all methods compared to the vanilla CMS; see Figure A1. Figure A2 shows that, as expected, the conformal lower bounds no longer have a clear advantage over the bootstrap ones when the data are sketched with the vanilla CMS instead of the CMS-CU. In fact, although the conformal intervals obtained with the adaptive conformity scores can still be little shorter than the bootstrap ones even for the vanilla CMS, the latter have the advantage of (approximately, in the limit of large samples) satisfying an even stronger frequency-conditional coverage property equivalent to (8) with bins of size 1. Analogous results for the experiments with Pitman-Yor process data are also in Appendix C; see Figures A3–A6.
4.2. Analysis of 16-mers in SARS-CoV-2 DNA sequences

This example application involves a data set of nucleotide sequences from SARS-CoV-2 viruses made publicly available by the National Center for Biotechnology Information (Hatcher et al., 2017). These data include 43,196 sequences, each consisting of approximately 30,000 nucleotides. The goal is to estimate the empirical frequency of each possible 16-mer, a distinct sequence of 16 DNA bases found in contiguous nucleotides. Given that each nucleotide has one of 4 bases, there are $4^{16} \approx 4.3$ billion possible 16-mers. This means that exact tracking of all 16-mers is not unfeasible with a powerful computer, which allows us to validate the sketch-based queries. Note that sequences containing missing values are removed during pre-processing, for simplicity.

The experiments are carried out as in Section 4.1, but (1) a larger sample of 1,000,000 observations is sketched, and (2) the width $w$ of the hash functions is varied as a control parameter. Figure 3 shows the performance of all methods as a function of the hash width, measured in terms of marginal
coverage and mean confidence interval width. All methods appear to have marginal coverage above the nominal level, except for the Bayesian approach which yields slightly lower coverage if \( w \) is large. For small hash widths, all methods construct confidence intervals of similar width, because the distribution of SARS-CoV-2 16-mers frequencies is quite concentrated with relatively narrow support (see Figure A7 in Appendix C), which makes it especially difficult to compress the data without much loss. By contrast, the proposed conformal methods yield noticeably shorter confidence intervals if \( w \) is large. Figure A8 reports the same results stratified by the frequency of the queried objects, while Figure A9 confirms the advantage of sketching with the CMS-CU as opposed to the vanilla CMS. Table A1 visualizes a list of 10 common and 10 rare queries along with their corresponding deterministic upper bounds for \( w = 50,000 \), comparing the lower bounds obtained with each method. Table A2 shows analogous results obtained with \( w = 5,000 \).

![Figure 3: Performance of confidence intervals based on sketched SARS-CoV-2 sequence data. The results are shown as a function of the hash width. Other details are as in Figure 1.](image)

Figure A10 compares the performance of different frequency point-estimates, measured in terms of mean absolute deviation from the true frequency. With the classical method we take for simplicity the midpoint of the 95% confidence interval as a point estimate, although there exist of course also other approaches (Cormode and Yi, 2020). For the other methods, the point estimate is defined as the lower confidence bound at level \( \alpha = 0.5 \); in the Bayesian case, this is the posterior median. Although a conformal lower bound at level \( \alpha = 0.5 \) is not always a reliable estimator of conditional medians (Medarametla and Candès, 2021), because the conformal coverage guarantees treat the query as random, this approach consistently outperformed the benchmarks in all of our experiments.

4.3. Analysis of 2-grams in English literature

The second application considered in this paper is based on a data set consisting of the full texts of 18 open-domain classic pieces of English literature downloaded using the NLTK Python package (Bird et al., 2009) from the Gutenberg Corpus (Project Gutenberg). The goal is to count the frequencies of all possible 2-grams—consecutive pairs of English words—across this corpus. After some basic preprocessing to remove punctuation and unusual words (only those contained in a dictionary of size 25,487 common English words are retained), the total number of 2-grams left in this data set is approximately 1,700,000 (although the total number of all possible 2-grams within this dictionary is
approximately 650,000,000). The same experiments are then carried out as in Section 4.2, sketching 1,000,000 randomly sampled 2-grams and querying 10,000 independent 2-grams.

