CONCENTRATION INEQUALITIES FOR LEAVE-ONE-OUT CROSS VALIDATION

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Abstract. In this article we prove that estimator stability is enough to show that leave-one-out cross validation is a sound procedure, by providing concentration bounds in a general framework. In particular, we provide concentration bounds beyond Lipschitz continuity assumptions on the loss or on the estimator. We obtain our results by relying on random variables with distribution satisfying the logarithmic Sobolev inequality, providing us a relatively rich class of distributions. We illustrate our method by considering several interesting examples, including linear regression, kernel density estimation, and stabilized/truncated estimators such as stabilized kernel regression.

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1. Introduction

It is customary in many statistical and machine learning methods to use train-validation, where the data is split into a training set and a validation set. Then the training set is used for estimating (training) the model, while the validation set is used to measure the performance of the fitted model. The downside in splitting the data into the training set and the validation set is that one is wasting a lot of data to be used for either the training, leading to inaccuracy, or to the validation, leading to insufficient knowledge whether the model is performing well. One common technique to overcome this problem is to perform cross-validation, originally introduced by Stone in [39]. In the present paper, we consider the classical leave-one-out (LOO) cross validation. In LOO cross validation one leaves one fixed observation out, and uses the remaining ones as the training set. By using the remaining one observation as the validation set, one can then measure the performance of the fitted model on this single data point. However, by repeating this procedure through the whole data set of size n, one can then measure the performance by averaging over n data points. In this way one can, on each step, use most of the data for the training, while the performance is measured on n observation points as well.

Cross validation has many uses, but the most common ones are as a model selection procedure (see [39]) or as a method to estimate generalization error. In this paper we are interested in estimating the generalization error. For a discussion about model selection, see Section 7.

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Concentration and algorithm stability measures how well one estimates the true error (with respect to some given loss function) arising from fitting the model in the first place, and hence are crucially important topics for practical applications. Indeed, under- or over-fitting can lead to severe inaccuracies in making predictions by using the underlying model, thus reducing the prediction performance significantly. As such, the topic has been extensively studied in the literature from different perspectives. Several theoretical studies on the goodness of cross-validation include, among others, [8, 9, 14, 19, 21, 22, 26, 27, 31, 32] in various settings. The $L^2$-error is studied, under various settings, in [5, 7, 22, 23, 34]. For the results related to algorithmic stability, we refer to [12, 13, 16, 17, 18, 29, 36, 37, 1, 23, 24, 28] and references therein. For a very good history of the subject of algorithmic stability in the context of cross validation, see [1]. Finally, while we do not discuss the issue of cross-validation having relatively heavy computational burden in the present paper, the reader may consult [6, 15, 33, 38, 40] for efficient computations.

Despite the problem being well-studied in the literature, it seems that concentration bounds are not that well studied in a general framework, and most of the result presented in the literature assume various simplifying properties such as boundedness in the data or loss, e.g. [14], or Lipschitz in the Hamming distance, e.g. [5]. In this article we study concentration inequalities for LOO cross validation in a general unbounded framework using the gradient of the loss as information. For the data, we assume it to come independently from a distribution that satisfies the logarithmic Sobolev inequality, prototypically the Gaussian. This provides us a relatively simple proof that gives rather general concentration bounds under many interesting situations. Although in the theory of logarithmic Sobolev inequalities, the concentration of Lipschitz functions is a well known fact, it seems to the authors that in the context of algorithmic stability, the gradient is a new piece of information. We finally mention an interesting and related paper, [1], where the authors assume a Gaussian type moment bound on the LOO estimate, allowing for unbounded data. In comparison, for Gaussian data this allows one to use Lipschitz loss functions, while our framework allows us to go beyond and cover quadratic losses as well, with a small price in the exponential rate.

The logarithmic Sobolev inequality has its roots in the theory of hypercontractivity of the Ornstein-Uhlenbeck semigroup, and was essentially first discovered by L. Gross in [20]. The concentration of measure on the other hand was a term coined by Milman (for references see [35]) in his study of asymptotic theory of Banach spaces, essentially saying that most of the surface area of the sphere is concentrated on the equator. However, it was Herbst who made the connection between the log-Sobolev inequality and concentration of measure in an unpublished letter to Gross, for more information see [30]. The logarithmic Sobolev inequality is useful, because it tensorizes and is thus very suitable for the i.i.d. framework. The assumption is rather mild in the sense that many distributions satisfy it. On the other hand however, it says that the measure is essentially Gaussian in the sense that it needs to be strictly log-concave outside a large ball.
We obtain our results by posing certain assumptions on the gradient of our estimator and the loss function. In particular, our results can be applied beyond the Lipschitz case that is a common assumption present in the literature. We illustrate the applicability of our approach with several examples, including linear regression, kernel density estimation, and stabilized/truncated estimators such as stabilized kernel regression.

The rest of the article is organized as follows. In Section 2 we introduce our notation. In Section 3 we state our main theorems. We illustrate the applicability of our approach with several remarks in Section 7. Several numerical experiments are conducted in Section 5, while all the proofs are postponed to Section 6. We end the paper with concluding remarks in Section 7.

2. Setup and preliminaries for leave-one-out cross validation

In order to define the leave-one-out (LOO) cross validation we need first a definition:

**Definition 2.1.** Let \( Z_1, \ldots, Z_n \) be an i.i.d. sequence of random variables, \( Z_i = (X_i, Y_i) \in \mathbb{R}^k \times \mathbb{R}^m \). We will call \( D = \{Z_1, \ldots, Z_n\} \) a dataset of length \( n \). Furthermore, for any \( i = 1, \ldots, n \) we define the deleted dataset \( D_{(-i)} = \{Z_1, \ldots, Z_{i-1}, Z_{i+1}, \ldots, Z_n\} \).

Leave-one-out cross validation is often used to evaluate the prediction performance of a statistic.

**Definition 2.2.** For a statistic \( T_n : \mathbb{R}^{(k+m)n} \to C(\mathbb{R}^k; \mathbb{R}^m) \) and a dataset \( D \) of length \( n \), we denote \( T_D = T_n[D] \in C(\mathbb{R}^k; \mathbb{R}^m) \). We also denote \( T_{D_{(-i)}} = T_{n-1}[D_{(-i)}] \). Furthermore, we call any function \( L : \mathbb{R}^k \times \mathbb{R}^m \to \mathbb{R} \) a loss function. The risk is the expected loss w.r.t. a random variable \( Z = (X, Y) \) which is i.i.d. to \( (X_i, Y_i) \in D \).

**Definition 2.3.** Given a statistic \( T_n : \mathbb{R}^{(k+m)n} \to C(\mathbb{R}^k; \mathbb{R}^m) \), a dataset \( D \) of length \( n \), and a loss function \( L : \mathbb{R}^k \times \mathbb{R}^m \to \mathbb{R} \) we define the leave-one-out (LOO) cross validation of risk as

\[
\hat{L}_{\text{LOO}} := \frac{1}{n} \sum_{i=1}^{n} L(T_{D_{(-i)}}(X_i), Y_i) \sim L_{\text{LOO}} := \mathbb{E}[L(T_D(X), Y) \mid D],
\]

where \( Z = (X, Y) \) is i.i.d. to \( D \), and \( \sim \) means ’estimate of’.

Although the introduction of \( L \) and \( T_D \) is necessary, the notation is cumbersome. We will often without specific mention use the following shorthand instead: \( f_i(z) = L(T_{D_{(-i)}}(x), y), z = (x, y) \), and \( f_D(z) = L(T_D(x), y) \).

This is an a posteriori measurement of error (conditioned on \( D \)) and we consider the model \( (T) \) as fitted and fixed, we are just testing its prediction performance. Our main theorems below provide concentration inequalities for the error \( L_{\text{LOO}} - \hat{L}_{\text{LOO}} \).

In what follows, we use \( | \cdot | \) to denote the absolute value and \( \| \cdot \| \) to denote the Euclidean norm given by \( \| x \|^2 = \sum_{k=1}^{n} x_k^2 \), where \( n \) is the size of the vector.
2.1. Logarithmic Sobolev inequalities. Throughout, we consider our data to arise from a distribution that has a finite logarithmic Sobolev constant, given below:

**Definition 2.4.** We define the logarithmic Sobolev constant of a probability measure $\mu$ as

$$\sigma^2(\mu) := \sup_{f \in W^{1,2}(\mu)} \frac{1}{2} \text{Ent}_\mu(f^2),$$

where the entropy of $g$ is given by

$$\text{Ent}_\mu(g) = E_\mu[g \log(g)] - E_\mu[g] \log(E_\mu[g]),$$

and $W^{1,2}(\mu)$ is the Sobolev Hilbert space associated with $\mu$.

