Abstract

We study the estimation and concentration on its expectation of the probability to observe data further than a specified distance from a given iid sample in a metric space. The problem extends the classical problem of estimation of the missing mass in discrete spaces. We give some estimators for the conditional missing mass and show that estimation of the expected missing mass is difficult in general. Conditions on the distribution, under which the Good-Turing estimator and the conditional missing mass concentrate on their expectations are identified. Applications to anomaly detection, coding, the Wasserstein distance between true and empirical measure and simple learning bounds are sketched.

1 Introduction

What is the probability that lightning will strike more than a given distance from one of the previously observed strikes? In the genetic survey of some species, how large is the population of individuals, whose DNA differs from the previously observed sequences in more than a fixed number of positions? Have we seen all handwritten digits up to some given precision? Under the assumption of independent observations, these questions and a number of similar problems can be formalized as follows.

In a metric probability space \((X, d, \mu)\) an iid sample \(X = (X_1, ..., X_n)\) is drawn from \(\mu\). For \(r \geq 0\) we would like to estimate the conditional missing mass, defined as the random variable
\[
\hat{M}(X, r) = \mu \{ y : \forall i \in \{1, ..., n\}, d(y, X_i) > r \}.
\]
The conditional missing mass is the probability of finding a point at distance more than \(r\) from the given sample. The expected missing mass is its expectation \(M(\mu, n, r) = \mathbb{E} [\hat{M}(X, r)]\). It is a scale-dependent property of the distribution \(\mu\), and the conditional missing mass is a scale-dependent property both of the distribution and the sample.

In the discrete case \(X\) is at most countable, \(d(x, y) = 1\) for \(x \neq y\), and \(r < 1\). The pedagogical narrative underlying the discrete case is that we have seen zebras six times, elephants three times and a lions only once in independent sightings. What is the probability of running into a yet unseen species on the next sighting? The problem surfaced in a more serious context, when Alan Turing’s team was deciphering the enigma code during World War Two. They found what is now called the Good-Turing estimator \(G\), the relative number of species (or words or letters) having been encountered only once. Soon Turing’s co-worker Good showed that \(G\) has small bias, and various strong concentration results for both \(M\) and \(G\) have been established since ([14], [21], [20], [4] and [2], the latter being a particularly complete treatise).

In this paper we study the missing mass in the extended setting of metric spaces or spaces with more general distortion functions, thus opening the way to other applications. We show that in separable metric spaces the conditional missing mass converges to zero almost surely (Proposition 4.17), but the emphasis is on finite sample bounds. Potential examples are coding, anomaly detection, estimating the support of a distribution, or applications to ecology, when there is nearly a continuum
of species such as frequently mutating bacteria or viruses. Some application are sketched in Section 8.

It is clear, that the discrete case applies to neither of the initially posed problems (lightnings, genes and handwritten digits). In the discrete case the relation $d(x, y) \leq r < 1$ implies $x = y$ and is therefore transitive and an equivalence relation, partitioning the space into species, words or numbers. In the general setting the relation $d(x, y) \leq r$ is only reflexive and symmetric but not transitive. For this reason only weaker results can be expected and sometimes obtained only under additional conditions. In the discrete case the negative association of occupancy counts can be exploited, but in the general case it is not even clear, what should be defined as occupancy counts, and different techniques are called for.

There does not seem to be not much literature on the missing mass in metric spaces. One reference is 3, where Section 4 gives a bound on the rate of decrease of $\hat{M}(\mu, n, r)$ for totally bounded metric spaces. In 17 this is combined with a not quite correct application of the discrete-case results on the concentration of $\hat{M}(X, r)$ to the general environment of metric spaces (17), (16), probably a typo. In 15 this is corrected and bounds on $\hat{M}(X, r)$ are obtained by reduction to the discrete case of occupation numbers on a partition into sets of diameter less than $r/2$. These results are asymptotic and targeted to show the consistency of certain nearest-neighbor sample-compression algorithms.

A brief summary of our findings is the following: just as in the discrete case the conditional missing mass converges to zero almost surely and an extension of the Good-Turing estimator can be used to estimate $\hat{M}$, but no uniformly valid exponential bounds are available at this point, in fact such may not exist at all. Another simple estimator bounds $\hat{M}$ above with high probability, but with potentially large upward bias. This estimator may be very useful whenever $\hat{M}$ is expected to be very small. The estimation problem for the expected missing mass $\bar{M}$, is more difficult, and there is no uniform and universally valid bound for any estimator. Exponential bounds and tight bounds on the variance of $\hat{M}$ exist, but depend on an intrinsic dimensionality of the distribution.

We conclude this section with a summary of notation. The next section introduces our results in detail. Then follows a sketch of applications, and a section containing the proofs.

1.1 Notation and conventions

For $m \in \mathbb{N}$ we use the abbreviation $[m] = \{1, \ldots, m\}$. The indicator of a set $A$ is denoted $1_A$, its complement by $A^c$ and the difference $A \cap B^c$ with $A \setminus B$. Both cardinality of sets and absolute value of reals are denote by bars $|\cdot|$. Vectors are written in bold letters. If $x = (x_1, \ldots, x_n) \in X^n$, $k \in \left[\begin{array}{c} n \end{array}\right]$ and $y \in X$ then the substitution $S^k_y(x) \in X^n$ is defined by

$$S^k_y(x) = (x_1, \ldots, x_{k-1}, y, x_{k+1}, \ldots, x_n),$$

and the deletion by $x^\setminus k = (x_1, \ldots, x_{k-1}, x_{k+1}, \ldots, x_n) \in X^{n-1}$.

Random variables are written in upper case letters, $E$, and $\mathbb{V}$ are used for expectation and variance respectively and $\mathbb{P}$ for the probability of events. $\|Y\|_p := (\mathbb{E} |Y|^p)^{1/p}$ for real valued $Y$ and $p \geq 1$. If $Y$ is a random variable with values in $[0, 1]$ then we write the complementary variable $Y^\perp = 1 - Y$. The unit mass at a point $x$ will be denoted with $\delta_x$.

On $\mathbb{R}^D$ the letter $\lambda$ is used for the Lebesgue measure and $e_1, e_2, \ldots, e_D$ for the canonical basis vectors.

Throughout $(X, d, \mu)$ is a Hausdorff space with Borel-probability measure $\mu$ and a continuous distortion function $d : X \times X \to [0, \infty)$ satisfying $d(x, x) = 0$ and $d(x, y) = d(y, x)$. If $d$ is indeed a metric it will be specially mentioned.

For $r > 0$ and $x \in X$ we write $B(x, r) = \{y : d(x, y) \leq r\}$. Note that $x \in B(y, r) \iff y \in B(x, r)$. Often we write simply $B(x)$ if $r$ is understood and there is no ambiguity. A subset $S \subseteq X$ is called $r$-separated (for $r > 0$) is $d(x, y) > r$ for all $x, y \in S$ with $x \neq y$. If $A \subseteq X$ an $r$-net of $A$ is a maximal $r$-separated subset of $A$.

$X_1, \ldots, X_n, \ldots$ is a sequence of independent random variables distributed in $X$ as $\mu$. For $m_1, m_2 \in \mathbb{N}$, $m_1 < m_2$ we write $X_{m_1}^{m_2} = (X_{m_1}, X_{m_1+1}, \ldots, X_{m_2}) \sim \mu^{m_2-m_1+1}$. With $X$ we mean $X = X_1^\perp = (X_1, \ldots, X_n) \sim \mu^n$, when $n$ is understood.
For \( r \geq 0 \) the conditional missing mass is the \([0, 1]\)-valued random variable
\[
\hat{M}(X^n_1, r) = \mu \left( \bigcap_{k \in [n]} B(X_k, r)^c \right)
\]
and the expected missing mass \( M(\mu, n, r) = \mathbb{E} \left[ \hat{M}(X^n_1, r) \right] \). It is often more convenient to work with their "positive" counterparts, the conditional envelope mass
\[
\hat{M}^\perp(X^n_1, r) = 1 - \hat{M}(X^n_1, r) = \mu \left( \bigcup_{k \in [n]} B(X_k, r) \right)
\]
and the expected envelope mass \( M^\perp(\mu, n, r) = 1 - M(\mu, n, r) \). When there is no ambiguity we omit the dependences on \( X, r, \mu \) and \( n \).

2 Results

In this section we first state results on the estimation of the conditional missing mass by the extended Good-Turing estimator \( G \) and give exponential upper bounds on the conditional missing mass with a simple martingale-type estimator. Then we show that the estimation of the expected missing mass is more difficult and that there is no universal uniformly converging estimator. We then give tight bounds on the variance of \( \hat{M}(X^n_1, r) \) and \( G(X^n_1, r) \) and exponential concentration inequalities depending on an auxiliary statistic \( h(X^n_1, r) \), which can be interpreted as an empirical local packing number.

2.1 The Good-Turing estimator and the conditional missing mass

By independence we have for any \( k \in [n] \)
\[
\mu \left\{ \bigcap_{i \in [n]: i \neq k} B(X_i)^c \right\} = \mathbb{E} \left[ \mathbf{1} \left\{ X_k \in \bigcap_{i \in [n]: i \neq k} B(X_i)^c \right\} | X \setminus k \right].
\]
The indicator of the event on the right hand side is a crude leave-one-out estimate for the conditional missing mass. To reduce variance we average this estimate over all \( x_k \), which leads to the random variable
\[
G(X) = \frac{1}{n} \sum_{k=1}^{n} \mathbf{1} \left\{ X_k \in \bigcap_{i \in [n]: i \neq k} B(X_i)^c \right\},
\]
The random variable \( G(X) \) will also be called the Good-Turing estimator, because this is what it reduces to in the discrete case. It is the relative number of sample points, which are further than \( r \) from all other sample points.

**Theorem 2.1.** (Proof in Section 4.1) Define
\[
H(X, r) = \frac{1}{n} \sum_{k=1}^{n} \mu \left( \bigcap_{i \in [n]: i \neq k} B(X_i, r)^c \right).
\]
Then
(i) \( \hat{M}(X^n_1, r) \leq H(X^n_1, r) \leq \hat{M}(X^n_1, r) + 1/n \)
(ii) \( M(\mu, n, r) \leq \mathbb{E} \left[ G(X^n_1, r) \right] \leq M(\mu, n, r) + 1/n \)
(iii) \( \mathbb{V}[G(X^n_1, r) - H(X^n_1, r)] \leq 3/n \)
(iv) \( \left\| G(X^n_1, r) - \hat{M}(X^n_1, r) \right\|_2 \leq \sqrt{7/n} \).
The random variable $H$ is an approximation of $\hat{M}$ adapted to the Good-Turing estimator, since evidently $E[H] = E[H]$. The Conclusion (ii) is a simple extension of the bias bound by [14] to the extended setting considered in this paper. The variance bound (iii) and its tricky proof are due to Sourav Chatterjee (private communication). It is unclear if higher-moment or exponential bounds exist.

Parts (i) and (iii) of Theorem 2.1 in combination with Chebychev’s inequality show that, for $\delta > 0$ with probability at least $1 - \delta$

$$|\hat{M}(X, \epsilon) - G(X, \epsilon)| \leq \frac{1}{n} + \frac{\sqrt{3}}{n\delta}. \quad (1)$$

### 2.2 A martingale estimator

The strong dependence of (1) on the failure probability $\delta$ makes it unsuited for the union bounds often used for the purpose of model selection.

The conditional missing mass in some sense measures ignorance and it may in some applications be more important to bound it above than below. This can be done with the following estimator

$$T(X) = \frac{1}{n} \sum_{k=1}^{n} 1 \left\{ X_k \in \bigcap_{i<k} B(X_i) \right\}.$$

Notice the similarity to the Good-Turing estimator and $G(X) \leq T(X)$. It follows almost immediately from the Hoeffding-Azuma Lemma [22] that the difference $\hat{M}(X) - T(X)$ has a sub-Gaussian upper tail. But $T(X)$ may have a large bias. To reduce this we define for $m \in [n]$ the random variable

$$T_m(X) = \frac{1}{m} \sum_{k=n-m+1}^{n} 1 \left\{ X_k \in \bigcap_{i+1<k} B(X_i, r) \right\}.$$

For $m = n$ this reduces to $T$. The estimator $T_m$ is related to, but not the same as using $X_{n-m+1}^{n}$ as a test set to estimate $\hat{M}(X_{1}^{n-m})$.