Figure 4 shows the conformal intervals with adaptive scores achieve the desired coverage and tend to have the shortest width, while the Bayesian intervals are not valid unless the hashes are very wide. The conformal approach has a larger advantage here because these data can be compressed more efficiently compared to the one in the previous section because the frequency distribution of English 2-grams has power-law tails; see Figure A7. Additional results along the lines of those in the previous section are in Appendix C; see Figures A11–A13 and Tables A1–A2.

Figure 4: Performance of confidence intervals for random frequency queries, for a sketched data set of English 2-grams in classic English literature. Other details are as in Figure 3.

5. Discussion

Conformalized sketching is a non-parametric and data-adaptive statistical method for quantifying uncertainty in problems involving frequency estimation from sketched data. This paper has revolved around the CMS because that is a prominent technique for which several benchmarks are available. However, the key strength of conformalized sketching is that it operates under the sole assumption that the data are exchangeable with one another as well as with the future queries, without requiring anything from the sketching algorithm, which may be completely arbitrary and even unknown. Therefore, this methodology could be applicable quite broadly when one needs to retrieve information from large data sets that must be sketched due to memory or privacy constraints. Of course, exchangeability is not always an appropriate assumption, and therefore sometimes one has to rely on more conservative bounds based on hashing randomness. Yet there are interesting situations in which the sketched data can be seen as exchangeable random samples from a population. For example, in natural language processing one may wish to count the frequencies of non-contiguous tuples of words co-occurring in the same sentence within a large corpus, expanding on the example of Section 4.3. In that case, it would be unfeasible to keep track of all frequencies exactly, but sketching random samples would be relatively easy. One limitation of conformalized sketching is that it does not provide guarantees about the expected proportion of correct unique queries. In fact, if the queries are randomly sampled exchangeably with the sketched data points, some of them may be redundant. Even though the expected proportion of incorrect unique queries is sometimes below
\( \alpha \) (Figures A14–A15), this is not always the case (Figure A16). It may be possible to modify the procedure to achieve this additional guarantee, but we leave this intriguing problem for future work.

**Software availability**

Code and data needed to reproduce these experiments are available online at [https://github.com/msesia/conformalized-sketching](https://github.com/msesia/conformalized-sketching).

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Appendix A. Algorithms

A.1. CMS-CU

Algorithm 1 CMS-CU

Input: Data set $Z_1, \ldots, Z_m$. Sketch dimensions $d, w$. Hash functions $h_1, \ldots, h_d$. Query $z$.

Initialize: $C_{j,k} = 0$ for all $j \in [d], k \in [w]$.

for $i = 1, \ldots, m$ do
  Compute $j^* = \arg\min_{j \in [d]} C_{j,h_j(Z_i)}$.
  Increment $C_{j^*,h_{j^*}(Z_i)} \leftarrow C_{j^*,h_{j^*}(Z_i)} + 1$
end for

Compute $\hat{f}_{\text{CMS-CU}}^{\text{up}}(z) = \min_{j \in [d]} \{ C_{j,h_j(z)} \}$.

Output: deterministic upper-bound for the frequency of $z$ in the data set: $\hat{f}_{\text{CMS-CU}}^{\text{up}}(z)$. 
A.2. Conformalized sketching

Algorithm 2 Conformalized sketching

Input: Data set \( Z_1, \ldots, Z_m \). Sketching function \( \phi \). Warm-up duration \( m_0 \ll m \).
A (trainable) rule for computing nested intervals \([\hat{L}_{m,\alpha}(\cdot; t), \hat{U}_{m,\alpha}(\cdot; t)]\), \( t \in T \).
Number of data points \( m_0^{\text{train}} < m_0 \) used for training \([\hat{L}_{m,\alpha}(\cdot; t), \hat{U}_{m,\alpha}(\cdot; t)]\).
A partition \( B = (B_1, \ldots, B_L) \) of \( \{0, \ldots, m\} \) into \( L \) intervals.
Random query \( Z_{m+1} \). Desired coverage level \( 1 - \alpha \in (0, 1) \).