The log-Sobolev constant essentially measures the tail behavior of the measure, but it does so in a rather strong way. The log-Sobolev constant is related to the interplay between the geometry of the manifold of support and the log-concavity of the density at the tails. Examples include measures uniformly bounded from below and above on the unit sphere, the Gaussian measure, and densities which are solutions to Kolmogorov Fokker-Planck equations

$$u_t = \nabla \cdot (\nabla u + \nabla F u),$$

where $F$ has quadratic growth at infinity. However, it is still a fairly rich class of densities, and covers densities that are log-concave outside a large ball. See also [30] for Bakry-Emery and Holley-Stroock perturbations. Worth mentioning is also the Aida perturbation argument, see [2].

The fact that $\sigma^2(\mu) < \infty$ implies concentration is well known, see for instance [30].

**Lemma 2.5.** Let a measure $\mu$ satisfy $\sigma^2(\mu) < \infty$. Then for the sub-Gaussian constant of a measure $\mu$, defined as

$$\sigma^2_{SG}(\mu) = \inf \left\{ \sigma^2 : \int e^{2t^2} d\mu \leq e^{\sigma^2 t^2/2}, \quad \forall t \in \mathbb{R}, \quad \forall f : \| \nabla f \| \leq 1 \right\},$$

we have $\sigma^2_{SG}(\mu) \leq \sigma^2(\mu)$.

It is interesting to note that the log-Sobolev property tensorizes with the same constant for product measures, i.e. $\sigma^2(\mu^\otimes n) = \sigma^2(\mu)$. Thus, it suits the i.i.d. framework well.

2.2. Algorithmic stability. The main objects of study will be the following concept of stability.

**Definition 2.6.** If there exists functions $\delta_1(n, z), \delta_2(n, z), \delta_3(n)$ all non-negative and tending to zero as $n \to \infty$, such that for any point $D \in \mathbb{R}^{(k+m)n}$ and $z = (x, y) \in \mathbb{R}^{k+m}$, it holds

$$\| \nabla D L(T_D(x), y) \| \leq \delta_1(n, z) + \delta_2(n, z) \| D \|, \quad (2.1)$$

and for a dataset $D$ of length $n$ whose distribution $\mu$ satisfies $\sigma^2(\mu) < \infty$, it holds

$$| \mathbb{E}[L(T_{D_{(i-1)}}(X_i), Y_i)] - \mathbb{E}[L(T_D(X), Y)] | < \delta_3(n), \quad i = 1, \ldots, n. \quad (2.2)$$
Then we say that the pair \((T, L)\) is \((\delta_1, \delta_2, \delta_3)\)-stable.

**Remark 2.7.** The interpretation of \(\delta_1\) and \(\delta_2\) is the “variability” or “instability” of the loss when we alter the data (i.e. which fold). To see how this allows us to control the variability, note first that the log-Sobolev inequality (see [30]), specifically, for any smooth \(f\)

\[
\forall[f] \leq C E[|\nabla f|^2].
\]

Thus, if \(|\nabla_{D} f(D)| \leq \delta_1(n) + \delta_2(n)|D|\), and \(E[|D|^2] \approx n\), then for the variance of \(f\) to tend to zero we need \(\delta_2(n) = o(\sqrt{n}^{-1})\). Furthermore, concentration is equivalent to concentration of 1-Lipschitz functions (see [30]), and as such the introduction of \(\delta_1\) is very natural indeed. Finally, \(\delta_3\) measures the bias induced by the fact that one observation is removed.

Let us frame Definition 2.6 in a particular example. We first consider the simplest possible:

**Example 2.8.** Let \(D\) be a dataset of length \(n\). Let \(T_D\) be the empirical mean. Then, \(T_D\) is Lipschitz with respect to \(D\). Let \(L(x, y) = (x - y)^2\) be the quadratic loss. Then, the loss function evaluated on the estimator \((|T_D(x) - y|^2)\) now satisfies Definition 2.6 with \(\delta_1 \sim 1/\sqrt{n}\), \(\delta_2 \sim 1/n\), and \(\delta_3 \sim 1/n\). For a complete derivation, see Section 4.

On the other hand, a classical but a bit more complicated example is the following:

**Example 2.9.** Consider kernel density estimation with a given kernel \(K\) in \(\mathbb{R}\). Assume that the kernel \(K\) is differentiable and has a globally bounded derivative. Let our i.i.d. dataset of length \(n\) be denoted as \(D\). Then, denote the kernel density estimator \(\hat{g}_D\) with bandwidth \(h\) of a density \(g\). To estimate the integrated \(L^2\) loss, one needs to estimate \(L_{\text{LOO}} := \mathbb{E}[\hat{g}_D(Z) \mid D]\), where \(Z\) is a new data point. This is often done using leave-one-out cross-validation, which involves computing the corresponding \(L_{\text{LOO}}\) as defined in Definition 2.3, where the estimator \(T_D(z) = \hat{g}_D(Z)\) and the loss is \(L(T_D(z)) = |T_D(z)|\). In Section 4, we will see that \(\delta_1(n) = C/(h\sqrt{n})\), \(\delta_2 \equiv 0\), and \(\delta_3 \equiv 0\).

In Section 4, we will see that \(\delta_1(n) \sim 1/\sqrt{n}\) in many examples (which corresponds to the best case, as seen in Examples 2.8 and 2.9). Referring back to Remark 2.7, we need at least \(\delta_2 = o(\sqrt{n}^{-1})\) for the variance of the estimator to tend to zero as \(n \to \infty\).

To the authors, it seems that the introduction of \(\delta_1\) and \(\delta_2\) is new, while the error controlled by \(\delta_3\) appears in the literature. Historically, the error controlled by (2.2) has been measured in different norms, the strongest being uniform stability introduced in [12]. This corresponds to a.s. bounds in (2.2). Weaker notions of stability have been studied; for instance, \(L^1\) (hypothesis stability) and \(L^2\) (mean square stability) in [18, 23], respectively. Our formulation in (2.2) corresponds to the weakest notion of stability, customarily called error stability, which was first introduced in [24]. Under uniform stability, one gets Gaussian concentration bounds. This remains true if one has sufficient control of all the moments [1]. Under our weaker
assumption on (2.2), together with the new stability assumption involving \( \delta_1 \) and \( \delta_2 \), we obtain either Gaussian or exponential concentration.

3. MAIN RESULTS

In order to state our results, we begin with our main standing assumption:

**Assumption 3.1.** We assume that \( D \in \mathbb{R}^{(k+m)\otimes n} \) is a dataset of length \( n \) whose distribution \( \mu \) satisfies \( \sigma^2(\mu) < \infty \). We furthermore assume that the pair \((T, L)\) is \((\delta_1, \delta_2, \delta_3)\)-stable and that \( \mathbb{E}[L(T_D(x), y)] \) has linear or quadratic growth in \( z = (x, y) \).

3.1. The Lipschitz case. For illustration purposes, we begin with the following simplified version of our main result.

**Theorem 3.2** (Lipschitz case). Suppose that Assumption 3.1 holds, \( \delta_3(n, z) \equiv 0 \), and \( \|\nabla f\|_{\infty} < \infty \) with \( f(z) = \mathbb{E}[f_i(z)] \). Then for \( \varepsilon > 3\delta_3(n) \) we have

\[
P \left( L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon \right) \leq n \mathbb{E} \left[ e^{-\frac{\varepsilon^2 n}{8\sigma^2(\mu)\|\nabla f\|_{\infty}}} + e^{-\frac{\varepsilon^2 n}{8\sigma^2(\mu)\|\nabla f\|_{\infty}}} \right].
\]

Thus, if \( \delta_1(n, z) \leq \frac{\sigma}{\sqrt{n}} \), then for fixed \( \varepsilon > 0 \) there is an \( N_\varepsilon \) such that, for \( n \geq N_\varepsilon \), the following exponential concentration holds:

\[
P \left( L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon \right) \leq 3ne^{-C\varepsilon^2 n}. \tag{3.1}
\]

**Remark 3.3.** In Theorem 3.2, the right-hand side contains three error terms which control the following three errors respectively:

\[
L_{\text{LOO}} - \hat{L}_{\text{LOO}} = \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_i(Z_i) \mid Z_i] - f_i(Z_i) \right)
+ \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_i(Z_i)] - \mathbb{E}[f_i(Z_i) \mid Z_i] \right)
+ \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_D(Z) \mid D] - \mathbb{E}[f_i(Z_i)] \right). \tag{3.2}
\]

The first error measures how the empirical loss, as a function \( f_i \), differs from the expected loss function \( \mathbb{E}[f_i] \). The second error measures the difference between the Risk and the expected loss function \( \mathbb{E}[f_i] \) evaluated at the held out point \( Z_i \). The third error essentially measures the bias induced by the fact that one observation is removed together with the generalization error. Thus, we have to assume that the smallest measured deviation is bigger than the “bias/error stability”, i.e. \( \varepsilon > 3\delta_3(n) \).

