In this paper, we derive a new dimension-free non-asymptotic upper bound for the quadratic $k$-means excess risk related to the quantization of an i.i.d sample in a separable Hilbert space. We improve the bound of order $O(\frac{k}{\sqrt{n}})$ of Biau, Devroye and Lugosi, recovering the rate $\sqrt{\frac{k}{n}}$ that has already been proved by Fefferman, Mitter, and Narayanan and by Klochkov, Kroshnin and Zhivotovskiy but with worse log factors and constants. More precisely, we bound the mean excess risk of an empirical minimizer by the explicit upper bound $16B^2\log(\frac{n}{k})\sqrt{k\log(k)}/n$, in the bounded case when $P(\|X\| \leq B) = 1$. This is essentially optimal up to logarithmic factors since a lower bound of order $O(\sqrt{\frac{k}{1-4/d}}/n)$ is known in dimension $d$. Our technique of proof is based on the linearization of the $k$-means criterion through a kernel trick and on PAC-Bayesian inequalities. To get a $1/\sqrt{n}$ speed, we introduce a new PAC-Bayesian chaining method replacing the concept of $\delta$-net with the perturbation of the parameter by an infinite dimensional Gaussian process.

In the meantime, we embed the usual $k$-means criterion into a broader family built upon the Kullback divergence and its underlying properties. This results in a new algorithm that we named information $k$-means, well suited to the clustering of bags of words. Based on considerations from information theory, we also introduce a new bounded $k$-means criterion that uses a scale parameter but satisfies a generalization bound that does not require any boundedness or even integrability conditions on the sample. We describe the counterpart of Lloyd’s algorithm and prove generalization bounds for these new $k$-means criteria.

General notation. We will use the following notation throughout this document. On some measurable probability space $\Omega$, we will consider various random variables $X : \Omega \to \mathcal{X}, Y : \Omega \to \mathcal{Y}$, etc. that are nothing but measurable functions. We will also consider several probability measures on $\Omega$, and typically two measures $P$ and $Q \in \mathcal{M}_1^+(\Omega)$, where $P$ describes the usually unknown data distribution and $Q$ describes an estimation of $P$. Then we will use the short notation $P_X$ for the push forward measure $P \circ X^{-1}$, that is the law of $X$. Similarly we will let $Q_X = Q \circ X^{-1}$. In the same way $P_{X,Y} \in \mathcal{M}_1^+(\mathcal{X} \times \mathcal{Y})$ will be the joint distribution of the couple $(X,Y)$ under $P$ and $P_{Y|X}$ the corresponding regular conditional probability measure of $Y$ knowing $X$ when it exists. We will always work under sufficient hypotheses to ensure that the decomposition

$$P_{X,Y} = P_X P_{Y|X}$$

is valid, meaning that for any bounded measurable function $f(X,Y)$

$$\int f \, dP_{X,Y} = \int \left( \int f \, dP_{Y|X} \right) \, dP_X.$$
Moreover, we will use the short notation

$$\int f \, dP_{X,Y} = P_{X,Y}(f),$$

so that the previous formula becomes

$$P_{X,Y}(f) = P_X [P_{Y|X}(f)].$$

We will often use the Kullback Leibler divergence

$$\mathcal{K}(Q, P) = \begin{cases} Q \left[ \log \left( \frac{dQ}{dP} \right) \right] & \text{when } Q \ll P, \\ +\infty & \text{otherwise.} \end{cases}$$

We will always be in this article in a situation where the decomposition

**Lemma 1.**

$$\mathcal{K}(Q_{X,Y}, P_{X,Y}) = \mathcal{K}(Q_X, P_X) + Q_X [\mathcal{K}(Q_{Y|X}, P_{Y|X})]$$

$$= \mathcal{K}(Q_Y, P_Y) + Q_Y [\mathcal{K}(Q_{X|Y}, P_{X|Y})]$$

is valid.

**Proof.** It follows from the decomposition (1). A precise statement and a rigorous proof dealing with measurability issues can be found in [9, Appendix section 1.7 page 50]. \qed

**1. Introduction.** This paper is about the most widely used loss function for vector quantization, the $k$-means criterion. We will be interested in the statistical setting where the problem is to minimize the criterion for a random vector whose distribution is unknown but can be estimated through an i.i.d. random sample. Our main contribution will be to prove a new dimension free non-asymptotic generalization bound with a better $k/n$ dependence, where $k$ is the number of centers used for vector quantization and $n$ is the size of the statistical sample. We will also give an interpretation of the $k$-means criterion in terms of the Kullback-Leibler divergence and use it to embed it in a broader family of criteria with interesting properties. This will provide a specific algorithm for the quantization of conditional probability distributions ranging in an exponential family that can be used in particular to analyse bag of words models. This generalization will also provide a new robust criterion for the quantization of unbounded random vectors.

Our general setting is the following. Given a random variable $X \in H$ ranging in a separable Hilbert space $H$, we are interested in minimizing the risk function

$$\mathcal{R}(c_1, \ldots, c_k) = P_X \left( \min_{j \in [1:k]} \|X - c_j\|^2 \right), \quad (c_1, \ldots, c_k) \in H^k.$$

We will assume that the statistician does not know the distribution $P_X$, but has access instead to a sample $(X_1, \ldots, X_n)$ made of $n$ independent copies of $X$. If $P_X = \frac{1}{n} \sum_{i=1}^n \delta_{X_i}$, is the empirical measure of the sample, the empirical risk, or empirical $k$-means criterion, is defined as

$$\overline{\mathcal{R}}(c) = P_X \left( \min_{j \in [1:k]} \|X - c_j\|^2 \right) = \frac{1}{n} \sum_{i=1}^n \left( \min_{j \in [1:k]} \|X_i - c_j\|^2 \right), \quad c \in H^k.$$
NEW BOUNDS FOR K-MEANS

We will first consider the bounded case. Given a ball \( \mathcal{B} = \{ x \in H : \| x \| \leq B \} \), we will assume that \( \mathbb{P}(X \in \mathcal{B}) = 1 \). We will study the upper deviations of the random variable

\[
\sup_{c \in \mathcal{B}^k} \left[ \mathcal{R}(c) - \mathcal{R}(\hat{c}) \right].
\]

This will provide an observable upper bound for the risk that is uniform with respect to the choice of centers \( c \in \mathcal{B}^k \). Being uniform with respect to \( c \) covers the case where the centers have been computed from the observed sample through some algorithm. In order to study the excess risk of estimators, we will also study the upper deviations of

\[
\sup_{c \in \mathcal{B}^k} \left[ \mathcal{R}(c) - \mathcal{R}(c^*) - \mathcal{R}(\hat{c}) + \mathcal{R}(c^*) \right].
\]

This random variable compares uniformly with respect to \( c \) the excess risk of \( c \) with respect to a non random reference \( c^* \) and the corresponding empirical excess risk. In particular, the non random reference \( c^* \) can be chosen to be a minimizer, or more generally an \( \varepsilon \)-minimizer, of the risk \( \mathcal{R} \).

Indeed, we will consider \( \hat{c} \in \mathcal{B}^k \), depending on the sample, such that

\[
\mathcal{R}(\hat{c}) \leq \inf_{c \in \mathcal{B}^k} \mathcal{R}(c) + \varepsilon,
\]

and provide a bound for the excess risk \( \mathcal{R}(\hat{c}) - \inf_{c \in \mathcal{B}^k} \mathcal{R}(c) \). To complement deviation bounds, we will also provide corresponding bounds in expectation.

Regarding the sample size \( n \), we obtain a speed of order \( O(1/\sqrt{n}) \) as in [6], [16] and [17]. However, we get a better dependence in \( k \), with a rate of convergence of \( O(\sqrt{k/n}) \) up to log factors. This is essentially optimal up to log factors, at least in infinite dimension, since minimax lower bounds for the excess \( k \)-means risk are of order \( O(\sqrt{k^{1-4/d}/n}) \) in dimension \( d \), see [4] and [1]. We should mention that the speed \( \sqrt{k/n} \) has already been established in [15] (see Lemma 6), [18] and [21], but with worse log factors and less explicit constants.

These bounds will be obtained using PAC-Bayesian inequalities combined with a kernel trick and a new kind of PAC-Bayesian chaining method that we developed. In particular, borrowing ideas from the construction of the isonormal Gaussian process [26, section 3.5], we will use the distribution of an infinite sequence of shifted Gaussian random variables both for the prior and the posterior parameter distribution. We will also use some arguments from the proofs of [11] and [12], concerning the estimation of the mean of a random vector. Furthermore, we take inspiration from the classical chaining procedure for bounding the expected suprema of sub-Gaussian processes (see section 13.1 in [7]). We create a PAC-Bayesian version of chaining in which the concept of \( \delta \)-net and \( \delta \)-covering is replaced by the use of a sequence of Gaussian perturbations parametrized by a variance ranging on a logarithmic grid. We combine this PAC-Bayesian chaining with the use of the influence function \( \psi \) described in [10] to decompose the excess risk into a sub-Gaussian part and an other part representing extreme values. It is worth mentioning that we will work with weak hypotheses and will in particular not consider the kind of margin assumptions that are necessary to get bounds decreasing faster than \( \sqrt{1/n} \) for a given value of \( k \), as in [22], [23],[24], and [25].

2. Extensions of the \( k \)-means criterion. Before proving generalization bounds, let us embed the \( k \)-means criterion in a broader family of risk functions.