Initialize a sparse dictionary \( f^{\text{wu}}_{m_0}(z) = 0, \forall z \in Z \).
for \( i = 1, \ldots, m_0 \) do
  Increment \( f^{\text{wu}}_{m_0}(Z_i) \leftarrow f^{\text{wu}}_{m_0}(Z_i) + 1 \).
end for
Initialize a sparse dictionary \( f^{\text{sv}}_{m-m_0}(z) = 0, \forall z \in Z \).
Initialize an empty sketch \( \phi(\emptyset) \).
for \( i = m_0 + 1, \ldots, m \) do
  Update the sketch \( \phi \) with the new observation \( Z_i \).
  if \( f^{\text{wu}}_{m_0}(Z_i) > 0 \) then
    Increment \( f^{\text{sv}}_{m-m_0}(Z_i) \leftarrow f^{\text{sv}}_{m-m_0} + 1 \).
  end if
end for
Train \([\hat{L}_{m,\alpha}(\cdot; t), \hat{U}_{m,\alpha}(\cdot; t)]\) using the data in \( \{ (X_i, Y_i) \}_{i=1}^{m_0^{\text{train}}} \).
for \( i = m_0^{\text{train}} + 1, \ldots, m_0 \) do
  Set \( X_i = (Z_i, \phi(Z_{m_0+1}, \ldots, Z_m)) \) as in (12).
  Set \( Y_i = f^{\text{sv}}_{m-m_0}(Z_i) \).
  Compute the conformity score \( E(X_i, Y_i) \) with (5), using \([\hat{L}_{m,\alpha}(\cdot; t), \hat{U}_{m,\alpha}(\cdot; t)]\).
  Assign each score \( E(X_i, Y_i) \) to an appropriate frequency bin \( B \in B \) based on \( Y_i \).
end for
for \( l = 1, \ldots, L \) do
  Compute \( \hat{Q}^{n_l,1-\alpha}(B_l) \) as the \([(1 - \alpha)(n_l + 1)] \) smallest value among the \( n_l \) scores in bin \( B_l \).
end for
Set \( \hat{Q}^{1-\alpha} = \max_{l} \hat{Q}^{n_l,1-\alpha}(B_l) \).
Set \( X_{m+1} = (Z_{m+1}, \phi(Z_{m_0+1}, \ldots, Z_m)) \) as in (12).
Output: a \((1 - \alpha)\)-level confidence interval
\[
\left[ f^{\text{wu}}_{m_0}(Z_{m+1}) + \hat{L}_{m,\alpha}(X_{m+1}; \hat{Q}^{1-\alpha}_n), f^{\text{wu}}_{m_0}(Z_{m+1}) + \hat{U}_{m,\alpha}(X_{m+1}; \hat{Q}^{1-\alpha}_n) \right]
\]
for the unobserved frequency \( f_m(Z_{m+1}) \) of \( Z_{m+1} \) defined in (2).
A.3. Sampling from a Pitman-Yor predictive distribution

The data points are sampled sequentially from the following predictive distribution, which has parameters $\lambda > 0$ and $\sigma \in [0, 1)$. After sampling $Z_1$ from a standard normal distribution, $\mathcal{N}(0, 1)$, fix any $i \geq 1$ and let $Z_1, \ldots, Z_i$ indicate the data stream observed up to that point. Denote by $k_i$ the number of distinct elements within it, and by $V_i = (V_{i,1}, \ldots, V_{i,k_i})$ the set of such distinct values. Further, let $c_{i,l}$ indicate the number of times that object $V_{i,l}$ has been observed in $Z_1, \ldots, Z_i$, for $l \in \{1, \ldots, k_i\}$. Then, $Z_{i+1}$ is generated as follows:

$$Z_{i+1} \mid Z_1, \ldots, Z_i = \begin{cases} V_{i,l}, & \text{with probability } \frac{c_{i,l} - \sigma}{\lambda + i}, \text{ for } l \in \{1, \ldots, k_i\}, \\ \mathcal{N}(0, 1), & \text{with probability } \frac{\lambda + k_i \sigma}{\lambda + i}. \end{cases}$$

Above, the second case which occurs with probability $(\lambda + k_i \sigma)/(\lambda + i)$ corresponds to sampling a new unique value from the standard normal distribution.
Appendix B. Mathematical proofs