**Remark 3.4.** By examining our proof carefully, we actually observe two-sided concentration, i.e.

\[
P \left( |L_{\text{LOO}} - \hat{L}_{\text{LOO}}| > \varepsilon \right) \leq 6ne^{-C\varepsilon^2 n}.
\]

The same applies in the statements of Theorems 3.2, 3.6 and 3.9, where we multiply the estimates on the right-hand side by a factor two. Note that while (3.1) measures the probability of under-estimating the true risk \( L_{\text{LOO}} \), other sided concentration

\[
P \left( \hat{L}_{\text{LOO}} - L_{\text{LOO}} > \varepsilon \right)
\]

measures the probability of over-estimating the true risk \( L_{\text{LOO}} \).
3.2. The quadratic case. Theorem 3.2 is a special case of our main theorem, but before presenting our main theorem in full generality, it is necessary to introduce some further simplifying notation.

We define the following three rate functions that control the three different sources of error in the LOO cross validation (see Remark 3.3): Denote $C_1 = \sigma^2(\mu)$. Then there exists a constant $C$ depending on the linear or quadratic growth of $E[L(T_D(x), y)]$ and $C_1$, such that

$$
\theta_1(n, t, z) = e^{-\frac{1}{8C_1}(\delta_1^2(n, z)+\delta_2^2(n, z)+\delta_3^2(n, z))} \vee e^{-\frac{nt}{8C_1\delta_2(n, z)}} \quad (3.3)
$$

$$
\theta_2(n, t) = \begin{cases} 
\frac{e^{-\frac{2t^2}{2c}}}{2c} \sqrt{\mathbb{E}[f_1(z)]} \text{ has linear growth} \\
\frac{e^{-\frac{2t^2}{2c}}}{2c} \sqrt{\mathbb{E}[f_1(z)]} \text{ has quadratic growth} 
\end{cases} \quad (3.4)
$$

$$
\theta_3(n, t) = e^{-\frac{1}{8C_1}(\delta_1^2(n, z)+\delta_2^2(n, z)+\delta_3^2(n, z))} \vee e^{-\frac{nt}{8C_1\delta_3(n, z)}} \quad (3.5)
$$

**Remark 3.5.** The constant $C$ in (3.4) can be quantified as follows. In the linear case, i.e. under the assumption that $f(z) = \mathbb{E}[f_1(z)]$ satisfies $\|\nabla f\|_\infty < \infty$, then we can quantify $\theta_2$ as

$$
\theta_2(n, t) = e^{-\frac{nt^2}{8C_1\|\nabla f\|_\infty}}.
$$

For the quadratic case, we assume that $|f(z_1) - f(z_2)| \leq c_1|z_1 - z_2| + c_2|z_1 - z_2|^2$, and we can quantify $\theta_2$ as

$$
\theta_2(n, t) = e^{-\frac{nt^2}{8C_1(c_1^2+c_2^2\mathbb{E}[|X|^2]+16C_1)}} \vee e^{-\frac{nt}{8C_1c_2}}.
$$

Note that in the Lipschitz case we have $\delta_2(n, z) \equiv 0$, and both $\theta_1, \theta_2$ have the exponent quadratic in $t$, i.e. the first term dominates. On the other hand, if

$$
\frac{\delta_1^2}{\delta_2} + \delta_2 n \to 0,
$$

then for large enough $n$ the second term in $\theta_1, \theta_2$ will dominate. Finally, we would like to note that in order for $n\theta_1, \theta_2$ to approach 0 for fixed $t$ as $n \to \infty$, we need

$$
(\delta_1^2 + \delta_2^2 n) \vee \delta_2 \leq o((\log(n))^{-1}).
$$

We note again that in many examples, we can take $\delta_1 \sim \sqrt{n}^{-1}, \delta_2, \delta_3 \sim n^{-1}$, and thus we can find a constant $C$ in $\theta_2$ such that

$$
\theta_1 \vee \theta_3 \leq \theta_2.
$$

Our main result is the following.

**Theorem 3.6.** Suppose that Assumption 3.1 holds. Then for $\varepsilon > 3\delta_3(n)$ we have

$$
\mathbb{P}\left(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon\right) \leq n\mathbb{E}[\theta_1(n, \varepsilon/3, Z)] + \theta_2(n, \varepsilon/3) + \theta_3(n, \varepsilon/3 - \delta_3(n)).
$$
Remark 3.7. If we assume that the loss function $L$ is Lipschitz in its first component, i.e.
$$|L(A_1, B) - L(A_2, B)| \leq C \|A_1 - A_2\|,$$
then the Lipschitz condition on the estimator $T$ implies Lipschitz condition, i.e. $\delta_2(n, z) \equiv 0$ in Assumption 3.1.

3.3. Extensions beyond quadratic: conditioned concentration. In many cases of interest the rates $\delta_1(n, z)$ and $\delta_2(n, z)$ might depend on the data $D$ as well. Let us consider an example to highlight this fact:

Example 3.8. Consider the case of simple linear regression, i.e. for a dataset $D$ of length $n$ we let $T_D(x)$ be the estimated linear function and let the loss be the standard $L_1$ loss. We will see in Section 4 that $L(T_D(x), y)$ does not satisfy Assumption 3.1 on the space of all possible data configurations. To understand the issue without going too much into detail, we note that when the $X$ coordinates of the data are tightly grouped together, then the slope of $T_D(x)$ will change very rapidly and thus violate (2.1) unless we let $\delta_1$ and $\delta_2$ also depend on $D$.

In order to remedy the issue highlighted in Example 3.8 we will give an extension of Theorem 3.6 that is true when we condition on the data restricted to a set where the algorithm behaves nicely.

We end this section with a result that goes beyond Lipschitz continuity and log-Sobolev. Now the constant $\sigma^2(\mu)$ is not stable w.r.t. restrictions but $\sigma^2_{SG}(\mu)$ is: Specifically by [11, Theorem 1], for a set $A$ such that $\mu(A) > 0$, the restricted measure
$$\mu_A(B) = \frac{\mu(A \cap B)}{\mu(A)}$$
satisfies
$$\sigma^2_{SG}(\mu_A) \leq c \log \left( \frac{e^{\mu (K) \otimes n}}{\mu(A)} \right) \sigma^2_{SG}(\mu), \quad (3.6)$$
where $c = 3 \cdot 2^{12} e^2$.

The following result can be achieved as Theorem 3.6 by conditioning. Although the statement looks cumbersome, it is applicable in more situations, for instance when we cannot guarantee the Lipschitz condition everywhere, but only in a large part of the space.

Let $K \in \mathbb{R}^{(k+m)\otimes n}$ be a permutation symmetric set, and let
$$C_1 = c \log \left( \frac{e}{\mu^{\otimes n}(K)} \right) \sigma^2(\mu),$$
$$C_2 = 2c \sigma^2(\mu),$$
where $c$ is from (3.6). Then we define modified rate functions as
$$\hat{\theta}_{1,K}(n, \varepsilon, z) := \exp \left( -\frac{\varepsilon^2}{16C_2\delta^2_{1,K}(n, z)} \right),$$
$$\theta_{2,K}(n, \varepsilon) := \exp \left( -\frac{\varepsilon^2 n}{8C_1} \right).$$
\[
\theta_{3,K}(n, \varepsilon) := \exp\left(-\frac{(\varepsilon/6 - \delta_3(n))^2}{8C_1E[\delta_1,K(n,Z)]^2}\right),
\]
where \(\delta_1,K(n,z)\) is a function such that
\[
\|\nabla_D f_D(z)\| \leq \delta_1,K(n,z), \quad D \in K,
\]
with \(f_D(z) = L(T_D(x),y),\ z = (x,y)\). We further need a modified version of \(\delta_3\), which we state as
\[
|E[f_D(Z')| D \in K, D' \in K] - E[f(Z) | D \in K]| \leq \delta_3,K(n),
\]
with \(f(z) = E[f_i(z)] = E[L(T_D(-i)(x),y)]\), and finally we need \(\gamma(K)\) that is defined as
\[
\gamma(K) = E[f_D(Z)] - E[f_D(Z')| D \cup D' \in K],
\]
where \(D'\) is an independent copy of \(D\).

**Theorem 3.9.** Let \(D \in \mathbb{R}^{(k+m)\otimes n}\) be a dataset of length \(n\) with distribution \(\mu^{\otimes n}\). For any \(\varepsilon > 6(\delta_3,K(n) \wedge \gamma(K))\) we have
\[
\mathbb{P}(L_{LOO} - \hat{L}_{LOO} > \varepsilon) \leq n \mathbb{E}[\theta_{1,K}(n,\varepsilon/6,Z) + \theta_{2,K}(n,\varepsilon/6) + \theta_{3,K}(n,\varepsilon/6 - \delta_3,K(n))]
\]
\[
+ \theta_{3,K}(n,\varepsilon/6 - \gamma(K)) + \mathbb{P}(D \notin K)
\]
\[
+ \mathbb{P}(\mu^{\otimes(n-1)}(K_{1}(Z_1)) < 2^{-1} | D \in K),
\]
where \(K_1(z) = K \cap \{Z_1 = z\}\) is the \(z\) slice of \(K\).