**Theorem 2.2.** (Proof in Section 4.2) For $t > 0$ (i) $\mathbb{P}\left\{ \hat{M}(X) - T_m(X) > t \right\} \leq e^{-mt^2/2}$.

(ii) $\mathbb{P}\left\{ \hat{M}(X) - 2T_m(X) > t \right\} \leq \exp \left( -mt / (4(e - 2)) \right).$

(iii) For $m < n$, $\mathbb{E}\left[ T_m(X) - \hat{M}(X) \right] \leq \ln \frac{n}{n-m} \leq m / (n-m)$.

The two exponential tail bounds allow for some complicated union bounds incurring only logarithmic penalties. For one example we may optimize the bound in $m$. A union bound gives

**Corollary 2.3.** For $\delta > 0$

$$\mathbb{P}\left\{ \hat{M}(X) > \min_{m \in [n]} T_m(X) + \sqrt{\frac{\ln(n/\delta)}{2m}} \right\} \leq \delta.$$

On the other hand we may be interested in uniform estimates of the minimal conditional missing mass for sub-samples of a given size. For $S \subseteq \{1, ..., n\}$ denote with $X_S$ the vector $(X_i)_{i \in S}$. From Theorem 2.2 and a union bound we get

**Corollary 2.4.** For $m \in [n]$ and $\delta > 0$

$$\mathbb{P}\left\{ \sup_{S:|S|=m} \hat{M}(X_S) - T(X_S) > \sqrt{\frac{\min\{n-m,m\} \ln(n/\delta)}{m}} \right\} \leq \delta.$$
Corollary 2.5. (Proof in Section 4.2) For \( m \in [n] \) and \( \delta > 0 \), with probability at least \( 1 - \delta \) in \( X \), if there is an \( r \)-net \( Y \subset X \), with \( |Y| = m \) then
\[
\hat{M}(X, r) \leq \frac{m}{n} + \sqrt{\frac{m \ln(n/\delta)}{n}}.
\]

2.3 A negative result on the estimation of \( M \)

In the discrete case it has been established that both \( \hat{M} \) and \( G \) are exponentially concentrated on their expectations ([21], [20]). From this and the \( 1/n \)-bias of \( G \) it is immediate to obtain bounds on the estimation error \( G - \hat{M} \). In contrast to this Chatterjees’s proof of Theorem 2.1 (iii) and the analysis of the martingale estimator above adress the estimation error directly. This is in fact necessary, because \( \hat{M} \) and \( G \) may have large variance.

For intuition into this fact let \( \mu \) be a mixture of the uniform distribution on \( S^{D-1} \), the unit sphere of \( \mathbb{R}^D \) (with \( D \) very large), and a small mass at the origin of \( \mathbb{R}^D \). Take \( r \in (1, \sqrt{2}) \). If \( n \ll D \) and the origin is not in the sample, the conditional missing mass will be nearly one, because the \( X_i \) will be nearly mutually orthogonal and the spherical caps centered on them have very small mass (this follows from isoperimetric theorems on the sphere, see [18], for example). By approximate orthogonality most sample points will be alone in their respective balls, so \( G \) will also be large. But the entire support of the distribution is contained in the ball about the origin, so, if the origin is in the sample, both \( \hat{M} \) and \( G \) drop to zero. If the probability of the origin being in the sample is \( 1/2 \), then the variance of \( \hat{M} \) and \( G \) is near the maximal value \( 1/4 \).

Since this construction is possible for every sample-size \( n \), no universal and uniformly convergent estimator of \( M(\mu, n, r) \) exists in general.

Proposition 2.6. (Proof in Section 4.3) Let \( 1 < r < \sqrt{2} \). For every \( \epsilon \in (0, 1) \) and \( n \in \mathbb{N} \) with \( n \geq \ln(4/\epsilon) \) there exists \( D \in \mathbb{N} \) and \( \mu \) on \( \mathbb{R}^D \) such that
(i) for \( X \sim \mu^n \), \( \min \{ \mathbb{V}(\hat{M}(X, r)), \mathbb{V}(G(X, r)) \} \geq (1/4) - \epsilon \).
(ii) Let \( B \) be the event \( \{ \forall i, j \text{ with } i \neq j, \|X_i - X_j\| > r \text{ and } \|X_i\| \leq 1 \} \). Then \( \mathbb{P}(B) \geq 1/2 - \epsilon \).
(iii) For every \( f : X^n \rightarrow \mathbb{R} \) there exists \( \mu'' \) on \( \mathbb{R}^D \) such that for \( X \sim (\mu'')^n \), we have
\[
\mathbb{E}\left[ (f(X) - M(\mu'', n, r))^2 \right] \geq (1 - \epsilon)^2 / 16,
\]
and consequently \( \|M - f(X)\|_{L_2((\mu'')^n)} \geq (1 - \epsilon) / 4 \).

2.4 Local separation

It follows from Proposition 2.6 that estimators of the expected missing mass will only work well, if we can exclude a construction as in the previous section. We can either rule it out a priori by some constraint on the dimension, or, if we insist on dimension independence, at least rule it out with high probability with the use of an auxiliary statistic, which measures some intrinsic dimension of the distribution.

For \( r \geq 0 \) and \( k \in \mathbb{N} \) we say a sequence \( S = (x_1, ..., x_k) \in \mathcal{X}^k \) has the \( r \)-local-separation property, if

- There exists \( y \in \mathcal{X} \) such that \( \forall i \in [k], d(x_i, y) \leq r \) (locality)
- For all \( 1 \leq i < j \leq k \) we have \( d(x_i, x_j) > r \) (separation)

So any sequence of points mutually separated by more than \( r \) has this property, if the intersection of the \( r \)-balls about them is non-empty. We denote with \( \Pi_r \subseteq \bigcup_{k \in \mathbb{N}} \mathcal{X}^k \) the set of all sequences \( S \) having the \( r \)-local-separation property. Define the function \( h : \mathcal{X}^n \times [0, \infty) \rightarrow \mathbb{R} \) by
\[
h(x, r) = \max \{ |S| : S \subseteq (x_1, ..., x_n) \text{ such that } S \in \Pi_r \}.
\]
h \((x, r)\) is the largest cardinality of a sub-sample separated by more than \( r \), but contained in some closed ball of radius \( r \).
The next result shows that the random variable \( h(X, r) \) controls concentration of \( G \) and \( \hat{M} \) about their expectations. Its proof is somewhat complicated and uses some recent moment inequalities for functions of independent variables.

**Theorem 2.7.** (Proof in Section 4.4) Under the conventions of Section 1.1 let \( n \geq 16 \). Then

\[
\begin{align*}
\mathbb{V}[G(X, r)] &\leq \frac{2}{n} (1 + \mathbb{E}[h(X, r)]) \\
\mathbb{V}[\hat{M}(X, r)] &\leq \frac{2n^2 \mathbb{E}[h(X, r)] + 4(n - 2)(\ln n + 1)}{n - 1}.
\end{align*}
\]

Furthermore, for any \( t > 0 \),

\[
\mathbb{P}\left\{ \left| G(X, r) - \mathbb{E}[G(X, r)] \right| > 12 \sqrt{\frac{(1 + \mathbb{E}[h(X, r)])t}{n}} \frac{23t}{\sqrt{n}} \right\} \leq 15e^{-t}
\]

\[
\mathbb{P}\left\{ \left| \hat{M}(X, r) - \mathbb{E}[\hat{M}(X, r)] \right| > 12 \sqrt{\frac{\mathbb{E}[h(X, r)]t}{n}} \frac{37t}{\sqrt{n - 1}} \right\} \leq 2ne^{-t}.
\]

Remarks:

1. **Tightness of variance bound.** Under the event \( B \) described in Proposition 2.6 (ii) we have \( h(X, r) = n. \) Since \( \mathbb{P}(B) \geq 1/2 - \epsilon \) we have \( \mathbb{E}[h(X, r)] / n \geq 1/4 - \epsilon. \) With \( \epsilon = 1/8 \) we get from Proposition 2.6

\[
\frac{3}{64} \leq \frac{\mathbb{E}[h(X, r)]}{8n} \leq \frac{1}{8} \leq \mathbb{V}(\hat{M}(X, r)).
\]

so the variance bound (2) is unimprovable up to a constant factor and an additive term of \( O(\ln(n)/n) \).

2. **Finite dimensions.** In the discrete case, when \( d(x, y) = 1 \iff x \neq y \), and \( r < 1 \) we always have \( h(X, r) = 1 \). In one dimension \( h(X) \) is at most 2, in 2 dimensions it is at most 5. In general we have the following Proposition.

**Proposition 2.8.** (Proof in Section 4.6) Let \( (\mathbb{R}^D, \|\cdot\|) \) be a finite dimensional Banach space with closed unit ball \( \mathbb{B} \) and define the 1-packing number of \( \mathbb{B} \) as

\[
\mathcal{P}(\mathbb{B}, d_{\|\cdot\|}, 1) := \max \{ |S| : S \subseteq \mathbb{B}^D, \forall x, y \in S, x \neq y \implies \|x - y\| > 1 \}.
\]

Let \( r > 0 \). Then

(i) for every vector \( x \in (\mathbb{R}^D)^n \) we have \( h(X, r) \leq \mathcal{P}(\mathbb{B}, d_{\|\cdot\|}, 1) \leq 8^D \).

(ii) For the 2-norm the bound improves to \( 3^D \).

(iii) If \( \mu \) has a positive density w.r.t. Lebesgue measure on \( \mathbb{R}^D \) and \( X_1^n \sim \mu^n \) then \( h(X_1^n, r) \rightarrow \mathcal{P}(\mathbb{B}, d_{\|\cdot\|}, 1) \) almost surely as \( n \rightarrow \infty \).

For any metric space \( (\mathcal{X}, d) \) with finite doubling dimension \( \text{DDim} \) we have \( h(X, r) \leq 2^{\text{DDim}} \), since the packing number at scale \( r \) can be bounded by the covering number for \( r/2 \) (25, 4.2.8). In summary: Theorem 2.7 guarantees exponential concentration of \( G \) and \( \hat{M} \) on their expectations in all finite dimensional metric spaces.

3. **Effective low dimensionality.** The worst-case bound for finite dimensions is disappointing in its exponential dependence on the dimension. But the random variable \( h(X, r) \) depends on both the underlying distribution and the scale \( r \) and not on the dimension of the ambient space. In the simplest case \( \mu \) is supported on a low-dimensional linear subspace, and the corresponding packing numbers can be used to bound \( h(X, r) \). Linearity or smoothness however are not necessary for \( h(X, r) \) to be small, nor is differentiability. There is a distribution \( \mu \) in \( L_2(0, \infty) \) whose support is not totally bounded, nowhere smooth and not contained in any finite dimensional subspace of \( L_2(0, \infty) \), but \( h(X, r) \leq 5 \) for any \( r > 0 \) and \( X \sim \mu \) (Proposition 4.19). The assumption of effective low-dimensionality is not unreasonable in practice, since the generative processes underlying real-world distributions often have far fewer degrees of freedom than the dimension of the ambient space where data is presented, an observation which has given rise to the manifold hypothesis ([19], [13], [5]).

The next section addresses the question how the function \( h(X, r) \) can be estimated from the data.
2.5 Concentration of $h$

A subset $\Pi$ of the set of all sequences $\Pi \subseteq \bigcup_{k \in \mathbb{N}} \mathcal{X}^k$ is called hereditary, if, whenever for $S = \{x_1, \ldots, x_k\} \in \mathcal{X}^k$ we have $S \subseteq \Pi$, then $S' \subseteq \Pi$ for every subsequence $S' \subseteq S$. We write $\Pi(S)$ for $S \subseteq \Pi$. For example the property of a sequence of real numbers to be non-decreasing is hereditary. Another example is the local-separation property of a sequence of points $S = \{x_1, \ldots, x_k\}$ in a space with symmetric distortion function, as described in the previous section: if there exists $y$ such that $x_i \in B(y, r)$ and $d(x_i, x_j) > r$ for all $i \neq j$, then the same will clearly hold for any subsequence of $S$.