B.1. Proof of Proposition 1

**Proof** Consider \( ((X_{\pi(1)}, Y_{\pi(1)}), \ldots, (X_{\pi(m_0)}, Y_{\pi(m_0)}), (X_{\pi(m+1)}, Y_{\pi(m+1)})) \) for any permutation \( \pi \) of \( \{1, \ldots, m_0, m + 1\} \). This is equal to \( ((X'_{1}, Y'_{1}), \ldots, (X'_{m_0}, Y'_{m_0}), (X'_{m+1}, Y'_{m+1})) \), defined by applying the functions in (11)–(12) to a shuffled data set \( Z_{\tilde{\pi}(1)}, \ldots, Z_{\tilde{\pi}(m+1)} \), where \( \tilde{\pi} \) indicates a permutation of \( \{1, \ldots, m+1\} \) that agrees with \( \pi \) on \( \{1, \ldots, m, m+1\} \) and leaves \( \{m+1, \ldots, m\} \) unchanged. Therefore,

\[
((X_{\pi(1)}, Y_{\pi(1)}), \ldots, (X_{\pi(m_0)}, Y_{\pi(m_0)}), (X_{\pi(m+1)}, Y_{\pi(m+1)})) \\
= ((X'_{1}, Y'_{1}), \ldots, (X'_{m_0}, Y'_{m_0}), (X'_{m+1}, Y'_{m+1})) \\
\overset{d}{=} ((X_1, Y_1), \ldots, (X_{m_0}, Y_{m_0}), (X_{m+1}, Y_{m+1})),
\]

where the last equality in distribution follows directly from the assumption that \( Z_1, \ldots, Z_{m+1} \) are exchangeable.

\( \blacksquare \)

B.2. Proof of Theorem 2

**Proof** The following notation will be helpful: let \( B(Y_i) \in \mathcal{B} \) indicate the frequency bin into which \( Y_i \) belongs, for \( i \in \{1, \ldots, m_0, m + 1\} \). We begin by proving the result for the simpler case in which Algorithm 2 is applied using conformity scores that do not require training, in which case \( m_0^{\text{train}} = 0 \). For \( i \in \{1, \ldots, m_0, m + 1\} \), define the random variables \( Y_i \) and \( X_i \) as in (11)–(12), respectively. We already know from Proposition 1 that \( (X_1, Y_1), \ldots, (X_{m_0}, Y_{m_0}), (X_{m+1}, Y_{m+1}) \) are exchangeable. This implies that the conformity scores \( E(X_i, Y_i) \) are exchangeable with one another, for \( i \in \{1, \ldots, m_0, m + 1\} \), because each of them only depends on \( X_i, Y_i \) and on the separate data points in the sketch \( \phi(Z_{m_0+1}, \ldots, Z_m) \). Therefore, \( E_{m+1} \) is also exchangeable with the subset of conformity scores with indices in \( \{i \in \{1, \ldots, m_0\} : B(Y_i) = B(Y_{m+1})\} \). Now, fix any bin \( B^* \in \mathcal{B} \) and assume \( B(Y_{m+1}) = B^* \). Now, note that the interval output by Algorithm 2 does not cover the true frequency \( f_m(Z_{m+1}) \) if and only if \( E_{m+1} > Q_{n,1-\alpha} > Q_{n,1-\alpha}(B^*) \). However, a standard exchangeability argument for the conformity scores in \( \{i \in \{1, \ldots, m_0\} : B(Y_i) = B^*\} \) shows that \( \mathbb{P}[E_{m+1} > Q_{n,1-\alpha}(B^*) \mid B(Y_{m+1}) = B^*] \leq 1 - \alpha \); for example, see Lemma 1 of Romano et al. (2019). This completes the first part of the proof. The second part with \( m_0^{\text{train}} > 0 \) follows very similarly: Proposition 1 implies that \( (X_{m_0^{\text{train}}+1}, Y_{m_0^{\text{train}}+1}), \ldots, (X_{m_0}, Y_{m_0}), (X_{m+1}, Y_{m+1}) \) are exchangeable, and so must be the conformity scores \( E_i \) for \( i \in \{m_0^{\text{train}}+1, \ldots, m_0, m + 1\} \), because each of them only depends on the corresponding \( X_i, Y_i \) and on the separate set of observations indexed by \( \{1, \ldots, m_0^{\text{train}}\} \), as well as on the sketch \( \phi(Z_{m_0+1}, \ldots, Z_m) \). The rest of the proof is exactly the same as in the first part because the empirical quantiles \( Q_{n,1-\alpha}(B) \) are only computed on subsets of the data indexed by \( \{m_0^{\text{train}}+1, \ldots, m_0\} \).
Appendix C. Supplementary figures and tables