**Remark 3.10.** If we now have the situation such that
\[
|\nabla_D f_D(z)| \leq \delta_1(n,z,D) + \delta_2(n,z,D)|D|,
\]
we can, when restricted on \(K\), write it as
\[
|\nabla_D f_D(z)| \leq \text{diam}(K)(\delta_1(n,z,D) + \delta_2(n,z,D)),
\]
where \(\text{diam}(K)\) is the diameter of the set \(K\), provided that \(K\) is compact.

In practice Theorem 3.9 can be applied by choosing a set \(K\) growing in \(n\). Then possible growth in \(\delta_1,K\) and \(\delta_2,K\) in terms of the size of \(K(n)\) makes the rates \(\theta_{1,K}\) and \(\theta_{3,K}\) slightly worse, while now \(\mathbb{P}(D \notin K)\) decays exponentially by the log-Sobolev assumption. Hence, one can optimize by choosing suitable \(K = K(n)\), depending on the situation.

**Remark 3.11.** The log-Sobolev inequality does not in general hold for bounded data, and as such our result focuses on extending concentration bounds beyond known results for bounded data. In our case, the tail behavior is contained in the log-Sobolev constant and in the quantity \(\mathbb{P}(D \notin K)\), see also Section 7.

4. **Examples**

4.1. **The empirical mean.** Consider the empirical mean \(\bar{X}_n\). In this case we can consider \(f_D(z) = L(\bar{X}_n, z) := |\bar{X}_n - z|\). Then, by the triangle inequality and Hölder inequality, we get
\[
|f_{D_1}(z) - f_{D_2}(z)| \leq |\bar{X}_n,1 - \bar{X}_n,2| \leq \frac{|D_1 - D_2|}{\sqrt{n}}.
\]
which gives us $|\nabla_D f_D(z)| \leq \frac{1}{\sqrt{n}}$. With $f_i(z) = L(T_{D_{(-i)}}(x), y)$ we also have

$$|\mathbb{E}[f_i(Z_i)] - \mathbb{E}[f_D(Z)]| \leq \mathbb{E}|X_n - X_{n-1}| \leq 2\frac{\mathbb{E}|X_1|}{n - 1},$$

allowing us to choose $\delta_3(n) = \frac{C}{n-1}$. Hence, we obtain, by Theorem 3.2,

$$P\left(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon\right) \leq 3ne^{-C\varepsilon^2n}$$

for large enough $n$. We note that by using permutation symmetry of $X_n$, one can improve the upper bound to be $e_1 e^{-C\varepsilon^2n}$. Using our general approach without extra information on permutation symmetry, we obtain the multiplier $n$ in front of the exponential term.

4.2. Z dependent Lipschitz constant. Let $L(x, y) = (x - y)^2$. Then for $f_D(z) = L(T_D(x), y) = (T_D(x) - y)^2$ from which it follows that

$$|\nabla_D f_D(z)| = |\nabla_D L(T_D(x), y)| \leq 2|\nabla_D T_D(x)||y - T_D(x)|.$$

If now $T_D(x)$ has linear growth in $x$ and $|\nabla_D T_D(x)| \leq \delta_1(n)$, it follows that

$$|\nabla_D f_D(z)| \leq C\delta_1(n)(|y| + |x|) := \delta_1(n, z).$$

This provides an example where $\delta_1(n, z)$ depends on $z$ as well, highlighting the fact that in general the $z$-dependence should be taken into account.

4.3. Kernel density estimation. Consider kernel density estimation with given kernel $K$ in $\mathbb{R}$, for simplicity. Here $g$ is our true density function and $\hat{g}$ is our estimate given by

$$\hat{g}(x) = \frac{1}{n} \sum_{j=1}^{n} K_h(x - x_j) = \frac{1}{nh} \sum_{j=1}^{n} K\left(\frac{x - x_j}{h}\right),$$

where $h$ is a suitably chosen parameter (typically one chooses $h$ to depend on $n$ as well). A common loss is the integrated $L^2$ loss, i.e.

$$L(g, \hat{g}) = \int_{\mathbb{R}} (g(x) - \hat{g}(x))^2 dx.$$ 

The risk is then given by $R(g, \hat{g}) = \mathbb{E}[L(g, \hat{g})]$. Expanding the expression for the loss, we get

$$L(g, \hat{g}) = \int_{\mathbb{R}} g^2(x) dx - 2\int_{\mathbb{R}} g(x)\hat{g}(x) dx + \int_{\mathbb{R}} \hat{g}^2(x) dx.$$

In order to estimate the above, one typically omits the deterministic parts and instead focus on estimating the random parts, i.e. the last two integrals. The last term is computable, while the second term equals $2\mathbb{E}[\hat{g}(X) \mid D]$ which we need to estimate. One way to do this is to use leave-one-out estimation. In this case we have $f_i(z) = \hat{g}_{D_{(-i)}}(z)$. We obtain (provided that $K$ is differentiable kernel with bounded derivative)

$$|\nabla_{z_k} \hat{g}_{D_{(-i)}}(z)| = \frac{1}{n} |K'_h(x - x_k)| \leq \frac{C}{hn},$$

leading to

$$|\nabla_{D_{(-i)}} \hat{g}_{D_{(-i)}}(z)| \leq \frac{C}{h\sqrt{n}}.$$
That is, we have \( \delta_1(n, z) = C/[h\sqrt{n}] \) and \( \delta_2(n, z) = 0 \). Furthermore, now \( \mathbb{E}[f_i(Z_i)] = \mathbb{E}[f_D(Z)] \), so \( \delta_3(n) = 0 \). Hence, we may apply Theorem 3.6 with \( \delta_1(n, z) = C/[h\sqrt{n}] \).

### 4.4. Linear regression.

An example which requires Theorem 3.9 is simple linear regression. Consider the model \( y = \alpha + \beta x + \varepsilon \), where \( x \sim N(0, 1) \) is a random variable and \( \varepsilon \sim N(0, 1) \). Then the least squares estimators for parameters \( \alpha \) and \( \beta \) are given by

\[
\hat{\alpha} = \overline{y} - \hat{\beta}\overline{x},
\hat{\beta} = \frac{\sum_{i=1}^n (x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^n (x_i - \overline{x})^2}.
\]

Consider also the \( L^1 \)-loss, i.e. \( L(x, y) = |x - y| \).

We will now show how to apply Theorem 3.9 to this problem and thus showing that there exists constants \( C, c \) such that for a fixed \( \varepsilon \) we get

\[
P\left(L_{\text{LOO}} - \bar{L}_{\text{LOO}} > \varepsilon \right) \leq Cn\varepsilon^{-cn}. \tag{4.1}
\]

For this we need to estimate the gradient of the different terms involved in the loss, find a good choice of the set \( K \), and finally estimate \( \delta_1, \delta_2, \delta_3 \). We begin by computing the gradient of the correlation estimator \( \hat{\beta} \).

Now finally, let \( X = \{(x_i - \overline{x})\}_i \) and \( Y = \{(y_i - \overline{y})\}_i \), then \( \hat{\beta} = \frac{XY}{|X|^2} \). Now,

\[
\nabla_X\hat{\beta} = \nabla_X \frac{X \cdot Y}{|X|^2} = \frac{Y}{|X|^2} - \frac{X \cdot Y}{|X|^4},
\]

and hence

\[
\|\nabla_X\hat{\beta}\| \leq 2 \frac{|Y|}{|X|^2}, \quad \|\nabla_Y\hat{\beta}\| \leq \frac{1}{|X|}, \quad \|\nabla_D\hat{\beta}\| = (\nabla_D X \cdot \nabla_X \hat{\beta}, \nabla_D Y \cdot \nabla_Y \hat{\beta}).
\]

Consequently, the derivative of the predictor \( \hat{\alpha} + \hat{\beta}x \) is thus

\[
|\nabla_D(\hat{\alpha} + \hat{\beta}x)| \leq |\nabla_D \hat{\alpha}| + |\nabla_D \hat{\beta}| |x| \leq \frac{1}{\sqrt{n}} + \frac{|X|}{|X|^2} \left( \frac{|X|}{|X|^2} + |x| \right).
\]

The issue with the above derivative is that it is unbounded, namely when \( |X| \) gets arbitrarily small or \( |Y| \) arbitrarily large. On the other hand, conditioned on the event that \( |X|^2 \) and \( |Y|^2 \) are close to their expectations, we obtain that the natural scaling of all terms involved is \( 1/\sqrt{n} \). Consider now the permutation symmetric set \( K_{\varepsilon} \) defined as

\[
K_{\varepsilon} := \left\{ \frac{1}{n} |X|^2 - 1 < \varepsilon, \frac{1}{n} |Y|^2 - 1 < \varepsilon \right\}.
\]