The function $f_{\Pi} : \mathcal{X}^k \to \mathbb{N}_0$, which for $x = \{x_1, \ldots, x_n\}$ gives the length $f_{\Pi}(x)$ of the longest subsequence of $x$, which has hereditary property $\Pi$, is called the configuration function of $\Pi$ ([7], Section 3.3, see also [23], [22] or [9]). The function giving the length of the longest increasing subsequence in a sequence of real numbers is such a configuration function, as is the function $h(x, r)$ defined in the previous section. Such functions have strong concentration properties. Here we quote Theorem 6.12 in [7].

**Theorem 2.9.** If $X = (X_1, \ldots, X_n)$ is a vector of independent variables in $\mathcal{X}$ and $f_{\Pi} : \mathcal{X}^n \to \mathbb{R}$ is the configuration function corresponding to the hereditary property $\Pi$ above then

(i) for every $t > 0$

$$\Pr \left\{ f_{\Pi}(X) - \mathbb{E}\left[ f_{\Pi}(X) \right] > t \right\} \leq \exp \left( \frac{-t^2}{2\mathbb{E} \left[ f_{\Pi}(X) \right] + 2t^3/3} \right),$$

(ii) and for every $0 < t \leq \mathbb{E} \left[ f_{\Pi}(X) \right]$

$$\Pr \left\{ \mathbb{E} \left[ f_{\Pi}(X) \right] - f_{\Pi}(X) > t \right\} \leq \exp \left( \frac{-t^2}{2\mathbb{E} \left[ f_{\Pi}(X) \right]} \right).$$

We can immediately substitute $h(\cdot, r)$ for $f_{\Pi}$. For our purpose the most important consequences are summarized in the following.

**Corollary 2.10.** (Proof in Section 2.6) For $t > 0$

(i) $\Pr \left\{ \sqrt{\mathbb{E}[h(X, r)]} \leq \sqrt{h(X, r)} + \sqrt{2t} \right\} \geq 1 - e^{-t}$

(ii) $\Pr \left\{ h(X, r) - 2\mathbb{E}[h(X, r)] > t \right\} \leq e^{-6t/7}$.

Part (i) means that, if we are able to compute $h(X, r)$, then $\mathbb{E}[h(X, r)]$ can be estimated with high probability from the sample. Consequently the bounds in Theorem 2.7 can be independent of assumptions on the distribution $\mu$ and determined with high probability by the observed data $X$, as can be seen by combining part (i) with the exponential inequalities of Theorem 2.7 in a union bound.

Part (ii) gives a sub-exponential bound in the other direction, which will be instrumental in the proof of Theorem 2.7.

At this point we have no efficient algorithm to compute $h(x, r)$, if this number is large, most likely this problem is NP-hard. But for our bounds it might be sufficient to determine if $h(x, r) \geq h_0$ for some fixed value $h_0$ and to compute it otherwise. In the euclidean space $\mathbb{R}^d$ one could execute an algorithm for the minimum enclosing ball problem (e.g. [27]) of $O(nD)$ on the $O(n^{h_0})$ candidate subsequences of size $h_0$, which would take polynomial execution time $O(n^{h_0+1}D)$. The generation of candidate subsequences could be further accelerated as they have to satisfy $r < d(x_i, x_j) \leq 2r$.

If we relax the locality condition to $d(x_i, x_j) \leq 2r$ then the cumbersome minimum-enclosing-ball problem can be avoided, and computation of the relaxed statistic is equivalent to the $h_0$-clique problem for the graph with $n$ vertices and edges whenever $r < d(x_i, x_j) \leq 2r$. In this case an efficient algorithm is given in [24]. In any case the computation of $h(x, r)$, or a good upper bound thereof, remains an interesting problem for further research.
3 Applications

Since $h(x) = 1$ in the discrete case, many of the applications of the discrete case are covered by Theorem 2.7 albeit with larger constants. In this section we sketch a few applications not covered by the classical results.

3.1 Anomaly detection

Kontorovich et al [16] propose a method of anomaly detection, where they assume that the metric space $(\mathcal{X}, d)$ is partitioned into disjoint sets corresponding to "normal" and "anomalous" ones, being separated by some minimal separation distance $\gamma$, so that $d(x, y) > \gamma$ for every pair of a normal point $x$ and an anomalous point $y$. Training data $X$ is drawn from an unknown distribution $\mu$ supported on the normal points. If the separation distance $\gamma$ is known, the simplest rule for anomaly detection is the proximity classifier, which decides a point $y$ to be anomalous iff $d(y, X_i) > \gamma$ for all $X_i$ in the sample. Then the "false alarm rate" (the probability that a normal point is labeled as anomalous) is the conditional missing mass $\hat{M}(X)$ and a data-dependent bound may be given either with the Good Turing estimator or any of the estimators in Section 2.2.

3.2 Nearest neighbor coding

Given a sample $X \sim \mu^n$ we encode every point $x \in \mathcal{X}$ by the index of the nearest neighbor in the sample, that is by $i(x) = \arg \min_{x_i \in [n]} d(x, X_i)$. Given a code $i(x)$ we reconstruct the point $x$ as $X_i(x)$ and incur a reconstruction error $d(x, X_i(x))$. Then the probability that the reconstruction error exceeds some specified accuracy $\epsilon$ is clearly $\mu(X : d(X, X_i(x)) > \epsilon) = \hat{M}(X, \epsilon)$. Using Theorem 2.1 it may be estimated by the Good-Turing estimator $G$ as

$$\hat{M}(X, \epsilon) - G(X, \epsilon) \leq \sqrt{\frac{3}{n\delta}}$$

with probability at least $1 - \delta$ in the sample $X$. Alternatively we may upper bound the reconstruction error with probability at least $1 - \delta$ as

$$\hat{M}(X, \epsilon) \leq T_n(X, \epsilon) + \sqrt{\frac{\ln (1/\delta)}{2n}} \text{ or}$$

$$\hat{M}(X, \epsilon) \leq \min_{m \in [n]} T_m(X, \epsilon) + \sqrt{\frac{\ln (n/\delta)}{2m}},$$

using Theorem 2.2 or Corollary 2.4(i). If the distortion function is bounded, say $d(x, y) \leq \Delta$, then the expected reconstruction error can be bounded by $E[d(X, X_i(x))] \leq \Delta \hat{M}(X, \epsilon) + \epsilon$ and estimated in the same way.

In high dimensions these estimates are, albeit correct, manifestly sample dependent and not necessarily reproducible. It follows from Proposition 2.6 that two samples $X$ and $X'$ may differ in a single point with $\hat{M}(X, \epsilon) = 0$ and $\hat{M}(X', \epsilon)$ arbitrarily close to 1. Theorem 2.7 then gives exponential guarantees of reproducibility in terms of the quantity $E[h(X, \epsilon)]$, which depends on the intrinsic dimension of $\mu$, the scale $\epsilon$ and the sample size $n$.

If we are content with any reconstruction error smaller than $\epsilon$, the coding scheme above is redundant and inefficient, whenever sample points cluster at scales much smaller than $\epsilon$. In this case we can construct an $\epsilon/2$-net $Y$ of $X$ (a maximal $\epsilon/2$-separated subsequence of $X$) and encode with nearest neighbors of $Y$. Since every point in $X$ is within $\epsilon/2$ from some point of $Y$, the probability that the reconstruction error of this coding scheme exceeds $\epsilon$ is then bounded by $\hat{M}(X, \epsilon/2)$ and can again be estimated as above.

Similar coding schemes, which use sub-sampled nets, underlie the nearest-neighbor sample-compression classification algorithm developed in [17]. The recent paper [15] proves that a minor modification of this algorithm, called OPTINET, is universally Bayes consistent in all essentially separable metric spaces. In this proof a bound on the conditional missing mass in the general setting of metric spaces, as defined by training sample and input marginal, is essential. The authors use a partitioning scheme as in the proof of Proposition 4.17 to reduce the estimation problem to the
discrete case, which is overly pessimistic. This does no harm however, as the results to be proven are asymptotic. The same method is used in the recent paper [10]. In the next section similar ideas are used together with the results in this paper to obtain finite sample bounds.

3.3 The Wasserstein distance to the empirical distribution

Suppose \((X, d)\) is a metric space. The Wasserstein distance \(W_1(\mu, \nu)\) on probability measures \(\mu\) and \(\nu\) is usually defined in terms of couplings or optimal transport. By the Kantorovich-Rubinstein Theorem it can be equivalently defined as

\[
W_1(\mu, \nu) = \sup_{\|f\|_{Lip}=1} \int f(\mu - \nu),
\]

where \(\|f\|_{Lip}\) is the usual Lipschitz seminorm. One quantity which has attracted attention is \(W_1(\mu, \hat{\mu})\), where \(\hat{\mu}\) is the empirical distribution

\[
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i} \text{ for } X = (X_1, ..., X_n) \sim \mu^n.
\]

Dudley [12] has shown that \(W_1(\mu, \hat{\mu}) \approx n^{-1/D}\) if \(\mu\) is compactly supported on \(\mathbb{R}^D\). This result has since been refined by several authors. Notably Weed and Bach [26] have sharpened and generalized this by moving to general bounded metric spaces and replacing \(D\) by an intrinsic dimension of the probability measure \(\mu\). In this section we give a simple and purely empirical bound on \(W_1(\mu, \hat{\mu})\).

First of all note that

\[
W_1(\mu, \hat{\mu}) \geq r \hat{M}(X, r) \quad \text{for every } r > 0.
\]

This is obvious from the optimal transport interpretation, as the missing mass has to be moved at least a distance \(r\) to arrive at the sample. Formally the supremum in the definition above is then witnessed by the Lipschitz function \(x \mapsto \min_{i \in [n]} d(x, X_i)\).

The estimate in the other direction is more complicated, because we have to control the error within the envelope \(\bigcup B(X_i, r)\). For this we require an \(r\)-net of the sample, and the analysis we provide is strongly inspired by the nearest-neighbor sample-compression methods developed in [15] or [10].

**Theorem 3.1.** (Proof in Section 4.7) Let \((X, d)\) be a complete, separable metric space with diameter 1 and Borel probability measure \(\mu\). For \(\delta > 0\), with probability at least \(1 - \delta\) in \(X \sim \mu^n\), if there exists an \(r\)-net \(Y \subset X\) with cardinality \(m, m \leq (n-3)/2\), then

\[
W_1(\mu, \hat{\mu}) \leq \hat{M}(X, r) + 3r + 2 \sqrt{\frac{m}{n-m}} \left(1 + \sqrt{\ln (n/\delta)}\right)
\]

or

\[
W_1(\mu, \hat{\mu}) \leq 3r + 3 \sqrt{\frac{m}{n-m}} \left(1 + \sqrt{2n/\delta}\right).
\]

This bound can be optimized by generating the \(r\)-nets of \(X\) using a farthest-first traversal algorithm. The price of data-dependence and simplicity is that we don’t quite recover the \(n^{-1/D}\)-bound for \(\mu\) compactly supported on \(\mathbb{R}^D\). But in that case we can always find a \(n^{-1/(D+2)}\)-net of cardinality \(O(nD/(D+2))\) for any sample from such a distribution, and Theorem 3.1 then gives a bound of \(O\left(\ln (n) / n^{-1/(D+2)}\right)\).

3.4 Elementary learning bounds for \(\beta\)-smooth functions

We give a very easy data-dependent learning bound involving a rather large hypothesis class, where the conditional missing mass controls generalization as a data dependent complexity measure. It shows how learning is possible for "easy" data, even if standard complexity measures on the hypothesis class fail.