We will do this while considering the square of the Euclidean distance, or more generally in possibly infinite dimension the square of the Hilbert norm, as the Kullback divergence between two Gaussian measures. In this interpretation, vector quantization according to the \( k \)-means criterion will appear as a special case of conditional probability measure quantization according to an entropy criterion.
To describe things at a more technical level, we need first to define the classification function underlying vector quantization. To a set of centers \( c \in H^k \) indeed corresponds a classification function \( \ell : H \to [1, k] \) into Voronoï cells defined as

\[
\ell(x) = \arg \min_{j \in [1, k]} \|x - c_j\|.
\]

This definition may not be unique if the minimum is reached more than once, in which case, we make an arbitrary choice, as for instance

\[
\ell(x) = \min \left\{ \arg \min_{j \in [1, k]} \|x - c_j\| \right\}.
\]

The corresponding vector quantization function is

\[
f(x) = c_{\ell(x)}, \quad x \in H.
\]

To study the quality of the quantization of a random variable \( X \in H \) in terms of conditional probability distributions, we introduce another random variable \( Y \in \mathbb{R}^N \) and consider on some probability space \( \Omega \) a realization \((X, Y) : \Omega \to H \times \mathbb{R}^N\) of the couple of random variables \((X, Y)\). We can for instance take \( \Omega = H \times \mathbb{R}^N \) and let \((X, Y)\) be the identity. Introduce now a probability measure \( P \in \mathcal{M}_1^c(\Omega) \) such that \( P_X \) is the law of \( X \) and such that \( P_{Y \mid X} \) is the law of the independent sequence \( \langle X, e_i \rangle + \sigma \varepsilon_i, i \in \mathbb{N} \), where \( \langle \varepsilon_i, i \in \mathbb{N} \rangle \) is an i.i.d. sequence of standard normal random variables, where \( \langle e_i, i \in \mathbb{N} \rangle \) is a basis of \( H \) and where \( \sigma > 0 \) is a standard deviation parameter. In other words, let

\[
P_{Y \mid X} = \bigotimes_{i \in \mathbb{N}} \mathcal{N}(\langle X, e_i \rangle, \sigma^2).
\]

Let us also introduce a probability measure \( Q^{(c)} \in \mathcal{M}_1^c(\Omega) \) such that \( Q^{(c)} = P_X \) and

\[
Q^{(c)}_{Y \mid X} = \bigotimes_{i \in \mathbb{N}} \mathcal{N}(\langle c_{\ell(X)}, e_i \rangle, \sigma^2),
\]

where \( \ell \) is defined from \( c \) as explained above. In other words, \( Q^{(c)}_{Y \mid X} \) is the distribution of the random sequence \( \langle c_{\ell(X)}, e_i \rangle + \sigma \varepsilon_i, i \in \mathbb{N} \). We see that \( Q^{(c)}_{Y \mid X} \) is a quantization of \( P_{Y \mid X} \) that takes \( k \) values, in the same way as \( f(X) = c_{\ell(X)} \) is a quantization of \( X \) itself.

**Proposition 2.** The k-means criterion \( \mathcal{R} \) can be expressed as

\[
\mathcal{R}(c) = 2\sigma^2 P_X \left[ \mathcal{K}(Q^{(c)}_{Y \mid X}, P_{Y \mid X}) \right] = 2\sigma^2 \mathcal{K}(Q^{(c)}_{X, Y}, P_X, P_Y).
\]

**Proof.** The first equality comes from the fact that

\[
\mathcal{K}(Q^{(c)}_{Y \mid X}, P_{Y \mid X}) = \sum_{i \in \mathbb{N}} \mathcal{K}(\mathcal{N}(\langle c_{\ell(X)}, e_i \rangle, \sigma^2), \mathcal{N}(\langle X, e_i \rangle, \sigma^2))
\]

\[
= \sum_{i \in \mathbb{N}} \frac{1}{2\sigma^2} \left( \langle c_{\ell(X)}, e_i \rangle - \langle X, e_i \rangle \right)^2 = \frac{1}{2\sigma^2} \|X - c_{\ell(X)}\|^2 = \frac{1}{2\sigma^2} \min_{j \in [1, k]} \|X - c_j\|^2.
\]

The second equality is a consequence of the decomposition stated in Lemma 1 on page 2, that says that

\[
\mathcal{K}(Q^{(c)}_{X, Y}, P_X, P_Y) = \mathcal{K}(Q^{(c)}_{X, Y}, P_X) + Q^{(c)}_X \left[ \mathcal{K}(Q^{(c)}_{Y \mid X}, P_{Y \mid X}) \right]
\]

and of the fact that \( Q^{(c)}_X = P_X \) by definition of \( Q^{(c)} \).

\[\square\]
The two equalities of Proposition 2 will be interesting to extend the k-means criterion. Let us draw the consequences of the first one first. Introduce

\[ \mu_j^{(c)} = \bigotimes_{i \in \mathbb{N}} \mathcal{N}(c_j, e_i, \sigma^2) \in \mathcal{M}_+^1(\mathbb{R}^N), \quad j \in [1, k]. \]

The first part of equation (2) can be written as

\[ \mathcal{R}(c) = 2\sigma^2 \mathbb{P}_X \left[ \mathcal{K}(\mu_j^{(c)}, \mathbb{P}_{Y|X}) \right] = 2\sigma^2 \mathbb{P}_X \left[ \min_{j \in [1, k]} \mathcal{K}(\mu_j^{(c)}, \mathbb{P}_{Y|X}) \right], \]

since

\[ 2\sigma^2 \mathcal{K}(\mu_j^{(c)}, \mathbb{P}_{Y|X}) = \|X - c_j\|^2. \]

Note that we could also have used \( 2\sigma^2 \mathcal{K}(\mathbb{P}_{Y|X}, \mu_j^{(c)}) = \|X - c_j\|^2 \), since the Kullback divergence between Gaussian measures is symmetric. This would have lead to another interpretation of the k-means criterion in a space of conditional probability measures. The choice we made is quite unusual, but is justified by the following property.

**Proposition 3.** The minimization of \( \mathcal{R}(c) \) seen as a function of \( \mu^{(c)} \) can be extended to the larger set \( \mathcal{M}_+^1(\mathbb{R}^N)^k \). In other words, if we put

\[ \tilde{\mathcal{R}}(\mu) = 2\sigma^2 \mathbb{P}_X \left[ \min_{j \in [1, k]} \mathcal{K}(\mu_j, \mathbb{P}_{Y|X}) \right], \quad \mu \in \mathcal{M}_+^1(\mathbb{R}^N)^k, \]

we can see that \( \mathcal{R}(c) = \tilde{\mathcal{R}}(\mu^{(c)}) \) and the minimum of \( \tilde{\mathcal{R}} \) coincides with the minimum of \( \mathcal{R} \) in the sense that

\[ \inf_{c \in H^k} \mathcal{R}(c) = \inf_{c \in H^k} \tilde{\mathcal{R}}(\mu^{(c)}) = \inf_{\mu \in \mathcal{M}_+^1(\mathbb{R}^N)^k} \tilde{\mathcal{R}}(\mu). \]

**Proof.** Given \( \mu \in \mathcal{M}_+^1(\mathbb{R}^N)^k \), we have to find \( c \in H^k \) such that \( \tilde{\mathcal{R}}(\mu) \geq \mathcal{R}(c) \). This will prove that

\[ \inf_{c \in H^k} \mathcal{R}(c) = \inf_{c \in H^k} \tilde{\mathcal{R}}(\mu^{(c)}) \leq \inf_{\mu \in \mathcal{M}_+^1(\mathbb{R}^N)^k} \tilde{\mathcal{R}}(\mu), \]

and since the reverse inequality is obvious from the fact that we take the infimum on a larger set, this will prove the proposition.

Consider then

\[ \ell(X) = \min \left\{ \arg \min_{j \in [1, k]} \mathcal{K}(\mu_j, \mathbb{P}_{Y|X}) \right\} \]

and

\[ c_j = \mathbb{P}_{X|\ell(X)=j}(X), \quad j \in [1, k]. \]

It is easy to check that the centers \( c_j \) are such that

\[ \frac{d\mu_j^{(c)}}{d\mu_j^{(0)}} = Z_j^{-1} \exp \left\{ \mathbb{P}_{X|\ell(X)=j} \left[ \log \left( \frac{d\mathbb{P}_{Y|X}}{d\mu_j^{(0)}} \right) \right] \right\}, \]

where \( Z_j \) is a normalizing constant and \( \mu^{(0)} \) is \( \mu^{(c)} \) with \( c = 0 \in H^k \), the centered Gaussian measure. Indeed, Gaussian measures with the same covariance form an exponential family indexed by their means. Taking the arithmetic mean of the parameter in an exponential family
results in taking the geometric mean of the probability measures. Thus, \( \mu_j^{(c)} \) is the geometric mean of \( P_{Y|X} \) with weights \( P_{X|\ell(X)=j} \). As a consequence, for any \( j \in [1,k] \),

\[
P_{X|\ell(X)=j} \left[ \mathcal{K}(\mu_\ell(X), P_{Y|X}) \right] \\
= P_{X|\ell(X)=j} \left\{ \mu_j \left[ \log \left( \frac{d\mu_j}{dP_{Y|X}} \right) \right] \right\} \\
= \mu_j \left[ \log \left( \frac{d\mu_j}{d\mu_j^{(0)}} \right) \right] - \mu_j \left\{ P_{X|\ell(X)=j} \left[ \log \left( \frac{dP_{Y|X}}{d\mu_j^{(0)}} \right) \right] \right\} \\
= \mu_j \left[ \log \left( \frac{d\mu_j}{d\mu_j^{(0)}} \right) \right] - \mu_j \left[ \log \left( \frac{d\mu_j}{d\mu_j^{(0)}} \right) \right] - \log(Z_j) = \mu_j \left[ \log \left( \frac{d\mu_j}{d\mu_j^{(c)}} \right) \right] - \log(Z_j).
\]

Moreover, considering the case when \( \mu = \mu^{(c)} \), we see that

\[
P_{X|\ell(X)=j} \left[ \mathcal{K}(\mu^{(c)}_\ell(X), P_{Y|X}) \right] = -\log(Z_j).
\]

Therefore

\[
P_X \left[ \min_{j \in [1,k]} \mathcal{K}(\mu_j, P_{Y|X}) \right] = P_X \left[ \mathcal{K}(\mu_\ell(X), P_{Y|X}) \right] = P_{\ell(X)} P_X|\ell(X) \left[ \mathcal{K}(\mu_\ell(X), P_{Y|X}) \right] \\
= P_X \left[ \mathcal{K}(\mu_\ell(X), \mu^{(c)}_\ell(X)) \right] + P_X \left[ \mathcal{K}(\mu^{(c)}_\ell(X), P_{Y|X}) \right] \\
\geq P_X \left[ \mathcal{K}(\mu^{(c)}_\ell(X), P_{Y|X}) \right] \geq P_X \left[ \min_{j \in [1,k]} \mathcal{K}(\mu_j^{(c)}, P_{Y|X}) \right],
\]

showing that \( \widetilde{R}(\mu) \geq \widetilde{R}(\mu^{(c)}) \). \( \square \)

So Proposition 3 shows that the \( k \)-means algorithm also solves a quantization problem for Gaussian conditional probability measures \( P_{Y|X} \). This is an invitation to study more generally the quantization problem for conditional probability measures, using what we will call the information \( k \)-means criterion \( \widetilde{R}(\mu) \). This is what will be done in section 4 on page 8.