Then on the set \( K_{\varepsilon} \) we have

\[
|\nabla_D(\hat{\alpha} + \hat{\beta}x)| \leq \frac{(1 + \varepsilon)}{(1 - \varepsilon)^{\sqrt{n}}\varepsilon} ((1 + \varepsilon) + |x|).
\]

Also, from Theorem 6.1 we get

\[
P(D \in K_{\varepsilon}) \geq 1 - 4e^{-\varepsilon n/|C|}.
\]

We now wish to apply Theorem 3.9 and as such, all that remains is to verify the slice-wise size of \( K_{\varepsilon} \). Namely, we need to estimate

\[
P(\mu^{\Phi(n^{-1})}(K_{\varepsilon,1}(Z_1)) < 2^{-1} | D \in K_{\varepsilon})
\]
i.e. if $D'$ is an independent copy of $D_{n-1}$ with $Z = (X, Y)$, then
\[ \mathbb{P}(\mathbb{P}(D' \in K_{x_1}(Z_1) \mid Z_1) < 1/2 \mid D \in K_x). \]

We will now only deal with, for $z = (x, y)$, the part
\[ K_x(z) := \left\{ X' \in \mathbb{R}^{n-1} : X = (x, X'), \left| \frac{1}{n} X - 1 \right| < \varepsilon \right\}, \]
as the $Y$ part can be treated similarly. Now, the condition that $X' \in K_x(z)$
can be written as
\[ \frac{n}{n-1} (1 - \varepsilon - x^2/n) \leq \frac{1}{n-1} \sum_{i=1}^{n-1} (X_i')^2 \leq \frac{n}{n-1} (1 + \varepsilon - x^2/n). \]
That is,
\[ \mathbb{P}(X' \in K_x(z)) = 1 - \mathbb{P}(X' \notin K_x(z)) \]
and, by Theorem 6.1,
\[ \mathbb{P}(X' \notin K_x(z)) = \mathbb{P} \left( \frac{1}{n-1} \sum_{i=1}^{n-1} x_i^2 - 1 > \frac{1}{n-1} \left( 1 + n\varepsilon - x^2 \right) \right) \]
\[ + \mathbb{P} \left( \frac{1}{n-1} \sum_{i=1}^{n-1} x_i^2 - 1 < -\frac{1}{n-1} \left( n\varepsilon + x^2 - 1 \right) \right) \]
\[ \leq e^{-\left( n\varepsilon + x^2 - 1 \right)} + e^{-\left( 1 + n\varepsilon - x^2 \right)} \leq 4e^{-\left( n\varepsilon - x^2 \right)}. \]

Finally, we estimate
\[ \mathbb{P}(\mathbb{P}(X' \in K_x(Z_1) \mid Z_1) < 1/2 \mid D \in K_x) \]
\[ = 1 - \mathbb{P}(\mathbb{P}(X' \notin K_x(Z_1) \mid Z_1) < 1/2 \mid D \in K_x) \]
\[ \leq 1 - \mathbb{P}(4e^{-\left( n\varepsilon - X_1^2 \right)} < 1/2 \mid D \in K_x) \]
and
\[ \mathbb{P}(4e^{-\left( n\varepsilon - X_1^2 \right)} \geq 1/2 \mid D \in K_x) = \mathbb{P}(e^{X_1^2} \geq 8^{-1}e^{n\varepsilon} \mid D \in K_x) \]
\[ = \mathbb{P}(X_1^2 \geq \log(8^{-1} + n\varepsilon) \mid D \in K_x) \]
\[ \leq 2 \frac{\mathbb{P}(X_1 \geq \sqrt{\log(8^{-1} + n\varepsilon)} \mid D \in K_x)}{\mathbb{P}(D \in K_x)} \]
\[ \leq 2 e^{-\left( \log(8^{-1} + n\varepsilon) \right)} \frac{1}{1 - 4e^{-n/C}}. \]

Hence, we may apply Theorem 3.9 using the estimates above which leads to (4.1).

4.5. Truncation. Many standard estimators are almost stable. It seems that they still concentrate but are not covered by our result. We here provide a simple method to stabilize them via truncation allowing us to apply our results. Consider the truncator $g_b(x) = \max(\min(x, b), -b)$ and consider $D_b = \{(g_b(X_1), g_b(Y_1)), \ldots, (g_b(X_n), g_b(Y_n))\}$. Now, if
\[ |\nabla f(D)| \leq C \frac{1}{n^{(q+1)/2}} |D|^q, \]
and hence, for a fixed 

and a tuning parameter

If now $K$ is the Gaussian kernel, we get

where $\delta > 0$ is a stabilization parameter. Consider also the $L^1$-loss, i.e. $L(x, y) = |x - y|$. We get as in Section 4.4 that for $\delta < 1$, it holds

which, as in Section 4.4, leads to

This allows to apply Theorem 3.6.

4.7. Stabilized kernel regression. Consider a stabilized form of kernel regression. For simplicity, let $g(X) = E[Y | X]$ be the regression function. Let $T_D$ be an estimate of $g(X)$ produced as the kernel regression estimate on the dataset $D$, and consider the $L^1$ prediction loss. That is, let $L(T_D(x), y) = |T_D(x) - y|$ and define the stabilized kernel regression estimator as

with a tuning parameter $h$. Computing first the $x_i$ derivative gives

If now $K$ is the Gaussian kernel, we get

and hence, for a fixed $h$, we get

\[
\sum_{j=1}^n K_h(x - x_j) + n\delta)
\]

\[
\sum_{j=1}^n K_h(x - x_j) + n\delta)
\]

\[
\sum_{j=1}^n K_h(x - x_j) + n\delta)
\]

\[
\sum_{j=1}^n K_h(x - x_j) + n\delta)
\]
Since now $|T_D(x)| \leq C|D|/\sqrt{n}$, we obtain
\[
\left| \frac{1}{n} (-y_i + T_D(x)) \right| \leq \frac{C|y_i| + C|D|}{n\sqrt{n}}.
\]
Similarly, derivatives in $y_i$ directions satisfy
\[
|\nabla y_i T_D(x)| = \left| \frac{K_h(x - x_i)}{\sum_{j=1}^n K_h(x - x_j) + n\delta} \right| \leq \frac{C(h, \delta)}{n}.
\]
From this it follows that, using also $\sum_{j=1}^n |y_j| \leq \sqrt{n} |D|$, we have
\[
|\nabla D T_D(x)|^2 \leq C(h, \delta) \sum_{j=1}^n \left( \left| \frac{|y_j|}{n} + \frac{|D|}{n\sqrt{n}} \right|^2 + \frac{1}{n^2} \right)
\]
\[
= C \sum_{j=1}^n \left[ \frac{|y_j|^2}{n^2} + \frac{2|y_j||D|}{n^2\sqrt{n}} + \frac{|D|^2}{n^2} + \frac{1}{n^2} \right]
\]
\[
\leq \frac{C}{n} + \frac{C|D|^2}{n^2}.
\]
Hence, we observe that, for all $x$,
\[
|\nabla D T_D(x)| \leq \frac{C}{\sqrt{n}} + \frac{C|D|}{n}.
\]
As such, we may set $\delta_1(n, z) = \frac{C}{\sqrt{n}}$ and $\delta_2(n, z) = \frac{C}{n}$. For $\delta_3$ we compute for $f_i, f_D$ defined as usual,
\[
\mathbb{E}[f_i(Z_i)] - \mathbb{E}[f_D(Z)]
\]
\[
= \mathbb{E}\left[ \left| \frac{\sum_{j=1}^n K_h(X - x_j)}{\sum_{j=1}^n K_h(X - x_j) + n\delta} - Y \right| - \left| \frac{\sum_{j=1}^n K_h(X - x_j) y_j}{\sum_{j=1}^n K_h(X - x_j) + n\delta} - Y \right| \right| Z \right]
\]
\[
\leq \frac{C}{\sqrt{n}},
\]
where in the last line we have used Lipschitz continuity of $T_D(x)$ in the $y_i$ direction. This allows us to set $\delta_3(n) = \frac{C}{\sqrt{n}}$ and hence we may again apply Theorem 3.6.

5. Numerical experiments

The aim of this section is to provide numerical evidence for the rate at which the level sets of the error $L_{\text{LOO}} - \hat{L}_{\text{LOO}}$ tend to zero w.r.t. $n$. Namely, for a given $\epsilon > 0$ we are interested in
\[
\mathbb{P}(|L_{\text{LOO}} - \hat{L}_{\text{LOO}}| > \epsilon).
\]
Furthermore, we provide simulations of the rate of the standard deviation, since if the probability above is bounded by $C e^{-c n \epsilon^2}$ for some constants $c, C$ and all $\epsilon > 0$, then the standard deviation would converge to 0 with rate $1/\sqrt{n}$, which is what one would expect. However, the bounds appearing in Theorems 3.2, 3.6 and 3.9 all holds for large enough $\epsilon$, and as such is purely of large deviation type. Note also that, the probability above should be
linear in $n$ in the log-scale, provided that the upper bounds are relatively sharp.