Let \(\mathcal{F}\) be a loss-class on \((X, d)\). By this we mean that \(\mathcal{F}\) is the set of functions obtained from composing the hypothesis functions with a fixed, non-negative loss function. Draw a training sample \(X \sim \mu^n\) and let \(\mathcal{F}_X\) be the class of loss functions which have zero empirical error, that is

\[
\mathcal{F}_X = \{f \in \mathcal{F} : \forall i \in [n], f(X_i) = 0\}.
\]
Given a test variable $X \sim \mu$, which is independent of $X$, and a tolerance parameter $s$ we define an error functional by
\[
R(X,s) = \mathbb{P} \{ \exists f \in F_X, f(X) > s \mid X \}.
\]
As it stands the loss may be arbitrarily large on the bad event, whose probability we want to bound, but on the good event it is uniformly bounded. This is different from conventional risk bounds, which would involve the expectation $\mathbb{E} [ f(X) ]$. If the loss functions were uniformly bounded, we could convert a bound on $R(X,s)$ into a risk bound of the form
\[
\forall f \in F_X, \mathbb{E} [ f(X) ] \leq s + R(X,s) \sup_{f \in F} \| f \|_\infty.
\]
Now take $(X,d)$ to be a Hilbert-space and assume that the functions in $F$ are $\beta$-smooth, which means that their gradients $f'$ are $\beta$-Lipschitz. Such a condition is standard for optimization algorithms involving gradient descent. For $\beta$-smooth functions the fundamental theorem of calculus implies the inequality
\[
f(x) - f(y) \leq \langle f'(y), x - y \rangle + \frac{\beta}{2} \| x - y \|^2.
\]
Now if $f \in F_X$ then $f'(X_i) = f(X_i) = 0$, since $f$ is non-negative, differentiable and vanishes at $X_i$. Therefore
\[
R(X,s) = \mathbb{P} \{ \exists f \in F_X, f(X) > s \mid X \} \\
\leq \Pr \{ \exists f \in F : \forall i \in [n], f(X) - f(X_i) > s \mid X \} \\
\leq \Pr \left\{ \forall i \in [n], \frac{\beta}{2} \| X - X_i \|^2 > s \mid X \right\} = \hat{M} \left( X, \sqrt{\frac{2s}{\beta}} \right).
\]
\[
\hat{M} \left( X, \sqrt{\frac{2s}{\beta}} \right)
\]
can be estimated by the methods described. Using Corollary 2.4 it is also possible to allow a certain fraction of errors, where $f(X_i) > 0$.

## 4 Proofs

For the reader’s convenience the various theorems and propositions are restated.

### 4.1 The Good-Turing estimator

**Theorem 4.1 (= Theorem 2.1).** Define
\[
H(X,r) = \frac{1}{n} \sum_{k=1}^{n} \mu \left( \bigcap_{i \in [n] \setminus i \neq k} B(X_i, r)^c \right).
\]

Then
\[
(i) \hat{M}(X,r) \leq H(X,r) \leq \hat{M}(X,r) + 1/n
\]
\[
(ii) M(\mu, n, r) \leq \mathbb{E} [ G(X,r) ] \leq M(\mu, n, r) + 1/n
\]
\[
(iii) \forall [G(X,r) - \hat{M}(X,r)] \leq 3/n
\]
\[
(iv) \left\| G(X,r) - \hat{M}(X,r) \right\|_2 \leq \sqrt{7/n}.
\]

**Proof.** We introduce a shorthand notation for some random subsets of $X$. For $i \in [n]$ we write $B_i = B(X_i, r)$ and for $i, j \in [n]$, $i \neq j$
\[
U = \bigcup_{k \in [n]} B_k, U_i = \bigcup_{k \in [n] \setminus \{i\}} B_k, \text{and } U_{ij} = \bigcup_{k \in [n] \setminus \{i,j\}} B_k.
\]
Then $\hat{M}_+ = \mu(U)$, $G_+ = (1/n) \sum_{i \in [n]} 1 \{ X_i \in U_i \}$ and $H_+ = (1/n) \sum_{i \in [n]} \mu(U_i)$. Since $U_i$ is independent of $X_i$ we have $\mathbb{E} [ 1 \{ X_i \in U_i \} | X_i^c ] = \mu(U_i)$, so that $\mathbb{E} [G_+] = \mathbb{E} [H_+]$. Also $\mathbb{E} [ 1 \{ X_i \in U_{ij} \} | X_i^c ] = \mu(U_{ij}) = \mathbb{E} [ 1 \{ X_i \in U_{ij} \} | X_i^c ]$. Note that
\[
U_{ij} \subseteq U_i \subseteq U, U \setminus U_i = B_i \setminus U_i, U_j \setminus U_{ij} = B_i \setminus U_{ij}.
\]
(4)
The collection of sets \( \{ B_i \setminus U_i \}_{i \in [n]} \) and for fixed \( j \in [n] \) the collection \( \{ B_i \setminus U_{ij} \}_{i \in [n] \setminus \{ j \}} \) and the collection of events \( \{ X_j \in B_i \setminus U_{ij} \}_{i \in [n] \setminus \{ j \}} \) are all disjoint.

We address the bias first. By (4) \( H^+ \leq \hat{M}^+ \) and

\[
\hat{M}^+ - H^+ = \frac{1}{n} \sum_{i \in [n]} (\mu(U) - \mu(U_i)) = \frac{1}{n} \sum_{i \in [n]} \mu(U \setminus U_i)
\]

\[
= \frac{1}{n} \sum_{i \in [n]} \mu(B_i \setminus U_i) = \frac{1}{n} \mu \left( \bigcup_{i \in [n]} B_i \setminus U_i \right) \leq \frac{1}{n}.
\]

This gives (i). Taking the expectation gives (ii).

We now come to Chatterjee’s variance bound. Fix \( j \in [n] \) for the moment. For \( i \in [n] \setminus \{ j \} \) we have \( \mathbb{E} \left[ 1 \{ X_j \in U_j \} - 1 \{ X_j \in U_{ij} \} \right] = \mu(U_j) - \mu(U_{ij}) \). In view of the inclusions in (4) the unconditional expectation gives

\[
\mathbb{E} \left[ \mu(U_j) - \mu(U_{ij}) \right] = \mathbb{E} \left[ \mu(U_j) - \mu(U_{ij}) \right] = \mathbb{E} \left[ 1 \{ X_j \in U_j \} - 1 \{ X_j \in U_{ij} \} \right] = \mathbb{E} \left[ 1 \{ X_j \in U_j \} - 1 \{ X_j \in U_{ij} \} \right] \leq \mathbb{P} \left( \{ X_j \in B_i \setminus U_{ij} \} \right).
\]

Since \( X_j \) and \( U_{ij} \) are independent of \( X_i \)

\[
\mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right] \mathbb{E} \left[ 1 \{ X_j \in U_{ij} \} - \mu(U_{ij}) \right] = \mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right] \mathbb{E} \left[ 1 \{ X_j \in U_{ij} \} - \mu(U_{ij}) \right] = 0.
\]

On the other hand \( 1 \{ X_i \in U_i \} - \mu(U_i) \leq 1 \), so that, for any \( i \neq j \),

\[
\mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right] \mathbb{E} \left[ 1 \{ X_j \in U_{ij} \} - \mu(U_{ij}) \right] \leq \mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right] \mathbb{E} \left[ 1 \{ X_j \in U_{ij} \} - \mu(U_{ij}) \right] = 2 \mathbb{P} \left( X_j \in B_i \setminus U_{ij} \right),
\]

where the last equality follows from (5). Thus

\[
\forall \left[ G - H \right] = \mathbb{E} \left[ G^+ - H^+ \right]
\]

\[
= \frac{1}{n^2} \sum_{i} \mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right]^2
\]

\[
+ \frac{1}{n^2} \sum_{i \neq j} \mathbb{E} \left[ 1 \{ X_i \in U_i \} - \mu(U_i) \right] \mathbb{E} \left[ 1 \{ X_j \in U_j \} - \mu(U_j) \right] \leq \frac{1}{n} + \frac{2}{n^2} \sum_{j} \mathbb{P} \left( \bigcup_{i \neq j} \{ X_j \in B_i \setminus U_{ij} \} \right)
\]

\[
= \frac{1}{n} + \frac{2}{n^2} \sum_{j} \mathbb{P} \left( \bigcup_{i \neq j} \{ X_j \in B_i \setminus U_{ij} \} \right)
\]

\[
\leq \frac{1}{n} + \frac{2}{n^2} = \frac{3}{n}.
\]

The identity in (*) holds, since the events \( \{ X_j \in B_i \setminus U_{ij} \} \) in the sum over \( i : i \neq j \) in the line before are disjoint. This proves (iii), and together with (i) and \( (a + b)^2 \leq 2a^2 + 2b^2 \) it shows that

\[
\mathbb{E} \left[ \left( G - \hat{M} \right)^2 \right] \leq \mathbb{E} \left[ \left( (G - H) + (H - \hat{M}) \right)^2 \right] \leq \frac{6}{n} + \frac{2}{n^2} \leq \frac{7}{n}.
\]

\( \square \)
4.2 A martingale estimator

**Theorem 4.2 (= Theorem 2.2).** For $t > 0$ (i) $\mathbb{P} \left\{ \hat{M}(X) - T_m(X) > t \right\} \leq e^{-mt^2/2}$.

(ii) $\mathbb{P} \left\{ \hat{M}(X) - 2T_m(X) > t \right\} \leq \exp \left( -mt/ (4(e - 2)) \right)$.

(iii) For $m < n$, $\mathbb{E} \left[ T_m(X) - \hat{M}(X) \right] \leq \ln \frac{n}{n-m} \leq m/(n-m)$.

For the proof of the relative bound (ii) (and also of Lemma 4.1 below) we need the following lemma, which is a minor modification and application of Theorem 1 of [10].

**Lemma 4.3.** Let $R_1, ..., R_n$ be random variables $0 \leq R_j \leq 1$ and let $\mathcal{F}_j$ be the $\sigma$-algebra generated by $R_1, ..., R_j$. Let $V = \frac{1}{n} \sum_j R_j$, $F = \frac{1}{n} \sum_j \mathbb{E} [R_j | \mathcal{F}_{j-1}]$. Then

$$1 \geq \mathbb{E} \left[ \exp \left( \frac{n}{4(e-2)} (F - 2V) \right) \right].$$

**Proof.** Let $Y_j := \frac{1}{n} (\mathbb{E} [R_j | \mathcal{F}_{j-1}] - R_j)$, so $\mathbb{E} [Y_j | \mathcal{F}_{j-1}] = 0$.

Then $\mathbb{E} \left[ Y_j^2 | \mathcal{F}_{j-1} \right] = (1/n^2) \left( \mathbb{E} \left[ R_j^2 | \mathcal{F}_{j-1} \right] - \mathbb{E} \left[ R_j | \mathcal{F}_{j-1} \right]^2 \right) \leq (1/n)^2 \mathbb{E} [R_j | \mathcal{F}_{j-1}]$, since $0 \leq R_j \leq 1$. For $\beta < n$ we have, using $e^x \leq 1 + x + (e - 2) x^2$ for $x \leq 1$,

$$\mathbb{E} \left[ e^{\beta Y_j | \mathcal{F}_{j-1}} \right] \leq \mathbb{E} \left[ 1 + \beta Y_j + (e - 2) \beta^2 Y_j^2 | \mathcal{F}_{j-1} \right] = 1 + (e - 2) \beta^2 \mathbb{E} \left[ Y_j^2 | \mathcal{F}_{j-1} \right] \leq \exp \left( (e - 2) \beta^2 \mathbb{E} \left[ Y_j^2 | \mathcal{F}_{j-1} \right] \right) \leq \exp \left( (e - 2) \left( \frac{\beta}{n} \right)^2 \mathbb{E} [R_j | \mathcal{F}_{j-1}] \right),$$

where we also used $1 + x \leq e^x$. Defining $Z_0 = 1$ and for $j \geq 1$

$$Z_j = Z_{j-1} \exp \left( \beta Y_j - (e - 2) \left( \frac{\beta}{n} \right)^2 \mathbb{E} [R_j | \mathcal{F}_{j-1}] \right)$$

then

$$\mathbb{E} [Z_j | \mathcal{F}_{j-1}] = \exp \left( - (e - 2) \left( \frac{\beta}{n} \right)^2 \mathbb{E} [R_j | \mathcal{F}_{j-1}] \right) \mathbb{E} [e^{\beta Y_j | \mathcal{F}_{j-1}}] \leq Z_{j-1}.$$

It follows that $\mathbb{E} [Z_n] \leq 1$. Spelled out this is

$$1 \geq \mathbb{E} \left[ \exp \left( \beta (F - V) - \frac{(e - 2) \beta^2 F}{n} \right) \right].$$

If we choose $\beta = n / (2(e - 2)) < n$, then

$$1 \geq \mathbb{E} \left[ \exp \left( \frac{n}{4(e-2)} (F - 2V) \right) \right].$$

The proof of part (iii) needs one more lemma.