Let us now come back to the second equality of equation (2) on page 4. It relates the minimization of the \( k \)-means criterion with the estimation of the joint probability measure \( P_{X,Y} \). Instead of considering the single distribution \( Q^{(c)}_{X,Y} \) we can optimize the value of \( Q^{(c)}_{X,Y} \), considering the model

\[
\mathcal{Q}(c) = \{ Q \in \mathcal{M}_+(\Omega) : Q_{Y|X} = \mu^{(c)}_\ell(X) \} \ni Q^{(c)}_{X,Y}.
\]

In order to get a better approximation of \( P_{X,Y} \), it is natural to consider instead of \( \mathcal{R}(c) \) the criterion

\[
\mathcal{C}_2(c) = 2\sigma^2 \inf_{Q \in \mathcal{Q}(c)} \mathcal{K}(Q_{X,Y}, P_{X,Y}) \leq \mathcal{R}(c) = 2\sigma^2 \mathcal{K}(Q^{(c)}_{X,Y}, P_{X,Y}).
\]

It turns out that this infimum can be computed.

**Proposition 4.** Consider the classification function

\[
\ell_c(x) = \min \left\{ \arg \min_{j \in [1,k]} \| X - c_j \| \right\}.
\]
The above criterion is equal to
\[
\mathcal{C}_2(c) = 2\sigma^2 \inf_{Q \in \mathcal{Q}(c)} \mathcal{K}(Q_X, Y, P_{X,Y}) = -2\sigma^2 \log \mathbb{P}_X \left\{ \exp \left[ -\mathcal{K}(\mu_{\ell,c}(X), P_{Y|X}) \right] \right\} \\
= -2\sigma^2 \log \mathbb{P}_X \left\{ \exp \left[ -\frac{1}{2\sigma^2} \| X - c_{\ell,c}(X) \|^2 \right] \right\} \\
= -2\sigma^2 \log \mathbb{P}_X \left\{ \exp \left[ -\frac{1}{2\sigma^2} \min_{j \in [1:k]} \| X - c_j \|^2 \right] \right\}.
\]

**Proof.** For any \( Q \in \mathcal{Q}(c) \), use the decomposition stated in Lemma 1 on page 2, to obtain that
\[
(4) \quad \mathcal{K}(Q_X, Y, P_{X,Y}) = \mathcal{K}(Q_X, P_X) + Q_X \left[ \mathcal{K}(P_{Y|X}) \right] \\
= \mathcal{K}(Q_X, P_X) + Q_X \left[ \mathcal{K}(\mu_{\ell,c}(X), P_{Y|X}) \right].
\]

Minimizing this last expression with respect to \( Q_X \in \mathcal{M}_+^1(H) \) according to forthcoming Lemma 7 on page 10 gives the first equality of the proposition, the others being obvious. \( \square \)

The criterion \( \mathcal{C}_2(c) \) is not a risk function in the sense that it is not the expectation of a loss function, but it is closely related to one. Indeed we can introduce
\[
\mathcal{R}_2(c) = 2\sigma^2 \left[ 1 - \exp \left( -\frac{1}{2\sigma^2} \mathcal{C}_2(c) \right) \right] \leq \mathcal{C}_2(c) \leq \mathcal{R}(c)
\]
that is equal to
\[
\mathcal{R}_2(c) = 2\sigma^2 \mathbb{P}_X \left[ 1 - \exp \left( -\frac{1}{2\sigma^2} \min_{j \in [1:k]} \| X - c_j \|^2 \right) \right]
\]
according to the previous proposition. We see that the risk \( \mathcal{R}_2 \) is a natural modification of the risk \( \mathcal{R} \) when we relate \( \mathcal{R} \) to the estimation of \( P_{X,Y} \). This new risk \( \mathcal{R}_2 \) is smaller, meaning that it should be easier to minimize and indeed, as it is the expectation of a bounded loss function, we will get a generalization bound under weaker hypotheses than what we will ask for \( \mathcal{R} \). More specifically, we will assume no more that the sample is bounded.

3. **Study of the robust quadratic \( k \)-means criterion.** We can find a local minimum of the usual quadratic \( k \)-means criterion using Lloyd’s algorithm that updates the centers and the classification function alternately. In this section, we will describe a similar algorithm for the robust criterion of equation (5). According to this equation, \( \mathcal{R}_2(c) \) is an increasing function of \( \mathcal{C}_2(c) \), so that we can as well study the minimization of \( \mathcal{C}_2(c) \). The discussion will also cover the minimization of the corresponding empirical criteria, replacing the law of \( X, P_X \), by the empirical measure \( \mathbb{P}_X \).

According to the decomposition (4),
\[
\frac{1}{2\sigma^2} \mathcal{C}_2(c) = \inf_{Q_X \in \mathcal{M}_+^1(H)} \mathcal{K}(Q_X, P_X) + Q_X \left( \frac{1}{2\sigma^2} \| X - c_{\ell,c}(X) \|^2 \right).
\]

Moreover the infimum in \( Q_X \) is reached at \( Q_X^* \ll P_X \) defined by its density
\[
\frac{dQ_X^*}{d\mathbb{P}_X} = Z^{-1} \exp \left( -\frac{1}{2\sigma^2} \| X - c_{\ell,c}(X) \|^2 \right).
\]

This proves
Proposition 5 (Lloyd’s algorithm for the robust \( k \)-means criterion). For any \( c \in H^k \), consider the updated centers \( c' \in H^k \) defined as
\[
c'_j = Q^*_X |_{\ell_c(X) = j} (X) = \frac{\mathbb{P}_{X | \ell_c(X) = j} \left[ X \exp \left( -\frac{1}{2\sigma^2} \| X - c_j \|^2 \right) \right]}{\mathbb{P}_{X | \ell_c(X) = j} \left[ \exp \left( -\frac{1}{2\sigma^2} \| X - c_j \|^2 \right) \right]},
\]
where \( \ell_c \) is defined by equation (3) on page 6. Then
\[
\mathcal{E}_2(c') \leq \mathcal{E}_2(c) - Q^*_X \| c_{\ell_c(X)} - c'_{\ell_c(X)} \|^2 \leq \mathcal{E}_2(c).
\]
Accordingly \( \mathcal{R}_2(c') \leq \mathcal{R}_2(c) \).

Proof. We can see that
\[
\frac{1}{2\sigma^2} \mathcal{E}_2(c) = \mathcal{K}(Q^*_X, \mathbb{P}_X) + Q^*_X \left( \frac{1}{2\sigma^2} \| X - c_{\ell_c(X)} \|^2 \right)
= \mathcal{K}(Q^*_X, \mathbb{P}_X) + Q^*_X \left( \frac{1}{2\sigma^2} \| X - c'_{\ell_c(X)} \|^2 \right) + Q^*_X \left( \frac{1}{2\sigma^2} \| c_{\ell_c(X)} - c'_{\ell_c(X)} \|^2 \right)
\geq \mathcal{K}(Q^*_X, \mathbb{P}_X) + Q^*_X \left( \frac{1}{2\sigma^2} \| X - c'_{\ell_c(X)} \|^2 \right) + Q^*_X \left( \frac{1}{2\sigma^2} \| c_{\ell_c(X)} - c'_{\ell_c(X)} \|^2 \right)
\geq \frac{1}{2\sigma^2} \mathcal{E}_2(c') + Q^*_X \left( \frac{1}{2\sigma^2} \| c_{\ell_c(X)} - c'_{\ell_c(X)} \|^2 \right),
\]
keeping in mind that \( Q^*_X \) depends on \( c \).

4. Study of the information \( k \)-means criterion. In this section, we will study the information \( k \)-means criterion \( \mathcal{R}(\mu) \) of Proposition 3 on page 5 for more general models of regular conditional probability measures \( \mathbb{P}_{Y | X} \).

Consider a couple of random variables \( (X, Y) \in \mathcal{X} \times \mathcal{Y} \), where \( \mathcal{X} \) and \( \mathcal{Y} \) are complete separable metric spaces, so that we can define regular conditional probability measures. Suppose there exists a reference measure \( \nu \in \mathcal{M}^1_+ (\mathcal{Y}) \) such that \( \mathbb{P} \left( \mathbb{P}_{Y | X} \ll \nu \right) = 1 \). Define \( p_X = \frac{d\mathbb{P}_{Y | X}}{d\nu} \). We are interested in the case where \( \mathbb{P}_{Y | X} \) is known therefore providing a bag of words model. This means that each random sample \( X \) is described by a random probability measure \( \mathbb{P}_{Y | X} \). In the original bag of words model, \( \mathcal{Y} \) is a set of words, and \( \mathbb{P}_{Y | X} \) is the distribution of words in a text \( X \) drawn at random from some corpus of texts. Here we include the case where \( \mathcal{X} \) and \( \mathcal{Y} \) can be more general measurable spaces.