In the following we have provided experimental data on the case of linear regression, kernel density estimation and that of the stabilized kernel regression.

5.1. Kernel density estimation. In this context, referring back to Section 4.3, our goal is to estimate the density $g$ by using the dataset $D$. In order to evaluate the risk we need to compute

$$L_{LOO} := E[\hat{g}_D(Z) | D],$$

where $Z$ is an independent copy of $Z_1 \in D$. The estimator of this is the leave-one-out estimator, i.e.

$$\hat{L}_{LOO} := \frac{1}{n} \sum_{i=1}^{n} f_i(Z_i),$$

where $f_i(z) = \hat{g}_{D(-i)}(z)$. In Section 4.3 we verified that $\delta_1(n, Z) \approx \frac{1}{\sqrt{n}}$, which then gives us exponential concentration via Theorem 3.6. For numerical illustration, let $X \sim \text{Uniform}(0, 1)$ and consider the random variable $Y = \sin(10X)$. Now our goal is to estimate the density of $Y$, which we do by using the Gaussian kernel with a bandwidth 1/10.

In Fig. 1 there are two plots. The first plot shows the value of $\hat{L}_{LOO} - L_{LOO}$ for different choices of $n$ (the x-axis), and we can see that it indicates the rate $1/\sqrt{n}$ of the standard deviation. The second plot shows the empirical value of $\mathbb{P}(|\hat{L}_{LOO} - L_{LOO}| > .02)$ on the log-scale with respect to $n$. The second plot shows linear relationship as it should, by Theorem 3.6.

5.2. Linear regression. In this particular example we chose $X \sim N(0, 1)$ and $Y \mid X \sim N(5X, 1)$. Our fitted line on a dataset $D$ is $T_D$, and our loss is $L(x, y) = |x - y|$. In this case we measure the error

$$\hat{L}_{LOO} := \frac{1}{n} \sum_{i=1}^{n} L(T_{D(-i)}(X_i), Y_i),$$

where

$$L_{LOO} := E[L(T_D(X), Y) | D]$$

and $(X, Y)$ is an independent copy of $Z_1 \in D$. Even though we have to resort to conditioning in Section 4.4 and only obtain a weaker concentration through Theorem 3.9, Fig. 2 shows an exponential type concentration. Furthermore, the second image in Fig. 2 shows the empirical value
Figure 2. Leave one out cross validation error using linear regression.

Figure 3. Leave one out cross validation error using stabilized kernel regression.

5.3. Stabilized kernel regression. In this particular example we chose $X \sim \mathcal{N}(0,1)$ and $Y \mid X \sim \mathcal{N}(\sin(10X),1)$. Our fitted curve on a dataset $D$ is $T_D$, and our loss is $L(x,y) = |x-y|$.

We chose the bandwidth $h = 1/100$, the stabilization parameter $\delta = 0.01$, keeping otherwise the setting as in the previous subsection. The result can be found in Fig. 3. Again, we observe strong concentration as guaranteed by Theorem 3.6.

6. Proofs

**Theorem 6.1.** Let $X_1, \ldots, X_n \overset{i.i.d.}{\sim} \mu$ be $\mathbb{R}$-valued random variables satisfying

$$
\mathbb{E}[e^{s(X_i - \mathbb{E}[X_i])}] \leq e^{\frac{s^2}{2}}, \quad s \leq \frac{1}{\lambda}.
$$

Then for any $\varepsilon > 0$ we get, for $\overline{X}_n = \frac{1}{n} \sum_{i=1}^{n} X_i$, that

$$
\mathbb{P}(\overline{X}_n - \mathbb{E}[\overline{X}_n] \geq \varepsilon) \leq e^{-\frac{2n}{\lambda^2}} + e^{-\frac{2n}{16}}.
$$

The following lemma is the key estimate for our proofs.

**Lemma 6.2.** Let $F : \mathbb{R}^{n \times m} \to \mathbb{R}$, and let $(X_1, \ldots, X_n) \in \mathbb{R}^{n \times m}$ be an i.i.d sequence of random variables with distribution $\mu$, with $\sigma^2(\mu) < \infty$. Assume further that the following structural assumption

$$
|\nabla F| \leq \delta_1(n) + \delta_2(n) |X|
$$

holds. Then for all $\lambda < \frac{1}{4\sigma^2(\mu)}\delta_2^{-1}(n)$ we have

$$
\mathbb{E}(e^{\lambda(F - \mathbb{E}[F])}) \leq e^{2\sigma^2(\mu)\lambda^2[\delta_1^2(n) + \delta_2^2(n)n(\mathbb{E}[|X|^2] + 16\sigma^2(\mu))]}.
$$
Remark 6.3. In the case of a Lipschitz gradient we have $\delta_2(n) \equiv 0$, and the above is valid for all $\lambda$.

Remark 6.4. Note that we require $\delta_2(n) < \frac{1}{\sqrt{n}}$ or there will be no concentration. This highlights the fact that we actually need $\lim_{n \to \infty} F = c$ and $\lim_{n \to \infty} \|\nabla F\| \to 0$ for our estimators $F$. Indeed, if all $X_i$'s have variance 1 and mean 0, then if $\delta_2(n) = O(n^{-1/2})$, we get

$$E[|\nabla F|^2] \leq O(n^{-1}) E[|X|^2] = O(1)$$

meaning that changing one observation point into another has an impact regardless of the amount of observations.

Proof of Lemma 6.2. Since $\sigma^2(\mu) < \infty$, we get for any smooth $f$ that

$$\text{Ent}(e^f) \leq \sigma^2(\mu) E[|\nabla f|^2 e^f].$$

Now defining $\Gamma(f) = 2\sigma^2(\mu)|\nabla f|^2$ we have by [10] or [30, Theorem 2.7] that

$$E(e^{f - \mathbb{E}[f]}) \leq E[e^{\Gamma(f)}].$$

Fix $\lambda \leq \lambda_0$ where $\lambda_0$ is to be chosen. Then applying (6.1) to $f = F$ and using independence we observe

$$E[e^{\Gamma(\lambda F)}] = E[e^{\lambda^2 \Gamma(F)}] \leq E[e^{2\sigma^2(\mu)\lambda^2\delta_2^2(n) + \delta_2^2(n) \sum_{i=1}^n |X_i|^2}]$$

$$\leq e^{2\sigma^2(\mu)\lambda^2\delta_2^2(n) \sum_{i=1}^n E[|\nabla F|^2|X_i|^2]}$$

(6.2)

where the right-hand side is finite for $2\sigma^2(\mu)\lambda^2\delta_2^2(n) \leq \frac{1}{2\sigma^2(\mu)}$ (see [30, Proposition 1.2]). It is well known that if $\sigma^2(\mu) < \infty$, then for $s_0 = \frac{1}{8\sigma^2(\mu)}$ it holds that

$$E[e^{\lambda(X_1^2 - \mathbb{E}[X_1^2])}] \leq e^{32\sigma^2(\mu)^2s^2}, s \leq s_0.$$  

(6.3)

From (6.1)–(6.3) we finally have

$$E[e^{\lambda(\mathbb{E}[f] - f)]} \leq e^{2\sigma^2(\mu)\lambda^2\delta_2^2(n)} e^{32\sigma^2(\mu)^2(2\sigma^2(\mu)\lambda^2\delta_2^2(n)^2n + 2\sigma^2(\mu)\lambda^2\delta_2^2(n)E[|X_i|^2])^n}$$

$$\leq e^{2\sigma^2(\mu)\lambda^2\delta_2^2(n)(E[|X_i|^2] + 16\sigma^2(\mu))}$$

provided that $2\sigma^2(\mu)\lambda^2\delta_2^2(n) \leq \frac{1}{8\sigma^2(\mu)}$, or equivalently setting $\lambda_0 = C_0\delta^{-1}(n)$, for $C_0 = \sqrt{\frac{1}{16\sigma^4(\mu)}}$. Putting it all together gives the lemma. \hfill $\square$

Corollary 6.5. Suppose that Assumptions of Lemma 6.2 prevail. Then

$$P(F - \mathbb{E}[F] > t) \leq e^{-\frac{t^2}{8\sigma^2(\mu)\delta_2^2(n)}} e^{-\frac{t^2}{8\sigma^2(\mu)\delta_2^2(n)(E[|X_i|^2] + 16\sigma^2(\mu))}}$$

Proof. By applying Lemma 6.2 and using Markov’s inequality we get for $\lambda < \frac{1}{8\sigma^2(\mu)}\delta_2^{-1}(n)$ that

$$P(F - \mathbb{E}[F] > t) \leq e^{-\lambda t} e^{2\sigma^2(\mu)\lambda^2\delta_2^2(n)(E[|X_i|^2] + 16\sigma^2(\mu))}.$$  