**Lemma 4.4.** For $(X_1, ..., X_m)$ ~ $\mu^m$ and $k \in [m]$ we have

$$\mathbb{E} \left[ \mu \left( B(X_k, r) \setminus \bigcup_{i \in [m], i \neq k} B(X_i, r) \right) \right] \leq 1/m.$$
Proof. For $X$ iid to $X_i$, the events \( \{ X \in B(X_i, r) \setminus \bigcup_{i \in [m], i \neq k} B(X_i, r) \} \) are disjoint for different values of $k$. It follows that their probabilities sum to at most 1, and since by symmetry they have to be equal, the conclusion follows.

Proof of Theorem 2.2: (i) Let $X$ be iid to the $X_i$ and for $k \in \{ n - m + 1, n \}$ let $R_k = 1 \{ X_k \in \bigcap_{i < k} B(X_i) \}$, so $T_m(X) = (1/m) \sum_{k = n - m + 1}^n R_k$ and $\mu(\bigcap_{i < k} B(X_i)) = \mathbb{E}[R_k|X_k^{n-1}]$.

\[
\begin{align*}
\hat{M}(X) &= \frac{1}{m} \sum_{k = n - m + 1}^n \mu \left( \bigcap_{i = 1}^n B(X_i)^c \right) \\
&\leq \frac{1}{m} \sum_{k = n - m + 1}^n \mu \left( \bigcap_{i < k} B(X_i)^c \right) = \sum_{k = n - m + 1}^n \frac{1}{m} \mathbb{E}[R_k|X_k^{n-1}] .
\end{align*}
\]

Thus
\[
\hat{M}(X) - T_m(X) \leq \sum_{k = n - m + 1}^n \frac{1}{m} \left( \mathbb{E}[R_k|X_k^{n-1}] - R_k \right).
\]

Then $(1/m) \left( \mathbb{E}[R_k|X_k^{n-1}] - R_k \right)$ is a martingale difference sequence with values in $[-1/m, 1/m]$. It follows from the Hoeffding-Azuma Theorem that
\[
\mathbb{P} \left\{ \hat{M}(X) - T_m(X) > t \right\} \leq e^{-mt^2/2}.
\]

(ii) Use Lemma 4.3 with the same $R_k, F = \hat{M}(X), V = T_m(X)$ and $n$ replaced by $m$ to obtain
\[
1 \geq \mathbb{E} \left[ \exp \left( \left( \frac{m}{4(e - 2)} \right) \left( \hat{M}(X) - 2T_m(X) \right) \right) \right].
\]

Then (ii) follows from Markov’s inequality.

(iii) Observe that
\[
\mathbb{E}[T_m(X)] = \frac{1}{m} \sum_{k = n - m + 1}^n \mathbb{E} \left[ 1 \left\{ X_k \in \bigcap_{i = 1}^{n-m} B(X_i, r)^c \right\} \right] = \mathbb{E}\left[ \hat{M}(X_k^{n-m}) \right].
\]

On the other hand, using Lemma 4.3 and $\ln t \leq 1 - t$,
\[
\begin{align*}
\mathbb{E} \left[ \hat{M}(X_k^{n-m}) - \hat{M}(X_k^n) \right] &= \sum_{k = n - m + 1}^n \mathbb{E} \left[ \mu \left( B_k \setminus \bigcup_{j: j \leq k} B(X_j, r) \right) \right] \\
&\leq \sum_{k = n - m + 1}^n \frac{1}{k} \leq \int_{n-m}^n \frac{dt}{t} = \ln \frac{n}{n-m} \\
&\leq \frac{m}{n-m} .
\end{align*}
\]

Thus
\[
\mathbb{E}[T_m(X) - \hat{M}(X)] \leq \mathbb{E}\left[ \hat{M}(X_k^{n-m}) - \hat{M}(X_k^n) \right] \leq \ln(n/ (n-m)) \leq m/ (n-m) .
\]

Corollary 4.5. (Corollary 2.3) For $m \in [n]$ and $\delta > 0$, with probability at least $1 - \delta$ in $X$, if there is an $r$-net $Y \subset X$, with $|Y| = m$ then
\[
\hat{M}(X, r) \leq \frac{m}{n} + \sqrt{\frac{m \ln(n/\delta)}{n}} .
\]
Proof. For any fixed $r$-net $Y \subset X$ of cardinality $m$ reorder $X$ by putting $Y$ to the front of the sequence. Then
\[
T(X, r) \leq \frac{1}{n} \sum_{k=1}^{m} 1 \left\{ Y_k \in \bigcap_{i<k} B(Y_k, r) \right\} + \frac{1}{n} \sum_{k=m+1}^{n} 1 \left\{ X_k \notin \bigcup_{i=1}^{m} B(Y_k, r) \right\}
\]
\[
\leq \frac{m}{n},
\]
because the $Y_k$ are an $r$-net. The result follows from combining Theorem 2.2 with a union bound over all subsets of cardinality $m$. 

4.3 A negative result

**Proposition 4.6 (= Proposition 2.6).** Let $1 < r < \sqrt{2}$. For every $\epsilon \in (0, 1)$ and $n \in \mathbb{N}$ with $n \geq \ln(4)/\epsilon$ there exists $D \in \mathbb{N}$ and $\mu$ on $\mathbb{R}^D$ such that

(i) For $X \sim \mu^n$, $\min \left\{ \mathbb{V}(\hat{M}(X, r)), \mathbb{V}(G(X, r)) \right\} \geq (1/4) - \epsilon$.

(ii) Let $B$ be the event $\{ \forall i, j \text{ with } i \neq j, \|X_i - X_j\| > r \text{ and } \|X_i\| \leq 1 \}$. Then for $D$ sufficiently large $\mathbb{P}(B) \geq 1/2 - \epsilon$.

(iii) For every $f : X^n \rightarrow \mathbb{R}$ there exists $\mu''$ on $\mathbb{R}^D$ such that for $X \sim (\mu'')^n$, we have

\[
\mathbb{E} \left[ (f(X) - M(\mu'', n, r))^2 \right] \geq (1 - \epsilon)^2 / 16,
\]

and consequently $\|M - f(X)\|_{L^2(\mu^n)} \geq (1 - \epsilon)/4$.

**Proof.** Let $D \geq 2n/\epsilon$ and choose $r$ with $1 < r < \sqrt{2}$.

Now let $\mu = (1/2)^{1/n} (1/D) \sum_{i=1}^{D} \delta_{e_i} + (1 - (1/2)^{1/n}) \delta_0$ and let $X$ be an $n$-sample drawn from $\mu$. Let $A$ be the event that $0$ occurs in $X$. Then $\mathbb{P}(A) = 1/2$ by definition of $\mu$, since $\mathbb{P}(A^c) = \left( 1 - (1 - (1/2)^{1/n}) \right)^n = 1/2$. If $A$ occurs then $\hat{M}(X, r) = 0$, because all basis vectors are within $r$ from $0$. Under $A^c$ however the sample must miss $D - n$ basis vectors, so $\hat{M}(X, r) \geq (1/2)^{1/n} (1 - n/D)$. Thus $(1/2) - 2\epsilon \leq (1/2)^{1/n} (1 - n/D)/2 \leq M(\mu, n, r) \leq 1/2$ and

\[
\mathbb{V}(\hat{M}(X, r)) \geq \frac{1}{2} \left( \frac{1}{4} \right)^{1/n} (1 - n/D)^2 - 1/4 \\
\geq \frac{1}{2} \left( \frac{1}{4} \right) \left( 1 - n/D \right)^2 - 1/4 \\
\geq \frac{1}{2} \left( 1 - \epsilon \right)^2 - 1/4 \geq (1/4) - \epsilon.
\]

Before we come to the Good-Turing estimator we prove (ii). Let $B$ be the event in (ii) which just means that $X$ consists of $n$ distinct basis vectors. Similar to the reasoning in the birthday paradox the probability of $B$ is

\[
\mathbb{P}_{\mu^n}(B) = \frac{1}{2} \prod_{i=1}^{n} \left( 1 - i - 1 \right) D \geq \frac{1}{2} \left( 1 - n - 1 \right) D \geq \frac{1}{2} \exp \left( n \ln \left( 1 - n - 1 \right) D \right) \\
\geq \frac{1}{2} \left( 1 - \frac{n^2}{D} \right) \geq \frac{1}{2} - \epsilon,
\]

by making $D$ sufficiently large, which gives (ii). Under $B$ we have $G = 1$. But under $A$ we have $G = 0$ with probability $1/2$. It follows that $\mathbb{E}[G] \leq 1/2$ and

\[
\mathbb{V}(G) \geq (1/2) 0^2 + (1/2 - \epsilon) 1^2 - 1/4 = 1/4 - \epsilon,
\]

which completes the proof of (i).
(iii) Now define $\mu' = (1/D) \sum_{i=1}^{D} \delta_{e_i}$ and let $Y \sim (\mu')^n$. Then $M(\mu', n, r) \geq 1 - n/D \geq 1 - \epsilon/2$ and $M(\mu', n, r) - M(\mu, n, r) \geq (1 - \epsilon)/2$. But conditional on $A^c$ the samples $X$ and $Y$ are identically distributed, so
\[
\begin{align*}
E \left[ (f(Y) - M(\mu', n, r))^2 + (f(X) - M(\mu, n, r))^2 \right] \\
\geq E \left[ (f(Y) - M(\mu', n, r))^2 + (f(X) - M(\mu, n, r))^2 \right] \Pr(A^c) \\
\geq \frac{(M(\mu', n, r) - M(\mu, n, r))^2}{2} \geq \frac{(1 - \epsilon)^2}{8},
\end{align*}
\]
which gives (ii) with either with $\mu'' = \mu$ or $\mu'' = \mu'$. In the second inequality we used calculus to minimize $(x - M(\mu_1, n, r))^2 + (x - M(\mu_2, n, r))^2$.
\[\square\]

4.4 Local separation

**Theorem 4.7 (= Theorem 2.4).** Under the conventions of Section 1.7 let $n \geq 16$. Then
\[
\begin{align*}
\mathbb{V}[G(X, r)] & \leq 2 \left(1 + \mathbb{E}[h(X, r)]\right) \\
\mathbb{V}[\hat{M}(X, r)] & \leq \frac{2\mathbb{E}[h(X, r)]}{n} + 4(e - 2)(\ln n + 1).
\end{align*}
\]
Furthermore, for any $t > 0$,
\[
\begin{align*}
\Pr \left\{ |G(X, r) - \mathbb{E}[G(X, r)]| > 12 \sqrt{\frac{(1 + \mathbb{E}[h(X, r)])}{n} t + \frac{23t}{\sqrt{n}}} \right\} & \leq 15e^{-t} \\
\Pr \left\{ |\hat{M}(X, r) - \mathbb{E}[\hat{M}(X, r)]| > 12 \sqrt{\frac{\mathbb{E}[h(X, r)]}{n} t + \frac{37t}{\sqrt{n} - 1}} \right\} & \leq 2ne^{-t}.
\end{align*}
\]

Define a nonlinear operator $Q$ acting on bounded functions $f : \mathcal{X}^n \to \mathbb{R}$ by
\[
Qf(x) = f(x) - \min_{k, y \in \mathcal{X}} f(S^k_y(x)) = \max_{k, y \in \mathcal{X}} f(x) - f(S^k_y(x)).
\]
The proof of Theorem 2.4 uses the following general concentration inequality, which may be of independent interest. Its proof is given in the next section.