We introduce the following generalization of the criterion \( \mathcal{R} \) of Proposition 3 on page 5, that we will name the information \( k \)-means criterion:
\[
\inf_{q \in \left( L_{+,1} (\nu) \right)^k} \mathbb{P}_X \left( \min_{j \in [1,k]} \mathcal{K}(q_j, p_X) \right),
\]
where \( [1, k] = \{1, \ldots, k\} \), \( L_{+,1} (\nu) = \left\{ q \in L^1 (\nu) : q \geq 0, \int q \, d\nu = 1 \right\} \) and
\[
\mathcal{K}(q_j, p_X) = \begin{cases} \int q_j \log (q_j / p_X) \, d\nu, & \text{if } q_j \mathbb{1} (p_X = 0) \, d\nu = 0, \\ +\infty, & \text{otherwise} \end{cases}
\]
NEW BOUNDS FOR $K$-MEANS

is the Kullback divergence between densities. The purpose of this section is to discuss the general properties of the information $k$-means problem and to build a mathematical framework and algorithms to perform the minimization. As we have seen in the previous section, we chose to study this algorithm rather than the better known $k$-means divergence algorithm because of Proposition 3 on page 5, showing that our proposal contains the classical Euclidean $k$-means as a special case. More generally, using the divergence in the way we do when the conditional probability measures $P_{Y|X}$ belong to an exponential family ensures that the optimal centers for a given classification function $\ell$ belong to that same exponential family.

We should point out that clustering histograms or more generally probability distributions based on the Kullback divergence or other information criteria is not a new subject. It has been extensively used in text categorization and image indexing, especially in word clustering to extract features or reduce the original space dimension, see [31], [33], [32], [14], [8], [35], and [20]. The clustering is essentially performed using the aforementioned $k$-means divergence algorithm. However, in the information $k$-means framework we follow a different route since the grouping step is done by minimizing the Kullback divergence with respect to its first argument instead of its second one. This leads to very different centroids, computed as geometric means of distributions instead of arithmetic means, see [5] and [34]. This follows from the fact that the Kullback divergence is asymmetric. Nevertheless, symmetric extensions of the Kullback divergence built upon averaged symmetrizations have been studied. Especially, centroids and $k$-means type algorithms derived from symmetrized divergence functions are analyzed in [34], [27], [30] and [28].

Besides, following the set-up provided by the typical $k$-means divergence, [3] presents a general $k$-means framework based on the Bregman divergence. The authors show that such criteria can be minimized iteratively using a $k$-means centroid-based algorithm. The Bregman distance encompasses many traditional similarity measures such as the Euclidean distance, the Kullback divergence, the logistic loss and many others. However, in the Kullback case, the minimization is performed with respect to the second argument, and not the first as in our proposal. Nevertheless, the study of a symmetrized version of the Bregman divergence, and especially the resulting centroids coming from it, is undertaken in [29].

Our contribution in this paper is to provide a mathematical framework for the information $k$-means criterion. In particular, we will prove generalization bounds and deal with the infinite dimension case.

Let us state some version of the Bayes rule that will be useful in the following discussion.

**Lemma 6.** Let $P_{X,Y}$ be a joint distribution defined on the product of two Polish spaces. The following statements are equivalent:

1. There exists a measure $\mu$ such that $P_{Y|X} \ll \mu$, $P_X$ almost surely;
2. $P_{Y|X} \ll P_Y$, $P_X$ almost surely;
3. $P_{X,Y} \ll P_X \otimes P_Y$;
4. $P_{X|Y} \ll P_X$, $P_Y$ almost surely.

Moreover, they imply the following identities between Radon–Nikodym derivatives:

$$\frac{dP_{X,Y}}{d(P_X \otimes P_Y)} = \frac{dP_{Y|X}}{dP_X} = \frac{dP_{X|Y}}{dP_X}.$$
PROOF. To prove that 1. implies 2., it is sufficient to show that $P_{Y|X}(\frac{dP_Y}{d\mu} = 0) = 0$, $P_X$ almost surely. But when 1. is true

$$P_{Y|X}(\frac{dP_Y}{d\mu} = 0) = \int 1(\frac{dP_Y}{d\mu} = 0) \frac{dP_{Y|X}}{d\mu} d\mu.$$ 

Thus by the Tonelli-Fubini theorem

$$P_X\left(P_{Y|X}(\frac{dP_Y}{d\mu} = 0)\right) = P_X\left(\int 1\left(\frac{dP_Y}{d\mu} = 0\right) \frac{dP_{Y|X}}{d\mu} d\mu\right)$$

$$= \int 1\left(\frac{dP_Y}{d\mu} = 0\right) P_X\left[\frac{dP_{Y|X}}{d\mu}\right] d\mu$$

$$= \int 1\left(\frac{dP_Y}{d\mu} = 0\right) \frac{dP_Y}{d\mu} d\mu = 0.$$ 

Therefore $P_{Y|X}(\frac{dP_Y}{d\mu} = 0) = 0$, $P_X$ almost surely. Obviously 2. implies 1. with $\mu = P_Y$.

Now let us show that 2. implies 3. Let $f$ be a bounded measurable function, we have by Fubini’s theorem

$$\int f dP_{X,Y} = \int \left(\int f dP_{Y|X}\right) dP_X = \int \left(\int f \frac{dP_{Y|X}}{dP_Y} dP_Y\right) dP_X$$

$$= \int f \frac{dP_{Y|X}}{dP_Y} d(P_Y \otimes dP_X),$$

implying 3. and that $P_X$ almost surely

$$\frac{dP_{Y|X}}{dP_Y} = \frac{dP_{X,Y}}{d(P_X \otimes P_Y)}.$$ 

We will show now that 3. implies 2. Let $f$ be a bounded measurable function, we have by Fubini’s theorem

$$\int f dP_{X,Y} = \int f \frac{dP_{X,Y}}{d(P_X \otimes P_Y)} d(P_X \otimes dP_Y)$$

$$= \int \left(\int f \frac{dP_{X,Y}}{d(P_X \otimes P_Y)} dP_Y\right) dP_X$$

$$= \int \left(\int f dP_{Y|X}\right) dP_X,$$

showing that $P_X$ almost surely $P_{Y|X} \ll P_Y$ and

$$\frac{dP_{Y|X}}{dP_Y} = \frac{dP_{X,Y}}{d(P_X \otimes P_Y)}.$$ 

The equivalence between 3. and 4. is immediate by interchanging the roles of $X$ and $Y$. □

The following lemma will be useful to optimize the information $k$-means criterion and is related to the Donsker Varadhan representation.
LEMMA 7. Let \( \pi \in \mathcal{M}_+(\Omega) \) be a probability measure on the measurable space \( \Omega \). Let \( h : \Omega \to \mathbb{R} \cup \{+\infty\} \) be a measurable function such that

\[
Z = \int \exp(-h) \, d\pi < \infty.
\]

Let \( \pi_{\exp(-h)} \) be the probability measure whose density with respect to \( \pi \) is proportional to \( \exp(-h) \) so that

\[
\frac{d\pi_{\exp(-h)}}{d\pi} = \frac{\exp(-h)}{Z}.
\]

The identity

\[
\inf_{\eta \in \mathbb{Z}} \left( \mathcal{K}(\rho, \pi) + \int \max\{h, \eta\} \, d\rho \right) = -\log \left( \int \exp(-h) \, d\pi \right) + \mathcal{K}(\rho, \pi_{\exp(-h)}) \in \mathbb{R} \cup \{+\infty\}
\]

is satisfied for any \( \rho \in \mathcal{M}_+(\Omega) \) and implies that

\[
\inf_{\rho \in \mathcal{M}_+(\Omega)} \inf_{\eta \in \mathbb{Z}} \left( \mathcal{K}(\rho, \pi) + \int \max\{h, \eta\} \, d\rho \right) = -\log \left( \int \exp(-h) \, d\pi \right),
\]

the minimum being reached when \( \rho = \pi_{\exp(-h)} \).

Note that the lemma could also be written as

\[
\mathcal{K}(\rho, \pi) + \int h \, d\rho = -\log \left( \int \exp(-h) \, d\pi \right) + \mathcal{K}(\rho, \pi_{\exp(-h)})
\]

if we are willing to follow the convention that

\[
\int h \, d\rho = \inf_{\eta \in \mathbb{Z}} \int \max\{h, \eta\} \, d\rho
\]

and that \( +\infty - \infty = +\infty \).

PROOF. See [9, page 159]. Note that the role of \( \eta \in \mathbb{Z} \) in this lemma is only to make sure that the integrals are always well defined in \( \mathbb{R} \cup \{+\infty\} \) in the sense that the negative part of the integrand is integrable. When \( \rho \) is not absolutely continuous with respect to \( \pi \), it is also not absolutely continuous with respect to \( \pi_{\exp(-h)} \) since \( \pi(A) = 0 \) if and only if \( \pi_{\exp(-h)}(A) = 0 \). In this case \( \mathcal{K}(\rho, \pi) = \mathcal{K}(\rho, \pi_{\exp(-h)}) = +\infty \) and the identity is true, both sides being equal to \( +\infty \). When \( \rho \ll \pi \), then \( \rho \ll \pi_{\exp(-\max\{h, \eta\})} \) and

\[
\frac{d\rho}{d\pi_{\exp(-\max\{h, \eta\})}} = Z_{\eta} \exp(\max\{h, \eta\}) \frac{d\rho}{d\pi},
\]

where

\[
Z_{\eta} = \int \exp(-\max\{h, \eta\}) \, d\pi < +\infty.
\]

Therefore

\[
\mathcal{K}(\rho, \pi_{\exp(-\max\{h, \eta\})}) = \log(Z_{\eta}) + \int \left[ \max\{h, \eta\} + \log(d\rho/d\pi) \right] \, d\rho.
\]