(6.4)
The minimizer is given by 
\[ \lambda^* = \frac{t}{4\sigma^2(\mu) \big[ 2\delta_2(n) + \delta_2^2(n) n \mathbb{E}[\|X_i\|^2] + 16\sigma^2(\mu) \big] } \]
which by plugging into (6.4) yields, provided that 
\[ \lambda^* < \frac{1}{4\sigma^2(\mu) \delta_2^{-1}(n)} \],
\[ \mathbb{P}(F - \mathbb{E}[F] > t) \leq e^{-\frac{t^2}{8\sigma^2(\mu) \delta_2^{-1}(n)}}. \]
On the other hand, in the case that 
\[ \lambda^* \geq \frac{1}{4\sigma^2(\mu) \delta_2^{-1}(n)} \], we choose 
\[ \hat{\lambda} = \frac{1}{4\sigma^2(\mu) \delta_2^{-1}(n)} \] from which plugging into (6.4) gives
\[ \mathbb{P}(F - \mathbb{E}[F] > t) \leq e^{\frac{t^2}{8\sigma^2(\mu) \delta_2^{-1}(n)}} e^{-\frac{t^2}{8\sigma^2(\mu) \delta_2^{-1}(n)}}. \]
Combining both estimates completes the proof. \( \square \)

6.1. Proof of Theorem 3.6. Recall that we defined 
\[ f_D(z) = L(T_D(x), y), \]
for \( z = (x, y) \), and 
\[ f_i(z) = L(T_{D_i}(x), y). \]
We begin by decomposing the error into the following components
\[ L_{LOO} - \hat{L}_{LOO} = \frac{1}{n} \sum_{i=1}^{n} (\mathbb{E}[f_i(Z_i) | Z_i] - f_i(Z_i)) \]
\[ + \frac{1}{n} \sum_{i=1}^{n} (\mathbb{E}[f_i(Z_i)] - \mathbb{E}[f_i(Z_i) | Z_i]) \]
\[ + \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_D(Z) | D] - \mathbb{E}[f_i(Z_i)] \right) \]
\[ = I_1 + I_2 + I_3. \]
By using the union bound,
\[ \mathbb{P}(I_1 + I_2 + I_3 > \varepsilon) \leq \mathbb{P}(I_1 > \varepsilon/3) + \mathbb{P}(I_2 > \varepsilon/3) + \mathbb{P}(I_3 > \varepsilon/3) \]
it suffices to consider the terms \( I_1, I_2, \) and \( I_3 \) separately. Consider the term \( I_1 \) first. We have
\[ \mathbb{P}(I_1 > \varepsilon/3) \leq \sum_{i=1}^{n} \mathbb{P}(\mathbb{E}[f_i(Z_i) | Z_i] - f_i(Z_i) > \varepsilon/3). \]
Now for each fixed \( z \), we may apply Corollary 6.5 together with Assumption 3.1 to obtain
\[ \mathbb{P}(\mathbb{E}[f_i(z)] - f_i(z) > \varepsilon/3) \leq \theta_1(n, \varepsilon/3, z), \]
where \( \theta_1 \) is from (3.3). Hence, by using the towering property for conditional expectation, it follows that
\[ \mathbb{P}(\mathbb{E}[f_i(Z_i) | Z_i] - f_i(Z_i) > \varepsilon/3) \leq \mathbb{E}\theta_1(n, \varepsilon/3, Z), \]
and hence
\[ \mathbb{P}(I_1 > \varepsilon/3) \leq n\mathbb{E}\theta_1(n, \varepsilon/3, Z). \]
Consider next the term \( I_2 \) and denote \( f(z) = \mathbb{E}[f_i(z)] \). We have
\[ \mathbb{P}(I_2 > \varepsilon/3) = \mathbb{P} \left( \mathbb{E}[f(Z)] - \frac{1}{n} \sum_{i=1}^{n} f(Z_i) > \varepsilon/3 \right). \]
Let $\mu$ be the distribution of $Z$. By assumption $\sigma^2(\mu) < \infty$, and it thus follows from Lemma 2.5 and the linear growth of $f(Z)$, that
\[
P(I_2 > \varepsilon/3) \leq e^{-\frac{\varepsilon^2}{C}}.
\]
Similarly, if $f$ has quadratic growth, we use Theorem 6.1 to get
\[
P(I_2 > \varepsilon/3) \leq \max\left\{ e^{-\frac{\varepsilon^2}{C}}, e^{-\frac{\varepsilon^4}{C}} \right\}.
\]
Combining both estimates yields
\[
P(I_2 > \varepsilon/3) \leq \theta_2(n).
\]
It remains to consider the term $I_3$. We decompose
\[
P(I_3 \geq \varepsilon/3) = P\left( \mathbb{E}[f_D(Z) \mid D] - \mathbb{E}[f(Z)] > \varepsilon/3 \right)
\]
\[
= P\left( \mathbb{E}[f_D(Z)] - \mathbb{E}[f(Z)] + \mathbb{E}[f_D(Z) \mid D] - \mathbb{E}[f_D(Z) \mid Z] > \varepsilon/3 \right).
\]
Now
\[
|\mathbb{E}[f_D(Z)] - \mathbb{E}[f_D'(Z)]| = |\mathbb{E}[f_D(Z) - f_D'(Z)]| \leq \mathbb{E}[|f_D(Z) - f_D'(Z)|] \leq \mathbb{E}[\delta_3(n, Z)]|D - D'|^2.
\]
Hence, again by Corollary 6.5, we get
\[
P(I_3 \geq \varepsilon/3) \leq \theta_3(n, \varepsilon/3 - \delta_3(n))
\]
provided that $\varepsilon/3 > (\mathbb{E}[f_D(Z)] - \mathbb{E}[f(Z)])$, where $|\mathbb{E}[f_D(Z)] - \mathbb{E}[f(Z)]| \leq \delta_3(n)$. This handles the term $I_3$ as well, and collecting all bounds together proves the claim.

### 6.2. Proof of Theorem 3.2.

The claim follows directly from Theorem 3.6 by plugging in correct forms of $\theta_1$, $\theta_2$, and $\theta_3$ in the linear growth case and with $\delta_2(n, z) \equiv 0$.

### 6.3. Proof of Theorem 3.9.

**Step 1: Conditioning.** Consider
\[
P(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon) = P(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon, D \in K)
\]
\[
+ P(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon, D \notin K). \quad (6.5)
\]
The last term on the right we simply bound by $P(D \notin K)$. We define, with $D'$ as an independent copy of $D$,
\[
L_{\text{LOO}, K} = \mathbb{E}[f_D(Z_1') \mid D, D' \in K].
\]
We have
\[
P(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon, D \in K)
\]
\[
= P(L_{\text{LOO}} - \hat{L}_{\text{LOO}} > \varepsilon \mid D \in K) P(D \in K)
\]
\[
\leq P(L_{\text{LOO}, K} - \hat{L}_{\text{LOO}} + L_{\text{LOO}} - L_{\text{LOO}, K} > \varepsilon \mid D \in K). \quad (6.6)
\]
Now, using again the union bound, we get
\[
P(L_{\text{LOO}, K} - \hat{L}_{\text{LOO}} + L_{\text{LOO}} - L_{\text{LOO}, K} > \varepsilon \mid D \in K)
\]
\[
\leq P(L_{\text{LOO}, K} - \hat{L}_{\text{LOO}} > \varepsilon/2 \mid D \in K)
\]
\[
+ P(L_{\text{LOO}} - L_{\text{LOO}, K} > \varepsilon/2 \mid D \in K). \quad (6.7)
\]
Step 2: Splitting the error into $I_1, I_2, I_3$. For the first term on the right-hand side of (6.7) we get

$$L_{\text{LOO}, K} - \hat{L}_{\text{LOO}} = \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_i(Z_i) \mid Z_i, D \in K] - f_i(Z_i) \right)$$

$$+ \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_i(Z_i) \mid D \in K] - \mathbb{E}[f_i(Z_i) \mid Z_i, D \in K] \right)$$

$$+ \frac{1}{n} \sum_{i=1}^{n} \left( \mathbb{E}[f_{D}(Z_i') \mid D, D' \in K] - \mathbb{E}[f_i(Z_i) \mid D \in K] \right)$$

$$= I_1 + I_2 + I_3.$$

Step 2a: Dealing with $I_1$. This is the trickiest term in the conditioned case. For a fixed $z$ note that $f_i$ is Lipschitz with respect to $D_{(-i)}$ by Assumption 3.1, with Lipschitz constant $\delta_{1,K}(n, Z)$. We let $\rho^n$ be the density of $\mu^n$ and let

$$\rho_K = \frac{\rho^n}{\int_K \rho^n dD}$$

be the conditional density and denote the corresponding measure with $\mu_K$. Furthermore, denote the slice $K_i = K \cap \{Z_i = z\}$, and write the partial density as

$$\rho_{K_i}(z) = \frac{\rho_{n-1}^{n-1}}{\int_{K_i(z)} \rho_{n-1}^{n-1} dD_{(-i)}}.$$