**Proposition 4.8.** Let $X = (X_1, \ldots, X_n)$ be a vector of independent random variables with values in $\mathcal{X}$ and $f : \mathcal{X}^n \to [0, 1]$ be measurable and strongly $(a, 0)$-self-bounded in the sense that
\[
\forall x \in \mathcal{X}^n, \sum_{k=1}^{n} f(x) - \inf_{y \in \mathcal{X}} f(S^k_y(x)) \leq af(x)
\]
with $a \geq 1$. Then $\mathbb{V}[f(X)] \leq a\mathbb{E}[Qf(X)]$. Suppose also that for some $b \geq 1$ and $\lambda > 0$ and for all $t > 0$
\[
\Pr \{ Qf(X) > w + t \} \leq be^{-\lambda t}.
\]
Then with $C = 4.16$ we have for every $\delta \in (0, 1)$
\[
\Pr \left\{ |f(X) - \mathbb{E}[f(X)]| > \sqrt{Cae^2w\ln(b + 2e^2/\delta)} + e^2 \sqrt{\frac{Ca}{\lambda} \ln(b + 2e^2/\delta)} \right\} \leq \delta.
\]
and for $t > 0$
\[
\Pr \{ |f(X) - \mathbb{E}[f(X)]| > t \} \leq 2(b + e^2) \exp \left\{ \frac{-t^2}{e^2(Caw + 2\sqrt{Ca\lambda}^{-1}t)} \right\}.
\]
If $b = 1$ then $b$ can be deleted from these inequalities.
To apply this proposition we will show that $\hat{M}$ and $G$ satisfy the above hypotheses. Define for $k \in \{1, \ldots, n\}$ functions $W_k$ and $W : A^n \to \mathbb{R}$

$$W_k (x) := \Pr \left\{ \bigg( B (x_k) \setminus \bigcup_{i: i \neq k} B (x_i) \bigg) \right\} \quad \text{and} \quad W (x) := \max_k W_k (x).$$

**Lemma 4.9.** $\hat{M}^\perp$ is $(1, 0)$-self-bounded and $Q \hat{M}^\perp \leq W$.

**Proof.** With reference to any $k \in \{1, \ldots, n\}$

$$\hat{M}^\perp (x) = \mu \left( \bigcup_i B (x_i) \right) = \mu \left( \bigcup_{i: i \neq k} B (x_i) \right) + W_k (x).$$

It follows that $\hat{M}^\perp (x) - \inf_y \hat{M}^\perp (S^k_y x) \leq W_k (x)$ and thus $Q \hat{M}^\perp \leq W$. Also note that

$$\sum_k W_k (x) = \sum_k \mu \left( \bigg( B (x_k) \setminus \bigcup_{i: i \neq k} B (x_i) \bigg) \right) \leq \hat{M}^\perp (x),$$

since the events in the second sum are disjoint. $\square$

**Lemma 4.10.** $G^\perp$ is $(2, 0)$-self-bounded and $QG^\perp \leq (1 + h) / n$.

**Proof.** With reference to any $k \in \{1, \ldots, n\}$, with a disjoint decomposition as in the proof of Lemma 4.9

$$G^\perp (x) = \frac{1}{n} \sum_{j=1}^n 1 \{ x_j \in U_j \}$$

$$= \frac{1}{n} 1 \{ x_k \in U_k \} + \frac{1}{n} \sum_{j: j \neq k} 1 \{ x_j \in U_j \cup (U_j \setminus U_k) \}$$

$$= \frac{1}{n} 1 \{ x_k \in U_k \} + \frac{1}{n} \sum_{j: j \neq k} 1 \{ x_j \in U_j \} + \frac{1}{n} \sum_{j: j \neq k} 1 \{ x_j \in B_k \setminus U_j \}.$$

The middle term is independent of $x_k$ and the subsequence of points $x_j$, which contribute to the sum in the last term, has the local separation property, so this term is bounded by $h (x) / n$. It follows that

$$G^\perp (x) - \inf_y G^\perp (S^k_y x) \leq \frac{1}{n} 1 \{ x_k \in U_k \} + \frac{1}{n} \sum_{j: j \neq k} 1 \{ x_j \in B_k \setminus U_j \}$$

$$\leq (1 + h (x)) / n$$

and likewise $QG^\perp (x) \leq (1 + h (x)) / n$. Also from the above

$$\sum_k G^\perp (x) - \inf_y G^\perp (S^k_y x)$$

$$\leq \frac{1}{n} \sum_k 1 \{ x_k \in U_k \} + \frac{1}{n} \sum_k \sum_{j: j \neq k} 1 \{ x_j \in B_k \setminus U_j \}$$

$$= G^\perp (x) + \frac{1}{n} \sum_j \sum_{k: k \neq j} 1 \{ x_j \in B_k \setminus U_j \} \quad (*)$$

$$= G^\perp (x) + \frac{1}{n} \sum_j 1 \left\{ x_j \in \bigcup_{k: k \neq j} (B_k \setminus U_j) \right\}$$

$$\leq 2G^\perp (x),$$

since the sets in the sum over $k$ in (*) are disjoint. $\square$
Lemma 4.11. For $t > 0$ and $k \in \{1, \ldots, n\}$
\[
\Pr \left\{ W_k (X) - \frac{2h(X)}{n-1} > t \right\} \leq \exp \left( -\frac{(n-1)t}{4(e-2)} \right) \quad \text{and}
\Pr \left\{ W(X) - \frac{2h(X)}{n-1} > t \right\} \leq n \exp \left( -\frac{(n-1)t}{4(e-2)} \right).
\]

Proof. For $k, j \in \{1, \ldots, n\}, k \neq j$ let $R^k_j$ be the random variable
\[
R^k_j = 1 \left\{ X_j \in B_k \setminus \bigcup_{i:j \neq i} B_i \right\}
\]
$R^k_j$ has values in $[0, 1]$, and $R^k_j$ is $\mathcal{F}_j$-measurable, where $\mathcal{F}_j = \Sigma (X_k, X_i)_{i \leq j}$. Then
\[
W_k (X) = \frac{1}{n-1} \sum_{j:j \neq k} \mu \left( B_k \setminus \bigcup_{i:j \neq k} B_i \right)
\leq \frac{1}{n-1} \sum_{j:j \neq k} \mu \left( B_k \setminus \bigcup_{i:j \neq k, i<j} B_i \right)
= \frac{1}{n-1} \sum_{j:j \neq k} \mathbb{E} [R^k_j | X_k, X_1, \ldots, X_{j-1}] = F_k (X).
\]
Let
\[
V_k (X) = \frac{1}{n-1} \sum_{j:j \neq k} R^k_j = \frac{1}{n-1} \sum_{j:j \neq k} 1 \left\{ X_j \in B_k \setminus \bigcup_{i:j \neq k, i<j} B_i \right\}
\]
Note that the indices $j$ which contribute to the sum in $V_k (x)$ must be such that each $X_j$ is in the ball about $X_k$, but none of them may be in the ball about any other one of the contributing indices. It follows that the corresponding subsequence has the local separation property. Therefore $V_k (X) \leq h(X)/(n-1)$.

Lemma 4.3 applied conditional on $X_k$ gives us
\[
1 \geq \mathbb{E} \left[ \exp \left( \frac{n-1}{4(e-2)} (F_k (X) - 2V_k (X)) \right) | X_k \right].
\]
Of course the unconditional expectation of the R.H.S. will also be bounded by 1. Markov’s inequality then implies
\[
\Pr \left\{ W_k (X) - \frac{2h(X)}{n-1} > t \right\} \leq \Pr \{ F_k (X) > 2V_k (X) + t \}
\leq \exp \left( -\frac{(n-1)t}{4(e-2)} \right).
\]
The second statement follows from a union bound.

\[\square\]

Corollary 4.12. (= Corollary 2.10) For $t > 0$
(i) $\Pr \left\{ \sqrt{\mathbb{E} [h(X,r)]} \leq \sqrt{h(X,r)} + \sqrt{2t} \right\} \geq 1 - e^{-t}$
(ii) $\Pr \{ h(X,r) - 2\mathbb{E} [h(X,r)] > t \} \leq e^{-6t/5}.$

Proof. Equating the r.h.s. of Theorem 2.9(ii) to $\delta$ and solving for $t$ gives for $\delta > 0$ with probability at least $1 - \delta$ that $\mathbb{E} [h(X)] - h(X) \leq \sqrt{2\mathbb{E} [h(X)] \ln (1/\delta)}$. Bringing the r.h.s. to the left,
completing the square and taking the square root gives (i) with \( \delta = e^{-t} \). Similarly we get from Theorem 2.9(i) with probability at least \( 1 - \delta \) that
\[
\frac{\delta}{n - 1} - E[h(X)]] \leq \sqrt{2E[h(X)]} \ln(1/\delta) + \frac{2 \ln(1/\delta)}{3}.
\]
Then use \( \sqrt{2E[h(X)]} \ln(1/\delta) \leq E[h(X)] + \ln(1/\delta)/2 \) and set \( \delta = e^{-t} \) to get the second conclusion.

**Proof of Theorem 2.7** Lemma 4.11 and integration by parts gives for \( \delta > 0 \)
\[
E[W(X) - \frac{2h(X)}{n-1}] = \delta + \int_{\delta}^{\infty} \mathbb{P}\left\{ \max_k W_k(X) - \frac{2h(X)}{n-1} > t \right\} dt
\]
\[
\leq \delta + n \int_{\delta}^{\infty} \exp\left( -\frac{(n-1)t}{4(e-2)} \right) dt
\]
\[
= \delta + \frac{4n(e-2)}{n-1} \exp\left( -\frac{(n-1)t}{4(e-2)} \right).
\]
With \( \delta = 4n(e-2) \ln(n)/(n-1) \) we obtain
\[
E[QM(X)] \leq E[W(X)] \leq \frac{2E[h(X)]}{n-1} + \frac{4(e-2)(\ln n + 1)}{n-1},
\]
so Proposition 4.8 gives us the bound on the variance of \( \hat{M}(X) \). The variance bound for \( G \) follows from Proposition 4.8 and Lemma 4.10.

From Corollary 2.10 we get for \( t > 0 \)
\[
\mathbb{P}\left\{ \frac{1+h(X)}{n} > \frac{1+2E[h(X)]}{n} + t \right\} \leq e^{-(6/7)nt}.
\]
Combined with Lemma 4.11 we obtain
\[
\mathbb{P}\left\{ W(X) - \frac{4E[h(X)]}{n} > t \right\} \leq n \exp\left( -\frac{(n-1)t}{8(e-2)} \right) + e^{-(6/14)nt}
\]
\[
\leq (n+1) \exp\left( -\frac{(n-1)t}{8(e-2)} \right)
\]
We summarize:

Lemma 4.10 and (6) imply that we can use Proposition 4.8 with \( f = G^\perp \) and the values \( a = 2, b = 1, \lambda = (6/7)n \) and \( w = (1 + 2E[h(X)])/n \). Substitution gives
\[
\mathbb{P}\left\{ |G^\perp(X) - E[G^\perp(X)]| > \sqrt{\frac{2C^2(1 + 2E[h(X)])}{n} \ln(2e^2/\delta)} + e^2 \sqrt{\frac{14C^2}{6n} \ln(2e^2/\delta)} \right\} \leq \delta.
\]
With some simplifications we get for \( t > 0 \)
\[
\mathbb{P}\left\{ |G(X) - E[G(X)]| > 12 \sqrt{\frac{(1+2E[h(X)])}{n}} t + 23t \sqrt{n} \right\} \leq 15e^{-t}.
\]

Lemma 4.9 and (7) imply that we can use Proposition 4.8 with \( f = \hat{M}^\perp \) and the values \( a = 1, b = n + 1, \lambda = (n-1)/(8(e-2)) \) and \( w = 4E[h(X)]/n \). Substitution gives
\[
\mathbb{P}\left\{ |f(X) - E[f(X)]| > \sqrt{\frac{Ce^24E[h(X)]}{n} \ln(n+1 + 2e^2/\delta)} + e^2 \sqrt{\frac{8C(e-2)}{n-1} \ln(n+1 + 2e^2/\delta)} \right\} \leq \delta.
\]
Using \( n \geq 16 > 1 + 2e^2 \) we can simplify and resolve the constants to obtain for \( t > 0 \)
\[
\mathbb{P}\left\{ \hat{M}(X) - E[\hat{M}(X)] > 12 \sqrt{\frac{E[h(X)]}{n}} t + \frac{37t}{\sqrt{n-1}} \right\} \leq 2ne^{-t}.
\]
4.5 Proof of Proposition 4.8

The proof uses the following moment inequalities first given in [8].