Figure A1: Performance of confidence intervals for random frequency queries, based on data sketched with either the vanilla CMS or the CMS-CU. Other details are as in Figure 1.

Figure A2: Performance of confidence intervals for random frequency queries, based on data sketched with the vanilla CMS. Other details are as in Figure 1.
Figure A3: Empirical coverage and length of 95% confidence intervals for random frequency queries on a data set sampled from the predictive distribution of a Pitman-Yor process. The results are shown as a function of the Pitman-Yor process parameter $\sigma$. Other details are as in Figure 1.

Figure A4: Performance of confidence intervals for random frequency queries, stratified by the quintile of the true query frequency. Other details are as in Figure A3.
Figure A5: Performance of confidence intervals for random frequency queries, based on data sketched with either the vanilla CMS or the CMS-CU. Other details are as in Figure A3.

Figure A6: Performance of confidence intervals for random frequency queries, based on data sketched with the vanilla CMS. Other details are as in Figure A3.
Figure A7: True frequency distribution in two sketched data sets. Left: sequenced SARS-CoV-2 DNA 16-mers. Right: English 2-grams in a corpus of classic English literature.

Figure A8: Performance of confidence intervals for random frequency queries, stratified by the quintile of the true query frequency. Other details are as in Figure 3.
Figure A9: Performance of confidence intervals for random frequency queries, based on data sketched with either the vanilla CMS or the CMS-CU. Other details are as in Figure 3.

Figure A10: Median absolute deviation of point estimates for random frequency queries. Other details are as in Figure 3.
Figure A11: Performance of confidence intervals for random frequency queries, stratified by the quintile of the true query frequency. Other details are as in Figure 4.

Figure A12: Performance of confidence intervals for random frequency queries, based on data sketched with either the vanilla CMS or the CMS-CU. Other details are as in Figure 4.
Figure A13: Median absolute deviation of point estimates for random frequency queries. Other details are as in Figure 4.

Figure A14: Performance of confidence intervals for random frequency queries, keeping only unique queries. The coverage is defined as the empirical proportion of unique queries whose frequency is correctly covered by the output confidence intervals. Other details are as in Figure 3.
Figure A15: Performance of confidence intervals for random frequency queries, keeping only unique queries. The coverage is defined as the empirical proportion of unique queries whose frequency is correctly covered by the output confidence intervals. Other details are as in Figure 4.

Figure A16: Performance of confidence intervals for random frequency queries, keeping only unique queries. The coverage is defined as the empirical proportion of unique queries whose frequency is correctly covered by the output confidence intervals. Other details are as in Figure 1.
**Table A1:** True frequencies, deterministic upper bounds, and 95% lower bounds for some random queries in two sketched data sets. Sketching with CMS-CU with $w = 50,000$. Lower bounds written in green are below the true frequency; those in red are above. For each query, the highest lowest bound below the true frequency is highlighted in bold.