By the monotone convergence theorem

\[
\lim_{\eta \to -\infty} Z_{\eta} = Z \quad \text{and} \quad \lim_{\eta \to -\infty} \int \left[ \max\{h, \eta\} + \log(\frac{d\rho}{d\pi}) \right] \, d\rho = \int \left[ h + \log(\frac{d\rho}{d\pi}) \right] \, d\rho.
\]
since we know that
\[
\int \left[ \log(Z) + h + \log \left( \frac{d\rho}{d\pi} \right) \right] d\rho = \int \log \left( \frac{d\rho}{d\pi} \right) - \frac{d\rho}{d\pi \exp(-h)} d\pi \exp(-h) \leq \exp(-1) < +\infty
\]
and therefore that
\[
\int \left[ h + \log \left( \frac{d\rho}{d\pi} \right) \right] d\rho < +\infty.
\]
This proves that
\[
\lim_{\eta \to -\infty} \mathcal{K}(\rho, \pi_{\exp(-\max\{h,\eta\})}) = \log(Z) + \int \left[ h + \log \left( \frac{d\rho}{d\pi} \right) \right] d\rho = \mathcal{K}(\rho, \pi_{\exp(-h)})
\]
\[
= \log(Z) + \inf_{\eta \in \mathbb{Z}} \int \left[ \max\{h, \eta\} + \log \left( \frac{d\rho}{d\pi} \right) \right] d\rho
\]
\[
= \log(Z) + \inf_{\eta \in \mathbb{Z}} \left( \int \max\{h, \eta\} d\rho + \int \log \left( \frac{d\rho}{d\pi} \right) d\rho \right)
\]
and therefore that
\[
\mathcal{K}(\rho, \pi_{\exp(-h)}) - \log(Z) = \inf_{\eta \in \mathbb{Z}} \left( \mathcal{K}(\rho, \pi) + \int \max\{h, \eta\} d\rho \right)
\]
as stated in the lemma. The second statement of the lemma is a consequence of the fact that the Kullback divergence is non-negative. \[\square\]

Let us now formulate a precise definition of the geometric mean of conditional probability measures and show that it is their optimal center according to the information projection criterion.

**Lemma 8.** Let \( P_{X,Y} \) be a joint distribution defined on the product of two Polish spaces. Assume that \( P_X \mid P_Y \ll P_Y \) and \( P_X(\mid P_Y) = 1 \). Consider the normalizing constant
\[
Z = P_Y \left( \exp \left[ -\mathcal{K}(P_X, P_X \mid Y) \right] \right) = P_Y \left( \exp \left\{ P_X \left[ \log \left( \frac{dP_{Y \mid X}}{dP_Y} \right) \right] \right\} \right).
\]
Obviously, \( Z \in [0,1] \). If \( Z = 0 \), then
\[
\inf_{Q_Y \in \mathcal{M}_+^1(Y)} P_X \left[ \mathcal{K}(Q_Y, P_{Y \mid X}) \right] = +\infty.
\]
Otherwise, \( Z > 0 \) and for any \( Q_Y \in \mathcal{M}_+^1(Y) \),
\[
P_X \left[ \mathcal{K}(Q_Y, P_{Y \mid X}) \right] = \mathcal{K}(Q_Y, Q_Y) + P_X \left[ \mathcal{K}(Q_Y, P_{Y \mid X}) \right] = \mathcal{K}(Q_Y, Q_Y) + \log(Z^{-1}),
\]
where \( Q_Y \ll P_Y \) is defined by the relation
\[
\frac{dQ_Y}{dP_Y} = Z^{-1} \exp \left[ -\mathcal{K}(P_X, P_X \mid Y) \right]
\]
\[= Z^{-1} \exp \left\{ P_X \left[ \log \left( \frac{dP_{Y \mid X}}{dP_Y} \right) \right] \right\}. \tag{6} \]
Consequently
\[
\inf_{Q_Y \in \mathcal{M}_t(y)} \mathbb{P}_X \left[ \mathcal{K}(Q_Y, \mathbb{P}_{Y|X}) \right] = \mathbb{P}_X \left[ \mathcal{K}(Q^*_Y, \mathbb{P}_{Y|X}) \right] = \log(Z^{-1}) < \infty,
\]

The probability measure \(Q^*_Y\) represents the geometric mean of \(\mathbb{P}_{Y|X}\) with respect to \(\mathbb{P}_X\).

**Proof.** By Lemma 1 on page 2,

\[
\mathbb{P}_X \left[ \mathcal{K}(Q_Y, \mathbb{P}_{Y|X}) \right] = \mathcal{K}(\mathbb{P}_X \otimes Q_Y, \mathbb{P}_{X,Y}) = \mathcal{K}(Q_Y, \mathbb{P}_Y) + Q_Y \left[ \mathcal{K}(\mathbb{P}_X, \mathbb{P}_{X|Y}) \right].
\]

Thus, when (7) is finite, \(Q_Y \ll \mathbb{P}_Y\) and

\[
Q_Y \left[ \mathcal{K}(\mathbb{P}_X, \mathbb{P}_{X|Y}) < +\infty \right] = 1,
\]

so that

\[
\mathbb{P}_Y \left[ \mathcal{K}(\mathbb{P}_X, \mathbb{P}_{X|Y}) < +\infty \right] > 0,
\]

implying that \(Z > 0\). Assuming from now on that (7) is finite, introduce

\[
\mathcal{A} = \left\{ y : \mathcal{K}(\mathbb{P}_X, \mathbb{P}_{X|Y = y}) < +\infty \right\}.
\]

From Lemma 7 on page 10 and (7), for any \(Q_Y \in \mathcal{M}_t^1(\mathcal{A})\),

\[
\mathbb{P}_X \left[ \mathcal{K}(Q_Y, \mathbb{P}_{Y|X}) \right] = -\log \left( \mathbb{P}_Y(\mathcal{A}) \right) - \log \mathbb{P}_{Y|Y \in \mathcal{A}} \left( \exp \left[ -\mathcal{K}(\mathbb{P}_X, \mathbb{P}_{X|Y}) \right] \right) + \mathcal{K}(Q_Y, Q^*_Y)
\]

\[
= \log(Z^{-1})
\]

\[
= \mathbb{P}_X \left[ \mathcal{K}(Q^*_Y, \mathbb{P}_{Y|X}) \right] + \mathcal{K}(Q_Y, Q^*_Y).
\]

Moreover, when \(Q_Y(\mathcal{A}) < 1\), \(Q_Y \not\ll Q^*_Y\), so that both members are equal to \(+\infty\). The identity (6) is a consequence of Lemma 6 on page 9.

We are now ready to express the minimum of the information \(k\)-means criterion in different ways involving the underlying classification function and optimal centers.

**Proposition 9.** The information \(k\)-means problem can be expressed as

\[
\inf_{q \in (\mathbb{L}_{+,1}(\nu))^k} \mathbb{P}_X \left( \min_{j \in [1,k]} \mathcal{K}(q_j, p_X) \right) = \inf_{\epsilon : \mathbb{X} \rightarrow [1,k]} \inf_{(q_1, \ldots, q_k) \in (\mathbb{L}_{+,1}(\nu))^k} \mathbb{P}_X \left( \mathcal{K}(q_{\ell(X)}, p_X) \right)
\]

\[
= \inf_{(q_1, \ldots, q_k) \in (\mathbb{L}_{+,1}(\nu))^k} \mathbb{P}_X \left( \mathcal{K}(q_{\ell^*(X)}, p_X) \right)
\]

\[
= \inf_{\epsilon : \mathbb{X} \rightarrow [1,k]} \mathbb{P}_X \left( \mathcal{K}(q_{\ell^*(X)}^{*,\epsilon}, p_X) \right)
\]

\[
= \inf_{\epsilon : \mathbb{X} \rightarrow [1,k]} \mathbb{P}_X \left( \log(Z_{\ell(X)}^{-1}) \right),
\]
where the infimum in ℓ is taken on measurable classification functions ℓ, where \( \ell^*_q : \mathcal{X} \mapsto [1, k] \) is the best classification function for a fixed \( q = (q_1, \ldots, q_k) \) defined as
\[
\ell^*_q(x) = \arg \min_{j \in [1, k]} \mathcal{K}(q_j, p_x), \quad x \in \mathcal{X},
\]
whereas \( q_1^*, \ldots, q_k^* \) are the best information k-means centers with respect to \( \ell(X) \) defined as
\[
q_j^* = Z_j^{-1} \exp \left\{ \mathbb{P}_X | \ell(X) = j \left[ \log(p_X) \right] \right\}, \quad j \in [1, k],
\]
where
\[
Z_j = \int \exp \left\{ \mathbb{P}_X | \ell(X) = j \left[ \log(p_X) \right] \right\} d\nu,
\]
with the convention that \( q_j^* \) can be given any arbitrary value in the case when \( Z_j = 0 \), the corresponding criterion being in this case infinite. Besides, we have the following Pythagorean identity
\[
\mathbb{P}_X \left( \mathcal{K}(\ell(X), p_X) \right) = \mathbb{P}_X \left( \mathcal{K}(q_\ell^*(X), p_X) \right) + \mathbb{P}_X \left( \mathcal{K}(q_\ell(X), q_\ell^*(X)) \right).
\]

**Proof.** This proposition is a straightforward consequence of Lemma 8 on page 12 applied to \( \mathbb{P}_X, Y | \ell(X) = j \).

It may be of some help to state the empirical counterpart of the previous proposition, where formulas are somehow more explicit.