Theorem 4.13. (Theorems 15.5 and 15.7 in [7]) Let $X = (X_1, ..., X_n)$ be a vector of independent random variables with values in $\mathcal{X}$ and $f : \mathcal{X}^n \to \mathbb{R}$. For $q \geq 2$ with $\kappa \approx 1.271$

$$\| (f(X) - \mathbb{E}[f(X)])_+ \|_q \leq \sqrt{\kappa q \| V^+ f(X) \|_{q/2}}$$

and with $C \approx 4.16$

$$\| (f(X) - \mathbb{E}[f(X)])_- \|_q \leq \sqrt{C q \left( \| V^+ f(X) \|_{q/2} \lor q \| Q f(X) \|_q \right)}.$$

where

$$V^+ f(x) = \sum_{k=1}^n \mathbb{E}_X \left[ (f(x) - f(S^k_X(x)))^2 \right].$$

We also need a few lemmata, one to convert exponential tail bounds to moment bounds, and one to convert moment bounds to tail bounds.

Lemma 4.14. Suppose that $X, w, \lambda, b \geq 0, p \geq 1$ and $\forall t > 0$

$$\mathbb{P}\{X > w + t\} \leq b e^{-\lambda t}.$$

Then $\|X\|_p \leq 2\lambda^{-1}b^{1/p} + w$.

Proof. We have $|X| = |X - w + w| \leq (X - w)_+ + w$. Then for $p \geq 1$

$$\mathbb{E}\left[(\lambda(X - w)_+)^p\right] = \int_0^\infty \mathbb{P}\{(\lambda(X - w)_+) > s\} ds$$

$$\leq \int_0^\infty \mathbb{P}\{(\lambda(X - w)_+) > t\} pt^{p-1} dt \text{ with } s = t^p$$

$$\leq bp \int_0^\infty e^{-t} t^{p-1} dt = bp \Gamma(p) \leq bp(p)^p \leq b(2p)^p.$$

So $\|\lambda(X - w)_+\|_p \leq 2b^{1/p}p$ or $\|X\|_p \leq 2\lambda^{-1}b^{1/p}p + w$. \qed

Lemma 4.15. Suppose $c, d, t > 0$ and $\sqrt{cx + dx} \geq t$. Then

$$x \geq \frac{t^2}{c + 2dt}$$

Proof. If $t \leq dx$ then $x \geq t/d = t^2/(dt) \geq t^2/(c + 2dt)$, so we can assume $t > dx$. Then

$$\sqrt{cx + dx} \geq t \implies \sqrt{cx + dx}^2 \geq t dx \implies cx + dx^2 \geq (t - dx)^2 = t^2 - 2dx + (dx)^2 \implies (c + 2dt)x \geq t^2. \qed$$

Lemma 4.16. Suppose for $\alpha, \gamma > 0, b \geq 1$ and $p \geq p_{\text{min}} \geq 1$ we have $\|Y\|_p \leq \sqrt{\alpha p} + \gamma b^{1/p}$.

Then

(i) for $\delta \in (0, 1)$

$$\mathbb{P}\left\{ |Y| > \sqrt{e^2 \alpha \ln \left(b + e^{p_{\text{min}}} / \delta\right)} + e^{2\gamma} \ln \left(b + e^{p_{\text{min}}} / \delta\right) \right\} \leq \delta.$$ (ii) for $t > 0$

$$\mathbb{P}\{ |Y| > t \} \leq (b + e^{p_{\text{min}}}) \exp \left( \frac{-t^2}{e^2 (\alpha + 2\gamma t)} \right).$$

(iii) If $b = 1$ then $b$ can be deleted in both inequalities above.
Proof. If \( p \geq \max \{ p_{\text{min}}, \ln (1/\delta) \} \) then

\[
P \left\{ |Y| > e \left( \sqrt{\alpha p} + \gamma b^{1/p} p \right) \right\} \leq P \left\{ |Y| > e^{\frac{\ln(1/\delta)}{p}} \|Y\|_p \right\} \leq \left( \frac{\|Y\|_p}{\|Y\|_p e^{\frac{\ln(1/\delta)}{p}}} \right)^p = \delta.
\]

The first inequality follows from the assumed bound on \( \|Y\|_p \), the second is Markov’s. Setting \( p = \ln ((b + e^{p_{\text{min}}})/\delta) \) we have \( p \geq \max \{ p_{\text{min}}, \ln (1/\delta) \} \) and also \( p \geq \ln b \), so that \( b^{1/p} = e^{(\ln b)/p} \leq e \). Substitution gives (i).

Let \( \delta > 0 \) and set \( e = e^2 \alpha, d = e^2 \gamma \) and \( x (\delta) = \ln (b + e^{p_{\text{min}}}/\delta) \leq \ln ((b + e^{p_{\text{min}}})/\delta) \), so \( \delta \leq (b + e^{p_{\text{min}}}) e^{-x(\delta)} \). Furthermore set \( t (\delta) = \sqrt{cx(\delta)} + dx(\delta) \), so \( t \) is decreasing in \( \delta \). If \( t (\delta) > t (1) \), then \( \delta \in (0, 1) \) and by (i) and Lemma 4.15

\[
P \left\{ |Y| > t (\delta) \right\} \leq \delta \leq (b + e^{p_{\text{min}}}) e^{-x(\delta)} \leq (b + e^{p_{\text{min}}}) \exp \left( \frac{-t (\delta)^2}{e^2 (\alpha + 2\gamma t (\delta))} \right).
\]

Since the right hand side is trivial for smaller values of \( t (\delta) \), the inequality holds for all \( t > 0 \). This gives (ii). (iii) follows from retracing the arguments with \( b = 1 \). \( \square \)

Proof of Proposition 4.8 The definitions of \( V^+ f \) and \( Qf \) and the self-boundedness imply

\[
V^+ f (x) \leq \sum_{k=1}^n \left( f (x) - \inf_{y \in X} f (S^k_y x) \right)^2 \\
\leq \max_k \left( f (x) - \inf_{y \in X} f (S^k_y x) \right) \sum_{k=1}^n f (x) - \inf_{y \in X} f (S^k_y x) \\
\leq (Qf) (x) a f (x) \leq a (Qf) (x),
\]

where we used \( f (x) \in [0, 1] \). The Efron-Stein inequality (Theorem 3.1 in (7)) then proves the bound on the variance. Furthermore \( \|Qf (X)\|_q \leq 2 \lambda^{-1} b^{1/q} q + w \) by Lemma 4.14. Substitution in the moment inequalities of Theorem 4.13 gives, using \( \kappa \leq C \), for \( q \geq 2 \) the inequalities

\[
\| (f (X) - E [f (X)])_+ \|_q \leq \sqrt{\kappa a} (\lambda^{-1} b^{2/q} q^2 + q) \leq \sqrt{Ca} (\lambda^{-1} b^{2/q} q^2 + q) \leq \sqrt{Ca} (\lambda^{-1} b^{2/q} q^2 + q)
\]

and, using \( a, b \geq 1 \),

\[
\| (f (X) - E [f (X)])_+ \|_q \leq \sqrt{C} \left( \sqrt{a \lambda^{-1} b^{2/q} q^2 + awq} \right) \leq \sqrt{C} \left( \sqrt{a (\lambda^{-1} b^{2/q} q^2 + awq)} \right) \leq \sqrt{Ca} \left( \lambda^{-1} b^{2/q} q^2 + q \right) \leq \sqrt{Ca} \lambda^{-1} b^{1/p} q + C awq,
\]

To see the third inequality recall that the range of \( f \) is in \([0, 1] \), so the left hand side above can be at most 1. But for any \( x \geq 0 \) we have \( \sqrt{C} (\sqrt{x} + x) \leq 1 \implies \sqrt{x} + x < 1/2 \implies \sqrt{x} \leq 1/2 \implies 2x \leq \sqrt{x} \implies \sqrt{C} (\sqrt{x} + x) = \sqrt{Cx} \). We then use Lemma 4.16 with \( \gamma = \sqrt{Ca} \lambda^{-1} \), \( \alpha = C aw, b = b \) and \( p_{\text{min}} = 2 \) and a union bound to get the conclusion. \( \square \)

4.6 Miscellaneous

Proposition 4.17. \( \hat{M} (X^n, r) \) converges to zero almost surely as \( n \to \infty \).

At this point it is worth mentioning that for totally bounded \((X, d)\) Berend and Kontorovich (3) show that \( M (\mu, n, r) \leq |C (r)| / (cn) \), where \( C (r) \) is an \( r \)-cover in \( X \).
Lemma 4.18. For every \( r, \epsilon > 0 \) we can write \( X \) as the disjoint union of two sets \( F \) and \( R \) such that \( \mu (R) < \epsilon \) and \( F \) is a finite union \( F = \bigcup_{i=1}^{N} C_i \) where the \( C_i \) have diameter at most \( r \) and \( \mu (C_i) > 0 \).

Proof. Since \( X \) is separable we can cover \( X \) with open balls \( \{ D_i \}_{i \geq 1} \) of radius \( r/2 \) and write \( C_i = D_i \setminus \bigcup_{1 \leq j < i} D_j \). The \( C_i \) are disjoint and \( 1 = \mu (X) = \sum_{i \geq 1} \mu (C_i) \), so there is \( N \) such that \( \epsilon > \sum_{i \geq N+1} \mu (C_i) = \mu (\bigcup_{i \geq N} C_i) \). Set \( R := \bigcup_{i \geq N} C_i \cup \bigcup_{i \in \mathbb{P} (C_i) = 0} C_i \). \( F = \bigcup_{1 \leq i \leq N, \mu (C_i) > 0} C_i \).

\[ \square \]

In the proof below we use the following consequence of the Borel-Cantelli lemma (1): let \( Y_n \) be a sequence of random variables. If for every \( \epsilon > 0 \) we have \( \sum_{n=1}^{\infty} \mathbb{P} \{|Y_n| > \epsilon\} < \infty \) then \( Y_n \to 0 \) almost surely as \( n \to \infty \).

Proof of Proposition 4.17. Fix \( \epsilon > 0 \) and let \( F, R \) and \( C \) be as in Lemma 4.18. For each \( n \in \mathbb{N} \) consider the event \( A_n = \{ \hat{M} (X^n_1, r) > \epsilon \} \). In case of \( A_n \) we have

\[
\epsilon < \hat{M} (X^n_1, r) = \mu \left( \bigcap_{i=1}^{n} B(X_i, r)^c \right) = \mu \left( R \cap \bigcap_{i=1}^{n} B(X_i, r)^c \right) + \mu \left( F \cap \bigcap_{i=1}^{n} B(X_i, r)^c \right) < \epsilon + \sum_{j=1}^{N} \mu \left( \bigcap_{i=1}^{n} B(X_i, r)^c \cap C_j \right).
\]

Thus \( A_n \) implies that there exists \( C_j \) such that

\[
\bigcap_{i=1}^{n} (B(X_i, r)^c \cap C_j) \neq \emptyset. \tag{8}
\]

Now if there is any \( X_i \in C_j \) then \( C_j \subseteq B(X_i, r) \) (by the constraint on the diameter of \( C_j \)) whence \( B(X_i, r)^c \cap C_j = \emptyset \). Thus (8) implies that for all \( i \in [n] \) we have \( X_i \notin C_j \). It follows that

\[
\mathbb{P} A_n \leq \mathbb{P} \bigcup_{j=1}^{N} \left\{ \mathbf{X} : \mu \left( \bigcap_{i=1}^{n} B(X_i, r)^c \cap C_j \right) > 0 \right\} \leq \mathbb{P} \bigcup_{j=1}^{N} \bigcap_{i=1}^{n} \{ \mathbf{X} : X_i \notin C_j \} \leq N \left( 1 - \min_{j} \mu (C_j) \right)^n.
\]

Thus \( \sum_{n} \mathbb{P} A_n < \infty \), and thus \( \hat{M} (X^n_1) \to 0 \) a.s. \( \square \)

Proposition 4.19. For \( p \in (1, \infty) \) there exists a distribution \( \mu \) in \( L_p [0, \infty) \) whose support is not totally bounded, nowhere smooth and not contained in any finite dimensional subspace, but \( h (X, r) \leq 2^p + 1 \) for any \( r > 0 \) and \( X \sim \mu \).