| Data         | Frequency | Upper bound | Classical | Bayesian | Bootstrap | Conformal |
|--------------|-----------|-------------|-----------|----------|-----------|-----------|
| **SARS-CoV-2** |           |             |           |          |           |           |
| AATTATTATAAGAAAG | 81        | 81          | 26        | 81       | 52        | 50 36     |
| TCAGACAACTACTATT | 76        | 76          | 21        | 55 47    | 45 32     |
| AAAGTTGATGGTGTTG | 73        | 73          | 18        | 59 44    | 42 31     |
| CAATTATTATAAGAAA | 63        | 63          | 8         | 48 34    | 32 26     |
| ATCAGACAACTACTAT | 60        | 60          | 5         | 44 31    | 29 26     |
| ACCTTTGACAATCTTA | 55        | 55          | 0         | 52 26    | 24 27     |
| ATTTGAAGTCACCTAAT | 55       | 55          | 0         | 55 26    | 24 27     |
| CATGCAAAATTACATAT | 54       | 54          | 0         | 54 25    | 23 26     |
| GAAATTCAAGTATTT | 54        | 54          | 0         | 54 25    | 23 27     |
| TTTGTAGAAACCCAG | 53        | 53          | 0         | 53 24    | 22 27     |
| AGTTGCAGACTTTTTT | 24        | 24          | 0         | 13 0     | 0 20      |
| TCTTCACAATTTGAAAC | 24       | 24          | 0         | 12 0     | 1 20      |
| TTCTGCTCGCATAGTG | 24       | 24          | 0         | 12 0     | 0 20      |
| CTACCTTAGAGGCGAAG | 23       | 23          | 0         | 11 0     | 0 19      |
| GCTTGCTGTTCTATCTT | 23       | 23          | 0         | 23 0     | 1 19      |
| TTCTAAGAGGCTCCGG | 23       | 23          | 0         | 14 0     | 0 20      |
| GGGCTGTGTTGTCTTTT | 22       | 22          | 0         | 12 0     | 0 20      |
| ACCCTTGTGTGTTTT | 20        | 20          | 0         | 20 0     | 0 16      |
| GAAGTCTTTGGAGGATG | 20       | 20          | 0         | 20 0     | 0 16      |
| CAAACCTGGTAATTTT | 3         | 3           | 0         | 3 0      | 0 0       |

**Literature**

| of the | 12565 | 12568 | 12513 | 12544 | 12557 | 12556 | 12562 |
|--------|-------|-------|-------|-------|-------|-------|-------|
| in the | 6188  | 6190  | 6135  | 6169  | 6179  | 6179  | 6180  |
| and the | 6173  | 6175  | 6120  | 6151  | 6164  | 6164  | 6165  |
| the of | 6015  | 6017  | 5962  | 5990  | 6006  | 6006  | 6007  |
| the lord | 4186  | 4195  | 4140  | 4165  | 4184  | 4184  | 4184  |
| to the | 3465  | 3467  | 3412  | 3445  | 3456  | 3456  | 3463  |
| the and | 2250  | 2251  | 2196  | 2227  | 2240  | 2240  | 2248  |
| all the | 2226  | 2230  | 2175  | 2207  | 2219  | 2219  | 2224  |
| and he | 2169  | 2173  | 2118  | 2153  | 2162  | 2162  | 2167  |
| to be | 2062  | 2064  | 2009  | 2043  | 2053  | 2053  | 2060  |

| man on | 22    | 29    | 0     | 10    | 18    | 18    | 18    |
| their hand | 22    | 24    | 0     | 9     | 13    | 13    | 0     |
| no need | 20    | 28    | 0     | 9     | 17    | 17    | 16    |
| and brother | 12    | 14    | 0     | 2     | 3     | 3     | 0     |
| miss would | 10    | 13    | 0     | 3     | 2     | 2     | 0     |
| i please | 8     | 12    | 0     | 3     | 1     | 1     | 1     |
| also how | 3     | 13    | 0     | 2     | 2     | 2     | 0     |
| in under | 3     | 9     | 0     | 2     | 0     | 0     | 0     |
| ten old | 3     | 6     | 0     | 1     | 0     | 0     | 0     |
| fault he | 1     | 9     | 0     | 1     | 0     | 0     | 0     |
Table A2: True frequencies, upper and lower bounds for a few random queries in two sketched data sets. Hash width $w = 50,000$. Other details are as in Table A1.