**Corollary 10.** Let \( X_1, \ldots, X_n \) be an i.i.d sample drawn from \( \mathbb{P}_X \). Then, the empirical version of the information k-means problem tries to partition the observations \( p_{X_1}, \ldots, p_{X_n} \) into k-clusters, what is expressed here by

\[
\inf_{q \in \left( \ell^*_q \right)^k} \frac{1}{n} \sum_{i=1}^n \min_{j \in [1, k]} \mathcal{K}(q_j, p_{X_i}) = \inf_{\ell: [1, n] \mapsto [1, k]} \inf_{q \in \left( \ell^*_q \right)^k} \frac{1}{n} \sum_{i=1}^n \mathcal{K}(q_{\ell(i)}, p_{X_i})
\]

\[
= \inf_{q \in \left( \ell^*_q \right)^k} \frac{1}{n} \sum_{i=1}^n \mathcal{K}(q^{*, \ell}_j, p_{X_i}) = \inf_{\ell: [1, n] \mapsto [1, k]} \frac{1}{n} \sum_{i=1}^n \mathcal{K}(q^{*, \ell}_j, p_{X_i})
\]

\[
= \inf_{\ell: [1, n] \mapsto [1, k]} 1 \sum_{i=1}^n \mathcal{K}(q^{*, \ell}_j, p_{X_i}) = \inf_{\ell: [1, n] \mapsto [1, k]} \kappa \sum_{j=1}^k |\ell^{-1}(j)| \log(Z_j^{-1}),
\]

where \( \ell^*_q : \mathcal{X} \mapsto [1, k] \) is the best classification function for a fixed \( q = (q_1, \ldots, q_k) \) defined as
\[
\ell^*_q(i) = \arg \min_{j \in [1, k]} \mathcal{K}(q_j, p_{X_i})
\]
whereas \( q^{*, \ell}_j, j \in [1, k] \) are the information k-means centers defined as
\[
q^{*, \ell}_j = Z_j^{-1} \left( \prod_{i \in \ell^{-1}(j)} p_{X_i} \right)^{1/|\ell^{-1}(j)|},
\]
where
\[
Z_j = \int \left( \prod_{i \in \ell^{-1}(j)} p_{X_i} \right)^{1/|\ell^{-1}(j)|} d\nu.
\]
PROOF. Apply the previous proposition to the empirical measure \( \mathbb{P}_X = \frac{1}{n} \sum_{i=1}^{n} \delta_{X_i} \) of the sample \( X_1, \ldots, X_n \).

We will now see that when the sample is in \( L^2(\nu) \) and has a finite second moment, the optimal centers for a given classification function are also in \( L^2(\nu) \), so that the optimization of the centers can be reduced to this space.

**Lemma 11.** Let us assume that \( \mathbb{P}_X \left( \int p_X^2 \, d\nu \right) < \infty \). Then, the optimal centers \( q_j^{*,\ell} \) defined in the previous lemma verify \( q_j^{*,\ell} \in L^2(\nu) \). Furthermore, in this case

\[
\inf \left\{ \mathbb{P}_X \left( \min_{j \in [1,k]} \mathcal{K}(q_j, p_X) \right) : q \in \left( L_{+,1}^1(\nu) \right)^k \right\} = \inf \left\{ \mathbb{P}_X \left( \min_{j \in [1,k]} \mathcal{K}(q_j, p_X) \right) : q \in \left( L_{+,1}^1(\nu) \cap L^2(\nu) \right)^k \right\}.
\]

**PROOF.** Apply Jensen’s inequality and the Fubini-Tonelli theorem to obtain that \( q_j^{*,\ell} \in L^2(\nu) \). Indeed, for any \( j \in [1,k] \), if \( Z_j = 0 \), we can pick up any value for \( q_j^{*,\ell} \), and in particular a value in \( L^2(\nu) \), in the same way if \( \mathbb{P}_X(\ell(X) = j) = 0 \), we can make an arbitrary choice for \( q_j^{*,\ell} \), otherwise, \( Z_j > 0 \), and

\[
\int (q_j^{*,\ell})^2 \, d\nu = Z_j^{-2} \int \exp \left\{ 2 \mathbb{P}_X|\ell(X) = j \left[ \log(p_X) \right] \right\} \, d\nu 
\leq Z_j^{-2} \mathbb{P}_X|\ell(X) = j \left( \int p_X^2 \, d\nu \right) \leq Z_j^{-2} \mathbb{P}_X(\ell(X) = j)^{-1} \mathbb{P}_X \left( \int p_X^2 \, d\nu \right) < \infty
\]

Then according to Proposition 9 on page 13

\[
\mathbb{P}_X \left[ \min_{j \in [1,k]} \mathcal{K}(q_j, p_X) \right] = \inf_{\ell : \mathcal{X} \rightarrow [1,k]} \mathbb{P}_X \left[ \mathcal{K}(q_{\ell(X)}, p_X) \right] 
\geq \inf_{\ell : \mathcal{X} \rightarrow [1,k]} \mathbb{P}_X \left[ \mathcal{K}(q_j^{*,\ell}, p_X) \right] \geq \inf_{\ell : \mathcal{X} \rightarrow [1,k]} \mathbb{P}_X \left[ \min_{j \in [1,k]} \mathcal{K}(q_j^{*,\ell}, p_X) \right],
\]

showing that we can restrict the optimization to \( q_j \in L^2(\nu) \). □

### 5. PAC-Bayesian generalization bounds for the linear k-means criterion

In this section, we derive non-asymptotic generalization bounds for the linear k-means criterion defined hereafter.

**Definition 12.** Given a random vector \( W \) in a separable Hilbert space \( H \) and a bounded measurable set of parameters \( \Theta \subset H^k \), the k-means linear criterion is defined as

\[
\mathbb{P}_W \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right), \quad \theta \in \Theta.
\]

If \( W_1, \ldots, W_n \) are \( n \) independent copies of \( W \), the empirical linear k-means criterion is defined by taking the expectation with respect to the empirical measure \( \overline{\mathbb{P}}_W = \frac{1}{n} \sum_{i=1}^{n} \delta_{W_i} \), instead of integrating with respect to \( \mathbb{P}_W \).
Using a change of representation based on the kernel trick, we will show that all the criteria we defined so far can be rewritten as linear $k$-means criteria in suitable spaces of coordinates.

Consequently, our approach will be to prove a generalization bound for the linear $k$-means criterion and to study its consequences for the other criteria.

To reach a $O\left(\sqrt{\frac{k}{n}}\right)$ speed up to logarithmic factors, we will borrow ideas from the classical chaining method used to upper bound the expected supremum of Gaussian processes (see [7]). However, we will transpose the idea of chaining into the setting of PAC-Bayesian deviation inequalities. To obtain dimension free bounds, we will use a sequence of perturbations of the parameter by isonormal processes with a variance parameter ranging in a geometric grid. This multiscale perturbation scheme will play the same role as the $\delta$-nets in classical chaining.

Let us begin with an existence result.

**Proposition 13.** In the setting of Definition 12 on the preceding page, let us assume that $\|W\|_\infty = \text{ess sup}_P W \| W \| < +\infty$. There is $\theta^* \in \Theta$, the weak closure of $\Theta$, such that

$$P_W \left( \min_{j \in [1,k]} \langle \theta^*_j, W \rangle \right) = \inf_{\theta \in \Theta} P_W \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right).$$

Moreover $\|\theta^*\| \leq \|\Theta\| \overset{\text{def}}{=} \sup_{\theta \in \Theta} \|\theta\|$.

**Proof.** This is inspired by the proof of Theorem 3.2 in [16]. Let us begin with the second statement. Since $\theta \mapsto \|\theta\| = \sup_{\theta' \in H^k, \|\theta'\| = 1} \langle \theta', \theta \rangle$ is weakly lower semicontinuous, $\|\Theta\| \leq \|\Theta\|$, so that in particular $\|\theta^*\| \leq \|\Theta\|$. Moreover, for any $w \in H$,

$$H^k \rightarrow \mathbb{R}$$

$$\theta \mapsto \min_{j \in [1,k]} \langle \theta_j, w \rangle$$

is weakly continuous, since, by definition of the weak topology of $H^k$, $\theta \mapsto \langle \theta_j, w \rangle$ are weakly continuous, and taking a finite minimum is a continuous operation.

Let $(\theta_n)_{n \in \mathbb{N}}$ be a bounded sequence in $H^k$, converging weakly to $\theta$. By the dominated convergence theorem

$$\lim_{n \rightarrow \infty} P_W \left( \min_{j \in [1,k]} \langle \theta_n, W \rangle \right) = P_W \left( \lim_{n \rightarrow \infty} \min_{j \in [1,k]} \langle \theta_n, W \rangle \right)$$

$$= P_W \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right),$$

since $\min_{j \in [1,k]} \langle \theta_n, W \rangle \leq \|\theta_n\| \|W\|_\infty$. Thus

$$\mathcal{R} : \theta \mapsto P_W \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right)$$

is weakly continuous on $\overline{\Theta}$. But the unit ball, and therefore any ball of $H^k$, is weakly compact, so that $\overline{\Theta}$ being weakly closed and bounded is also weakly compact. Consequently, $\mathcal{R}$ reaches its minimum on $\overline{\Theta}$ at some (non necessarily unique) point $\theta^* \in \overline{\Theta}$. Therefore

$$\mathcal{R}(\theta^*) = \inf_{\theta \in \overline{\Theta}} \mathcal{R}(\theta) = \inf_{\theta \in \Theta} \mathcal{R}(\theta),$$
the last equality being due to the fact that $\mathcal{R}$ is weakly continuous.

Note that we used the weak topology, since the unit ball of $H^k$ is not strongly compact when the dimension of $H$ is infinite. □

We will prove generalization bounds based on the following PAC-Bayesian lemma. We will use it as a workhorse to produce all the deviation inequalities necessary to achieve our goals. Combined with Jensen’s inequality, it will also produce bounds in expectation.

**Lemma 14.** Consider two measurable spaces $\mathcal{F}$ and $W$, a prior probability measure $\pi \in \mathcal{M}_1^+(\mathcal{F})$ defined on $\mathcal{F}$, and a measurable function $h : \mathcal{F} \times W \to \mathbb{R}$. Let $W \in W$ be a random variable and let $(W_1, \ldots, W_n)$ be a sample made of $n$ independent copies of $W$. Let $\lambda$ be a positive real parameter.

\[
\mathbb{P}_{W_1, \ldots, W_n}\exp\left\{ \sup_{\rho \in \mathcal{M}_1^+} \sup_{\eta \in \mathbb{N}} \left\{ \int \min\left\{ \eta, -\lambda \sum_{i=1}^{n} h(\theta', W_i) \right\} - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} \right\} \leq 1.
\]

Consequently, for any $\delta \in [0, 1]$, with probability at least $1 - \delta$,

\[
\sup_{\rho \in \mathcal{M}_1^+} \sup_{\eta \in \mathbb{N}} \left\{ \int \min\left\{ \eta, -\lambda \sum_{i=1}^{n} h(\theta', W_i) \right\} - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} \mathbb{P}_{\rho} d\rho \leq \log(\delta^{-1}).
\]

Note that the role of $\eta$ in this formula is to give a meaning to the integration with respect to $\rho$ in all circumstances.