For the corresponding measure, we use the notation $d\mu_{K_i}$. Since $C_i(z) = \sigma_{\text{SG}}^2(\mu_{K_i}(z)) < \infty$ by (3.6), we get

$$\mathbb{P}(\mathbb{E}[f_i(z) \mid D_{(-i)} \in K_i(z)] - f_i(z) > \varepsilon/6 \mid D \in K, Z_i = z) \leq e^{-\frac{\varepsilon^2}{8C_i(z)\sigma^2_{\text{SG}}(n, z)}}.$$

Hence, if we let

$$\theta_{1,K}(n, \varepsilon) := \exp \left( -\frac{\varepsilon^2}{8C_i(Z_i)\sigma^2_{\text{SG}}(n, Z_i)} \right), \quad \mathbb{E}_K \theta_{1,K} := \mathbb{E}[\theta_{1,K} \mid D \in K],$$

we obtain

$$\mathbb{P}(\mathbb{E}[f_i(Z_i) \mid D \in K, Z_i] - f_i(Z_i) > \varepsilon/6 \mid D \in K] \leq \mathbb{E}_K \theta_{1,K}(n, \varepsilon/6). \quad (6.8)$$

Step 2b: estimating $I_2, I_3$. To deal with $I_2$, we recall that since $K$ is permutation symmetric, $\mathbb{E}[f_i(z) \mid D_{(-i)} \in K_i(z)]$ does not depend on $i$, and we can set $f(z) = \mathbb{E}[f_i(z) \mid D_{(-i)} \in K_i(z)]$. Let $D'$ be an independent copy of $D$, and consider

$$\mathbb{P}(I_2 > \varepsilon/6 \mid D \in K) = \mathbb{P} \left( \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} f(Z_i') \mid D' \in K \right] - \frac{1}{n} \sum_{i=1}^{n} f(Z_i) > \varepsilon/6 \mid D \in K \right).$$

By the linear or quadratic growth assumption we can bound the above by $\theta_{2,n}$, but with $C = \sigma_{\text{SG}}^2(\mu_K)$, i.e.

$$\mathbb{P}(I_2 > \varepsilon/6 \mid D \in K) \leq \theta_{2,K}(n, \varepsilon/6). \quad (6.9)$$

For the term $I_3$, i.e.

$$\mathbb{P}(I_3 > \varepsilon/6 \mid D \in K)$$
Then and we write \( (6.12) \) given by

\[
\text{In order to estimate the last term in Step 3: The cost of restriction.}
\]

Using now that \( g \) satisfies (cf. Proof of Theorem 3.6) we argue as in the proof of Theorem 3.6 and get, using also the fact that for \( \hat{\theta}^2 = \sigma^2_{SG} (\mu_K ) ( \mathbb{E} [ \delta_{1,K} (n, Z_1) \mid D \in K] )^2 \) we have the estimate

\[
\mathbb{P} ( I_3 > \varepsilon / 6 \mid D \in K ) \leq e^{- \frac{(\varepsilon / 6 - \delta_3 (n))^2}{\sigma^2_{SG}}} =: \theta_{3,K} (n, \varepsilon / 6 - \delta_3 (n)),
\]

where

\[
\mathbb{E} [ f_D (Z_i') \mid D \in K, D' \in K] - \mathbb{E} [ f (Z_i) \mid D \in K] \leq \delta_3 (n).
\]

Now assembling (6.5)–(6.11) leads to

\[
\mathbb{P} \left( L_{LOO} - \hat{L}_{LOO} > \varepsilon \right) \leq e^{K_{\theta_{1,K}} (n, \varepsilon / 6) + \theta_{2,K} (n, \varepsilon / 6) + \theta_{3,K} (n, \varepsilon / 6 - \delta_3 (n))} + \mathbb{P} ( D \notin K ) + \mathbb{P} ( L_{LOO} - L_{LOO,K} > \varepsilon / 2 \mid D \in K ).
\]

**Step 3: The cost of restriction.** In order to estimate the last term in (6.12) given by

\[
\mathbb{P} ( L_{LOO} - L_{LOO,K} > \varepsilon / 2 \mid D \in K ),
\]

we write

\[
g_K (D) = L_{LOO} - L_{LOO,K} = \mathbb{E} [ f_D (Z) \mid D] - \mathbb{E} [ f_D (Z_i') \mid D, D' \in K]
\]

and

\[
\gamma (K) = \mathbb{E} [ g_K (D) \mid D \in K].
\]

Then

\[
\mathbb{P} ( L_{LOO} - L_{LOO,K} > \varepsilon / 2 \mid D \in K ) = \mathbb{P} \left( g_K (D) - \gamma (K) > \varepsilon / 2 - \gamma (K) \mid D \in K \right).
\]

Using now that \( g_K (D) \), conditioned on \( D \in K \), satisfies (cf. Proof of Theorem 3.6)

\[
\| \nabla_D g_K (D) \| \leq \mathbb{E} [ \delta_{1,K} (n, Z_1) \mid D \in K],
\]

we may proceed as in (6.10) to get

\[
\mathbb{P} \left( g_K (D) - \mathbb{E} [ g_K (D) ] > \varepsilon / 2 - \gamma (K) \mid D \in K \right) \leq \theta_{3,K} (n, \varepsilon / 6 - \gamma (K)).
\]

Hence, we obtain from (6.12) and (6.13) that

\[
\mathbb{P} \left( L_{LOO} - \hat{L}_{LOO} > \varepsilon \right) \leq \mathbb{E} [ \theta_{1,K} (n, \varepsilon / 6) + \theta_{2,K} (n, \varepsilon / 6) + \theta_{3,K} (n, \varepsilon / 6 - \delta_3 (n)) + \theta_{3,K} (n, \varepsilon / 6 - \gamma (K)) + \mathbb{P} ( D \notin K ).
\]
**Step 4: Estimation of** $E_{K_1,K} \theta_{1,K}$. Let $K_i(z) = K \cap \{ Z_i = z \}$, and note that due to the permutation symmetry we have that $K_i(z) = K_j(z)$, for all $i, j$. As such, it suffices to consider $K_1$. From (3.6) we have that
\[
\sigma^2_{SG}(\mu_{K_1}) \leq c \log \left( \frac{e}{\mu^{\otimes(n-1)}(K_1)} \right) \sigma^2(\mu). \tag{6.15}
\]
We estimate
\[
E_{K_1,K} \theta_{1,K} \leq E[\theta_{1,K} \chi_{\mu^{\otimes(n-1)}(K_1) > 2^{-1}}(Z_1) \mid D \in K] + \mathbb{P}(\mu^{\otimes(n-1)}(K_1(Z_1)) < 2^{-1} \mid D \in K), \tag{6.16}
\]
where in the first term on the right we can use (6.15) and obtain that $\theta_{1,K}$ can be replaced with
\[
\hat{\theta}_{1,K} := \exp \left( -\frac{\varepsilon^2}{8C\delta_1^2(n,Z_1)} \right),
\]
where $C = 2c\sigma^2(\mu)$. This leads to
\[
E_{K_1,K} \theta_{1,K} \leq E[\hat{\theta}_{1,K} \mid D \in K] + \mathbb{P}(\mu^{\otimes(n-1)}(K_1) < 2^{-1} \mid D \in K), \tag{6.17}
\]
and hence assembling (6.14) and (6.17) completes the whole proof.

**7. Conclusions**

In this article we have provided concentration inequalities for LOO cross validation under a general framework. Our approach is applicable for data arising from distribution that satisfies the logarithmic Sobolev inequality, providing us a relatively rich class of distributions. While our approach *a priori* is not suitable for bounded data, we stress that in the case of bounded random variables, one can apply well-known concentration inequalities for bounded random variables, but one now has to measure the gradient w.r.t. the $l^\infty$ norm on $\mathbb{R}^d$.

We have also illustrated the applicability of our method by considering several interesting examples. Obviously, our approach could be used in other practical estimation schemes as well. Finally, while we have restricted our study to the case of LOO cross validation only, one could use similar methodology to study concentration for other cross validation procedures as well. For example, leave-$k$-out cross validation could be covered with suitable changes in our procedure.

We also note that our approach could be used for model selection under our stability assumptions. The quantity of interest in this case is not the cross validated value of the losses $\hat{L}^1_{LOO}$ and $\hat{L}^2_{LOO}$ for two different estimators, but rather the difference $\hat{L}^1_{LOO} - \hat{L}^2_{LOO}$ of errors (or sign if one is solely interested in which performs better) when comparing two different models. It can be noted that often one expects the difference to concentrate better compared to each individual terms, see for instance [3, 4]. Specifically, we note that we can apply our Theorems 3.2, 3.6 and 3.9 directly to the difference. If the difference has better stability in terms of Definition 2.6, we get...
better concentration around the mean of the difference. Concentration further implies that one can base the model selection directly on the quantity \( \hat{L}_{1, \text{LOO}} - \hat{L}_{2, \text{LOO}} \).

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