| Data                        | Frequency | Upper bound | Classical | Bayesian | Bootstrap | Conformal |
|-----------------------------|-----------|-------------|-----------|----------|-----------|-----------|
| **SARS-CoV-2**              |           |             |           |          |           |           |
| AATTATTATAAGAAAG            | 81        | 209         | 0         | 4        | 0         | 0         | 18        |
| TCAGACACAATCTATT            | 76        | 213         | 0         | 8        | 0         | 0         | 18        |
| AAGTGTGTGGGTGGTTGGG         | 73        | 130         | 2         | 2        | 1         | 18        |
| CAAAGGATTAAAGAA             | 63        | 233         | 0         | 4        | 11        | 6         | 19        |
| ATCATCCCCACTCTAT            | 60        | 179         | 0         | 2        | 0         | 0         | 18        |
| ACCTTTGACAAATCTTTA          | 55        | 292         | 15        | 70       | 67        | 22        |
| ATTTAAAGTCACCTCAA           | 55        | 258         | 0         | 11       | 36        | 31        | 20        |
| CATGCAAATACATAT             | 54        | 204         | 0         | 3        | 0         | 0         | 18        |
| GAATTTACAGTATTC             | 54        | 260         | 0         | 12       | 38        | 35        | 22        |
| TTGTTAGAHAACCCAG            | 53        | 246         | 7         | 24       | 0         | 18        | 20        |
| ATGCTGCAATCGTGCT            | 24        | 139         | 0         | 2        | 0         | 0         | 17        |
| ATTTCTTAATATTACA            | 24        | 92          | 1         | 0        | 0         | 0         | 17        |
| CTCTACTATTATTGGT            | 24        | 121         | 0         | 1        | 0         | 0         | 17        |
| TGTTTTATCTCTCTACA           | 24        | 199         | 0         | 3        | 0         | 1         | 19        |
| CAGTACACGTGATATCG           | 23        | 119         | 0         | 2        | 0         | 0         | 17        |
| TAATGTTGACTTTTTG            | 23        | 92          | 1         | 0        | 0         | 0         | 17        |
| CAACCATAAACGACGT            | 22        | 105         | 1         | 0        | 0         | 0         | 17        |
| AGTTATGACTCTCTG             | 21        | 97          | 1         | 0        | 1         | 1         | 18        |
| ATAAAAGGAGTTGCACC           | 19        | 218         | 0         | 5        | 0         | 0         | 18        |

**Literature**

| Word          | Frequency | Upper bound | Classical | Bayesian | Bootstrap | Conformal |
|---------------|-----------|-------------|-----------|----------|-----------|-----------|
| of the        | 12565     | 12630       | 12086     | 12325    | 12463     | 12454     | **12563** |
| in the        | 6188      | 6242        | 5698      | 5906     | 6075      | 6067      | **6096**  |
| and the       | 6173      | 6314        | 5770      | 5972     | 6147      | 6139      | **6169**  |
| the of        | 6015      | 6162        | 5618      | 5834     | 5995      | 5985      | **6014**  |
| the lord      | 4186      | 4289        | 3745      | 3975     | 4122      | 4114      | **4185**  |
| to the        | 3465      | 3558        | 3014      | 3217     | 3391      | 3380      | **3464**  |
| the and       | 2250      | 2413        | 1869      | 2081     | 2246      | 2237      | **2249**  |
| all the       | 2226      | 2346        | 1802      | 1993     | 2179      | 2170      | **2225**  |
| and he        | 2169      | 2293        | 1749      | 1937     | 2126      | 2117      | **2168**  |
| to be         | 2062      | 2121        | 1577      | 1770     | 1954      | 1945      | **2061**  |
| very for      | 15        | 59          | 2         | 0        | 0         | 0         | 0         |
| and faithful  | 14        | 94          | 3         | 0        | 0         | 0         | 0         |
| but found     | 9         | 74          | 2         | 0        | 0         | 0         | 0         |
| my speech     | 6         | 98          | 3         | 0        | 0         | 0         | 0         |
| of eight      | 5         | 66          | 2         | 0        | 0         | 0         | 0         |
| and soul      | 4         | 140         | 6         | 0        | 0         | 0         | 0         |
| her prow       | 3        | 79          | 2         | 0        | 0         | 0         | 0         |
| usual as      | 2         | 56          | 2         | 0        | 0         | 0         | 0         |
| a invitation  | 1         | 80          | 2         | 0        | 0         | 0         | 0         |
| angular log   | 0         | 146         | 5         | 0        | 0         | 0         | 0         |