**Proof.** We follow here the same arguments as in the proof of Proposition 1.7 in [19]. Remark that the supremum in $\rho$ can be restricted to the case when $\mathcal{K}(\rho, \pi) < \infty$, and recall that in this case $\rho \ll \pi$ and $\mathcal{K}(\rho, \pi) = \int \log \left( \frac{d\rho}{d\pi} (\theta') \right) d\rho(\theta')$. Note also that

\[
\int 1 \left( \frac{d\rho}{d\pi} (\theta') > 0 \right) d\rho(\theta') = \int 1 \left( \frac{d\rho}{d\pi} (\theta') > 0 \right) \frac{d\rho}{d\pi} (\theta') d\pi(\theta') = \int \frac{d\rho}{d\pi} (\theta') d\pi(\theta') = 1.
\]

Applying Jensen’s inequality, we get

\[
\begin{align*}
\exp\left\{ \sup_{\rho \in \mathcal{M}_1^+} \sup_{\eta \in \mathbb{N}} \int \min\left\{ \eta, -\lambda \sum_{i=1}^{n} h(\theta', W_i) \right\} - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} & \\
\leq \sup_{\eta \in \mathbb{N}} \sup_{\rho \in \mathcal{M}_1^+} \int \exp\left\{ \min\left\{ \eta, -\lambda \sum_{i=1}^{n} h(\theta', W_i) \right\} - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} d\rho(\theta')^{-1} d\rho(\theta')
\end{align*}
\]
Let us put

\[ Y' = \sup_{\rho \in \mathcal{M}_1^c(Y)} \sup_{\eta \in \mathbb{N}} \int \exp \left\{ \min \left\{ \eta, -\lambda \sum_{i=1}^{n} h(\theta', W_i) - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} \right\} d\pi(\theta') \]

and

\[ Y = \log \int \exp \left\{ -\lambda \sum_{i=1}^{n} h(\theta', W_i) - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} d\pi(\theta'). \]

We just proved that \( Y' \leq Y \). Moreover, \( Y \) is measurable, according to Fubini’s theorem for non-negative functions. Therefore \( Y \) is a random variable. Note that we did not prove that \( Y' \) itself is measurable. Remark now that

\[
\mathbb{P}_{W_1, \ldots, W_n}[\exp(Y)] = \mathbb{P}_{W_1, \ldots, W_n} \int \exp \left\{ -\lambda \sum_{i=1}^{n} h(\theta', W_i) - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} d\pi(\theta'),
\]

\[
= \mathbb{P}_{W_1, \ldots, W_n} \mathbb{F} \int \exp \left\{ -\lambda \sum_{i=1}^{n} h(\theta', W_i) - n \log \left[ \mathbb{P}_W \exp \left[ -\lambda h(\theta', W) \right] \right] \right\} d\pi(\theta')
\]

\[
= \int \left( \mathbb{I} \left( \mathbb{P}_W \left[ \exp \left( -\lambda h(\theta', W) \right) \right] < +\infty \right) \prod_{i=1}^{n} \frac{\mathbb{P}_W \left[ \exp \left( -\lambda h(\theta', W_i) \right) \right]}{\mathbb{P}_W \left[ \exp \left( -\lambda h(\theta', W) \right) \right]} \right) d\pi(\theta') \leq 1,
\]

proving the first part of the lemma. From Markov’s inequality,

\[
\mathbb{P}(Y \geq \log(\delta^{-1})) \leq \delta \mathbb{P}_{W_1, \ldots, W_n}[\exp(Y)] \leq \delta.
\]

Consequently \( \mathbb{P}(Y \leq \log(\delta^{-1})) \geq 1 - \delta \). We have proved that the non necessarily measurable event \( Y' \leq \log(\delta^{-1}) \) contains the measurable event \( Y \leq \log(\delta^{-1}) \) whose probability is at least \( 1 - \delta \).

We are now ready to state and prove our generalization bounds for the linear \( k \)-means criterion.
LEMA 15. Let $W$ be a random vector in a separable Hilbert space $H$. Let $(W_1, \ldots, W_n)$ be a sample made of $n$ independent copies of $W$. Let $\Theta \subset H^k$ be a bounded measurable set of parameters. Define

$$\|\Theta\| = \sup \left\{ \left( \sum_{j=1}^{k} \|\theta_j\|^2 \right)^{1/2} : \theta \in \Theta \right\} < \infty$$

and assume that, for some real valued parameters $a$ and $b$,

$$P_W\left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \in [a, b] \text{ for any } \theta \in \Theta \right) = 1.$$

Assume also that $\|W\|_\infty \overset{\text{def}}{=} \text{ess sup}_{P_W} \|W\| < \infty$.

Our first result gives an observable upper bound for the $k$-means criterion, provided that the above parameters are known or upper bounded by known quantities.

For any $k \geq 2$, any $n \geq 2k$ and any $\delta \in [0,1]$, with probability at least $1 - \delta$, for any $\theta \in \Theta$,

$$P_W\left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right) \leq P_W\left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right) + \left( \frac{\log(n/k)}{\log(2)} \frac{8 \log(k)}{n} + 2 \sqrt{\frac{\log(k)}{n}} \right) \|\Theta\| \|W\|_\infty$$

$$+ \sqrt{\frac{(\sqrt{2} + 1)(k(b - a)^2 + 2 \log(ek)\|W\|_2^2 \|\Theta\|^2)}{n}} + \sqrt{\frac{2 \log(\delta^{-1})}{2n}} (b - a),$$

where $P_{\delta W} = \frac{1}{n} \sum_{i=1}^{n} \delta_{W_i}$ is the empirical measure.

Our second result deals with the excess risk with respect to a non random reference parameter $\theta^* \in \Theta$.

If $\theta^* \in \Theta$ is a non random value of the parameter, with probability at least $1 - \delta$, for any $\theta \in \Theta$,

$$\left( P_W - P_W \right) \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle - \min_{j \in [1,k]} \langle \theta^*_j, W \rangle \right)$$

$$\leq \left( \frac{\log(n/k)}{\log(2)} \frac{8 \log(k)}{n} + 2 \sqrt{\frac{\log(k)}{n}} \right) \|\Theta\| \|W\|_\infty$$

$$+ \sqrt{\frac{(\sqrt{2} + 1)(k(b - a)^2 + 2 \log(ek)\|W\|_2^2 \|\Theta\|^2)}{n}} + \sqrt{\frac{2 \log(\delta^{-1})}{2n}} (b - a).$$

Our third result draws the consequences of this excess risk bound for an $\varepsilon$-minimizer $\hat{\theta}$.

In the case when the estimator $\hat{\theta}(W_1, \ldots, W_n) \in \Theta$ is such that $P_{W_1,\ldots,W_n}$ almost surely

$$P\left( \min_{j \in [1,k]} \langle \hat{\theta}_j, W \rangle \right) \leq \inf_{\theta \in \Theta} P\left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right) + \varepsilon,$$

$$P_W\left( \min_{j \in [1,k]} \langle \hat{\theta}_j, W \rangle \right) - \inf_{\theta \in \Theta} P_W\left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right) - \varepsilon \text{ satisfies the same bound with at least the same probability.}$$
Moreover, the expected excess risk satisfies

\[
\mathbb{P}_{W_1,\ldots,W_n} \left[ \mathbb{P}_W \left( \min_{j \in [1,k]} \langle \hat{\theta}_j, W \rangle \right) - \inf_{\theta \in \Theta} \mathbb{P}_W \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right) \right] \\
\leq \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8 \log(k)}{n} + 2 \frac{\log(k)}{n}} \right) \|\Theta\| \|W\|_{\infty} \\
+ \sqrt{\frac{(\sqrt{2} + 1) \left( k(b-a)^2 + 2 \log(e) \|W\|_{\infty}^2 \|\Theta\|^2 \right)}{n}} + \varepsilon.
\]

**Proof.** Assume without loss of generality that \( H = \ell^2 \subset \mathbb{R}^N \). Let

\[
\rho_{\theta'}|\theta = \mathbb{P}_{\theta + \beta^{-1/2}\varepsilon, i \in \mathbb{N}}, \quad \theta \in \mathbb{R}^N,
\]

be a Gaussian conditional probability distribution with values in \( \mathcal{M}_+^1(\mathbb{R}^N) \), where \( \varepsilon_i, i \in \mathbb{N} \) is an infinite sequence of independent standard normal random variables. When \( \theta \) and \( \theta' \in \mathbb{R}^{k \times N} \) are made of \( k \) infinite sequences of real numbers, let

\[
\rho_{\theta'}|\theta = \bigotimes_{j=1}^{k} \rho_{\theta'_j}|\theta_j
\]

be the tensor product of the previously defined conditional probability distributions. Let \( W \) be a random vector in the separable Hilbert space \( \ell^2 \subset \mathbb{R}^N \). Consider the measurable functions

\[
f(\theta, w) = \min_{j \in [1,k]} \langle \theta_j, w \rangle, \quad \theta \in \mathbb{R}^{k \times N}, w \in \ell^2,
\]

where the scalar product is extended beyond \( \ell^2 \) as follows. For any \( u, v \in \mathbb{R}^N \), let us define \( \langle u, v \rangle \) as

\[
\langle u, v \rangle = \begin{cases} 
\lim_{s \to \infty} \sum_{t=0}^{s} u_t v_t, & \text{when } \limsup_{s \to \infty} \sum_{t=0}^{s} u_t v_t = \liminf_{s \to \infty} \sum_{t=0}^{s} u_t v_t \in \mathbb{R}, \\
0, & \text{otherwise}.
\end{cases}
\]

Remark that this extension is measurable, but not bilinear.