Proof. Let \( \mu \) be the distribution of the random variable \( 1_{[0, X]} \) in \( L_p [0, \infty) \) with \( X \) any real random variable whose distribution has full support on \( [0, \infty) \) (the exponential distribution would do). It is easy to see that the support of \( \mu \) has the required properties. Then note that \( \| 1_{[0, a]} - 1_{[0, b]} \|_p = |a - b|^{1/p} \), so if \( h (X, r) \geq k \) then \( \exists f \in L_p [0, \infty) \) and \( x_1, \ldots, x_k \in [0, 1] \) with \( x_{i-1} < x_i \), \( \| 1_{[0, x_i]} - 1_{[0, x_{i-1}]} \|_p > r \) and \( \| 1_{[0, x_i]} - f \|_p \leq r \). Then \( 2r \geq \| 1_{[0, x_i]} - 1_{[0, x_k]} \|_p = |x_k - x_1|^{1/p} = \left( \sum_{i=2}^{k} (x_i - x_{i-1}) \right)^{1/p} > (k - 1)^{1/p} r, \) so \( k - 1 < 2^p \). \( \square \)
Proposition 4.20. Let $(\mathbb{R}^D, \|\|)$ be a finite dimensional Banach space with closed unit ball $B$ and define the 1-packing number of $B$ as

$$\mathcal{P}(B, d_{\|\|}, 1) := \max \left\{|S| : S \subset B^D, \forall x, y \in S, x \neq y \implies \|x - y\| > 1\right\}.$$ 

Let $r > 0$. Then

(i) for every vector $x \in (\mathbb{R}^D)^n$ we have $h(x, r) \leq \mathcal{P}(B, d_{\|\|}, 1) \leq 8^D$.

(ii) For the 2-norm the bound improves to $D^D$.

(iii) If $\mu$ has a positive density w.r.t. Lebesgue measure on $\mathbb{R}^D$ and $X_1^n \sim \mu^n$ then $h(X_1^n, r) \to \mathcal{P}(B, d_{\|\|}, 1)$ almost surely as $n \to \infty$.

Proof. (i) Let $z = (z_1, ..., z_m) \subseteq x$ satisfy the local separation property with $h(x, r) = m$. So there is $y \in \mathbb{R}^D$ such that $\|z_i - y\| \leq r$ and $\|z_i - z_j\| > r$ for all $i \neq j$. Let $z'_k = (1/r)(z_i - y)$. Then $z'_k \in B$ and $\|z'_k - z'_j\| > 1$. This is the first inequality of (i). The second follows from Proposition 5 in [11].

(ii) This follows from the first inequality in (i) and Proposition 4.2.12 in [25].

(iii) Let $B(y, r)$ be any ball of radius $r$ in $\mathbb{R}^D$, $z = (z_1, ..., z_K)$ be any $r$-separated vector of points in $B(y, r)$ with $K = \mathcal{P}(B(y, r), d_{\|\|}, r) = \mathcal{P}(B, d_{\|\|}, 1)$. Since the separation condition is defined by strict inequalities, there is some $\eta > 0$ such that every vector $z' = (z'_1, ..., z'_K)$ satisfying $z'_k \in B(z_k, \eta)$ for all $k \in [K]$, is also $r$-separated. Since $\mu$ has a positive density w.r.t. Lebesgue measure $\mu(B(z_k, \eta)) > 0$ for each $k$. 

Now let $A_n$ be the event $A_n = \{h(X_1^n, r) \geq \mathcal{P}(B, d_{\|\|}, 1) - \epsilon\}$. Since $h(X_1^n, r) \leq \mathcal{P}(B, d_{\|\|}, 1)$, under $A_n$ there must exist $k \in [K]$, such that for all $i \in [n]$, $X_i \notin B(z_k, \eta)$. Thus

$$\mathbb{P}(A_n) \leq K \left(1 - \min_k \lambda(B(z_k, \eta))\right)^n$$

and the conclusion follows from the Borel-Cantelli lemma, as in Proposition 4.17.

4.7 The Wasserstein distance

Theorem 4.21. (= Theorem 3.1) Let $(X, d)$ be a complete, separable metric space with diameter 1 and Borel probability measure $\mu$. For $\delta > 0$, with probability at least $1 - \delta$ in $X \sim \mu^n$, if there exists an $r$-net $Y \subset X$ with cardinality $m$, $m \leq (n - 3)/2$, then

$$W_1(\mu, \hat{\mu}) \leq \tilde{M}(X, r) + 3r + 2 \sqrt{\frac{m}{n-m}} \left(1 + \sqrt{\ln (n/\delta)}\right)$$

or

$$W_1(\mu, \hat{\mu}) \leq 3r + 3 \sqrt{\frac{m}{n-m}} \left(1 + \sqrt{\ln (2n/\delta)}\right).$$

Proof. Let $V : y = (y_1, ..., y_m) \in \Sigma^m \to \{V_1, ..., V_m\} \in \Sigma^m$ be the Voronoi partitioning associated with $y$ and tie breaking according to the order of indices in $y$. Define $E(y)_k = V(y)_k \cap B(y_k, 2r)$. Note that the $E(y)_k$ are disjoint and

$$\bigcup_{k=1}^m B(y_k, 2r) = \bigcup_{k=1}^m E(y)_k. \tag{9}$$

Let $I \subseteq [n]$ be a set of indices with $|I| = m$ and assume that $Y = (X_i)_{i \in I}$ is an $r$-net. We write $Y = (Y_1, ..., Y_m)$ and

$$\hat{\mu}_{X\setminus Y} = \frac{1}{n-m} \sum_{i \in [n] \setminus I} \delta_{X_i}.$$
We will use the triangle inequality to bound $W_1(\mu, \tilde{\mu}) \leq W_1(\tilde{\mu}, \tilde{\mu}) + W_1(\mu, \tilde{\mu})$. We begin with the first term.

Note that at most one $Y_k$ can be in $E(Y)_k$, so

$$W_1(\tilde{\mu}, \tilde{\mu}) \leq \frac{|\{i : X_i \in E(Y)_k\}| - 1}{n-m}.$$ 

Let $F$ be the class of all $f : X \to [0, 1]$ satisfying $\|f\|_{Lip} \leq 1$. Since $\text{diam}(X) \leq 1$, by replacing the Lipschitz function $f$ in (3) by $f - \inf_{x \in X} f(x)$ we can always assume that $f \in F$. Then for any such $f$

$$\int_X f(d\tilde{\mu} - d\tilde{\mu}) = \sum_{k=1}^m \left( f(Y_k) \tilde{\mu}_{X \backslash Y}(E(Y)_k) - \frac{1}{n} \sum_{i : X_i \in E(Y)_k} f(Y_k) \right) + \frac{1}{n} \sum_{k=1}^m \sum_{i : X_i \in E(Y)_k} (f(Y_k) - f(X_i)).$$

The second term is bounded by $r$ by the Lipschitz condition on $f$. The first term is

$$\sum_{k=1}^m \left( f(Y_k) \left( \frac{|\{i : X_i \in E(Y)_k\}| - 1}{n-m} - \frac{|\{i : X_i \in E(Y)_k\}|}{n} \right) \right)$$

$$\leq \sum_{k=1}^m \frac{m|\{i : X_i \in E(Y)_k\}| - n}{n - m |\{i : X_i \in E(Y)_k\}|} - \frac{m|\{i : X_i \in E(Y)_k\}| - n}{n}$$

$$= \sum_{k=1}^m \frac{m|\{i : X_i \in E(Y)_k\}| - n}{n - m |\{i : X_i \in E(Y)_k\}|}$$

$$\leq \frac{m|\{i : X_i \in E(Y)_k\}| + n}{n - m |\{i : X_i \in E(Y)_k\}|} = \frac{m}{n-m}.$$ 

Thus

$$W_1(\tilde{\mu}, \tilde{\mu}) \leq \frac{m}{n-m} + r \leq \sqrt{m/(n-m)} + r$$

by virtue of the condition $m \leq (n-3)/2$. Now define

$$\Phi(X \backslash Y) := \sum_{k=1}^m |\mu(E(Y)_k) - \tilde{\mu}_{X \backslash Y}(E(Y)_k)|.$$ 

From (3) and the fact, that the $E(Y)_k$ are mutually disjoint, we also obtain for $f \in F$

$$\int_X f(d\tilde{\mu} - d\tilde{\mu}) \leq \int_{B(Y_k, 2r)} f d\mu + \sum_{k=1}^n \int_{E(Y)_k} f(d\mu - d\tilde{\mu})$$

$$\leq \tilde{M}(X, r) + \sum_{k=1}^m \int_{E(Y)_k} (f - f(Y_k)) d\mu + \sum_{k=1}^m f(Y_k) (\mu(E(Y)_k) - \tilde{\mu}(E(Y)_k))$$

$$\leq \tilde{M}(X, r) + 2r + \Phi(X \backslash Y),$$

where the second inequality follows from the triangle inequality and the fact that $Y$ is an $r$-net of $X$, so that $\bigcap_{k=1}^n B(Y_k, 2r)^c \subseteq \bigcap_{i=1}^n B(X_i, r)^c$. The last inequality comes from the Lipschitz property of $f$, since $d(x, Y_k) \leq 2r$ for all $x \in E(Y)_k$. 

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From Jensen’s inequality we get

\[
\mathbb{E} \left[ \Phi(X \setminus Y | Y) \right] \leq \sum_{k=1}^{m} \left( \mathbb{E} \left( \frac{1}{n-m} \sum_{j \notin I_j} (\mu(E(Y)_k) - 1 \{X_j \in E(Y)_k\})^2 \right) \right)^{1/2} 
= \frac{1}{n-m} \sum_{k=1}^{m} \left( \sum_{j \notin I_j} \mathbb{E} (\mu(E(Y)_k) - 1 \{X_j \in E(Y)_k\})^2 \right)^{1/2} 
\leq \frac{1}{\sqrt{n-m}} \sum_{k=1}^{m} \sqrt{\mathbb{E} (\mu(E(Y)_k))} \leq \sqrt{\frac{m}{n-m}}.
\]

On the other hand modifying \( X_i \) for some \( i \notin Y \) can change the value of \( \Phi(X \setminus Y) \) at most for two values of \( k \), since the \( E(Y)_k \) are mutually disjoint, so the incurred difference in \( \Phi(X \setminus Y) \) is bounded by \( 2/(n-m) \). It follows from the bounded difference inequality that \( \mathbb{P} \{ \Phi(X \setminus Y) - \mathbb{E} [\Phi(X \setminus Y | Y)] > t \} \leq \exp \left( -(n-m) t^2 / 4 \right) \). We conclude from (10) and (11) that for any fixed \( r \)-net \( Y \subset X \) with cardinality \( m \leq (n-3)/2 \) and \( t > 0 \)

\[
\mathbb{P} \left\{ W_1(\mu, \hat{\mu}) > M(X, r) + 3r + 2 \sqrt{\frac{m}{n-m}} + t \right\} 
\leq \mathbb{P} \{ \Phi(X \setminus Y) - \mathbb{E} [\Phi(X \setminus Y | Y)] > t \} 
\leq \exp \left( -(n-m) t^2 / 4 \right).
\]

A union bound over all the \( \binom{n}{m} \leq n^m \) sub-samples \( Y \subset X \) with \( |Y| = m \) gives

\[
\mathbb{P} \left\{ \exists Y \subseteq X, |Y| = m, W_1(\mu, \hat{\mu}) > M(X, r) + 3r + 2 \sqrt{\frac{m}{n-m}} + t \right\} \leq n^m \exp \left( -(n-m) t^2 / 4 \right).
\]

The first conclusion follows from equating the bound on the probability to \( \delta \) and solving for \( t \). The second conclusion follows from a union bound with Corollary 2.5. \( \square \)

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