Our strategy will be to decompose the opposite of the centered empirical risk

\[
\left( \mathbb{P}_W - \mathbb{P}_W \right) \left[ f(\theta, W) \right]
\]

into

\[
(10) \quad \left( \mathbb{P}_W - \mathbb{P}_W \right) \left[ f(\theta, W) \right] = \left( \mathbb{P}_W - \mathbb{P}_W \right) \left( \delta_{\theta}|\theta - \rho_{\theta'}|\theta \right) \left[ f(\theta', W) \right]
\]

\[\text{small perturbation}\]

\[+ \sum_{q=1}^{p} \left( \mathbb{P}_W - \mathbb{P}_W \right) \left( \rho_{\theta'}^{2^q-1} - \rho_{\theta'}^{2^q} \right) \left[ f(\theta', W) \right]
\]

\[\text{chain of intermediate scales}\]

\[+ \left( \mathbb{P}_W - \mathbb{P}_W \right) \rho_{\theta'}^{2^p} \left[ f(\theta', W) \right],
\]

\[\text{big perturbation}\]

where \( \delta_{\theta'}|\theta \) is the Dirac (or identity) transition kernel and \( \rho_{\theta'}^{2^q} \) is the transition kernel \( \rho_{\theta'}|\theta \) iterated \( 2^q \) times.

Let

\[
\overline{f}(\theta, w) = f(\theta, w) - \mathbb{P}_W \left( f(\theta, W) \right), \quad \theta \in \mathbb{R}^{k \times N}, w \in \ell^2,
\]
be the centered loss function.

We will first apply the PAC-Bayesian inequalities of Lemma 14 on page 17 to the function 

\[ h(\theta', w) = (\delta_{\theta''|\theta'} - \rho_{\theta''|\theta'}) \left[ \bar{f}(\theta'', w) \right] = \bar{f}(\theta', w) - \rho_{\theta''|\theta'} \left[ \bar{f}(\theta'', w) \right], \quad \theta' \in \mathbb{R}^{k \times \mathbb{N}}, \ w \in \ell^2 \]

and to the reference measure \( \pi_{\theta'} = \rho_{\theta'|\theta=0} \).

**Lemma 16.** The function \( h \) satisfies

\[
(\pi_{\theta'} \otimes P_W) \left( |h(\theta', w)| \leq 2 \sqrt{2\log(k)/\beta} \|W\|_\infty \right) = 1,
\]

where \( \|W\|_\infty = \text{ess sup}_{P_W} \|W\| \).

**Proof.** Remark that for any \( w \in \ell^2 \), \( \pi_{\theta'} \) almost surely,

\[
(\delta_{\theta''|\theta'} - \rho_{\theta''|\theta'}) \left[ f(\theta'', w) \right] = \rho_{\theta''|\theta'} \left( \min_j \langle \theta_j', w \rangle - \min_j \langle \theta_j'', w \rangle \right) \leq \rho_{\theta''|\theta'} \left( \max_j \langle \theta_j'' - \theta_j', w \rangle \right),
\]

since in this situation, the first case in the extended definition of the scalar product applies with probability one (according to Kolmogorov’s three series theorem). Considering that under \( \rho_{\theta''|\theta'} \), \( \langle \theta_j'' - \theta_j', w \rangle \), \( j \in [1, k] \) are \( k \) independent centered real random variables with variance \( \|w\|^2/\beta \) and applying a classical maximal inequality for the expectation of the maximum of \( k \) standard normal variables (see section 2.5 in [7]), we get that

\[
(\delta_{\theta''|\theta'} - \rho_{\theta''|\theta'}) \left[ f(\theta', w) \right] \leq \sqrt{2 \log(k)/\beta} \|w\|.
\]

Reasoning in a similar way for the opposite, we get

\[
-(\delta_{\theta''|\theta'} - \rho_{\theta''|\theta'}) \left[ f(\theta', w) \right] \leq \rho_{\theta''|\theta'} \left( \max_j \langle \theta_j' - \theta_j'', w \rangle \right) \leq \sqrt{2 \log(k)/\beta} \|w\|.
\]

The lemma follows from the definition of \( h \). \qed

Applying Lemma 14 on page 17 to \( h : \mathbb{R}^{k \times \mathbb{N}} \times \ell^2 \rightarrow \mathbb{R}, \pi = \rho_{\theta'|\theta=0} \) and restricting the supremum in \( \rho \in \mathcal{M}_+(\mathbb{R}^{k \times \mathbb{N}}) \) to \( \rho \in \{ \rho_{\theta'|\theta} : \theta \in (\ell^2)^k \} \), we get

\[
P_{W, \ldots, W_n} \left\{ \exp \sup_{\theta \in (\ell^2)^k} \left[ n\lambda (P_W - P_W) (\rho_{\theta'|\theta} - \rho_{\theta''|\theta}) f(\theta', W) \right. \right.
\]

\[
\left. - n\rho_{\theta'|\theta} \left[ \log \left( P_W \left[ \exp \left( -\lambda h(\theta', W) \right) \right] \right) - \frac{\beta\|\theta\|^2}{2} \right] \right\} \leq 1,
\]

where we have let \( \eta \) go to \( +\infty \), using monotone convergence (since \( h \) is bounded from the previous lemma) and where we have computed

\[
\mathcal{K}(\rho_{\theta'|\theta}, \pi) = \sum_{j=1}^k \mathcal{K}(\rho_{\theta'|\theta}, \rho_{\theta_j'|0})
\]

\[
= \sum_{j=1}^k \sum_{i \in \mathbb{N}} \mathcal{K}(\mathcal{N}(\theta_{j,i}, \beta^{-1}), \mathcal{N}(0, \beta^{-1})) = \frac{\beta}{2} \sum_{j=1}^k \sum_{i \in \mathbb{N}} \theta_{j,i}^2 = \frac{\beta\|\theta\|^2}{2}.
\]
Apply now Jensen’s inequality and devide by $n\lambda$ to get
\[
\mathbb{P}_{W_1 \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \left[ \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta} - \rho_{\theta' | \theta}^2 \right) f(\theta', W) \right] - \lambda^{-1} \rho_{\theta' | \theta} \left[ \log \left( \mathbb{P}_W \left[ \exp \left( -\lambda h(\theta', W) \right) \right] \right) - \beta \|\theta\|^2/2n\lambda \right] \right\} \leq 0.
\]
From Hoeffding’s inequality, since $\mathbb{P}_W \left( h(\theta', W) = 0, \pi_{\theta'} \right)$ almost surely,
\[
\mathbb{P}_W \left[ \exp \left( -\lambda h(\theta', W) \right) \right] \leq \exp \left( \frac{\lambda^2}{2} \sup_{\theta \in \Theta} \mathbb{E} h(\theta', W)^2 \right) \leq \exp \left( \frac{4\lambda^2}{\beta} \log(k) \|W\|^2_{\infty} \right).
\]
Considering a measurable bounded subset $\Theta \subset (\ell^2)^k$, we deduce that
\[
\mathbb{P}_{W_1 \ldots, W_n} \left[ \sup_{\theta \in \Theta} \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta} - \rho_{\theta' | \theta}^2 \right) f(\theta', W) \right] \leq \frac{4\lambda}{\beta} \log(k) \|W\|^2_{\infty} + \frac{\beta \|\Theta\|^2}{2n\lambda}.
\]
In order to minimize the right-hand side, choose
\[
\lambda = \frac{\beta \|\Theta\|}{\sqrt{8n \log(k) \|W\|_{\infty}}}
\]
and define
\[
F = \|W\|_{\infty} \|\Theta\| \sqrt{\frac{1}{n} \log(k)}.
\]
We get
\[
\mathbb{P}_{W_1 \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \left[ \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta} - \rho_{\theta' | \theta}^2 \right) f(\theta', W) \right] \right\} \leq F.
\]
For any integer $q$, the iterated transition kernel $\rho_{\theta' | \theta}^{2^q}$ is equal to $\rho_{\theta' | \theta}$ with $\beta$ replaced by $2^{-q}\beta$. As $F$ is independent of $\beta$, we therefore deduce that
\[
\mathbb{P}_{W_1 \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \left[ \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta}^{2^q} - \rho_{\theta' | \theta}^{2^q} \right) f(\theta', W) \right] \right\} \leq F.
\]
Summing up for $q = 1$ to $p$, where $p$ is to be chosen later, and exchanging $\sum_q$ and $\sup_{\theta}$, we deduce that
\[
\mathbb{P}_{W_1 \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \left[ \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta} - \rho_{\theta' | \theta}^{2^q} \right) f(\theta', W) \right] \right\} \leq \mathbb{P}_{W_1 \ldots, W_n} \left\{ \sum_{q=1}^{p} \sup_{\theta \in \Theta} \left[ \left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \left( \rho_{\theta' | \theta}^{2^{q-1}} - \rho_{\theta' | \theta}^{2^q} \right) f(\theta', W) \right] \right\} \leq pF.
\]
As we are interested in bounding from above $\left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) f(\theta, W)$, according to the decomposition formula (10) on page 20, there remains to upper bound
\[
(\mathbb{P}_W - \overline{\mathbb{P}}_W) \left( \delta_{\theta' | \theta} - \rho_{\theta' | \theta} \right) \left[ f(\theta', W) \right]
\]
and $\left( \mathbb{P}_W - \overline{\mathbb{P}}_W \right) \rho_{\theta' | \theta}^{2^q} \left[ f(\theta', W) \right],$

or with a change of notation
\[
(\mathbb{P}_W - \overline{\mathbb{P}}_W) \rho_{\theta' | \theta} \left[ f(\theta', W) \right].
\]
An almost sure bound for (12) is provided by Lemma 16 on page 21, since (12) is equal to \( \mathbb{P}_W[h(\theta, W)] \). To bound (14), introduce the influence function

\[
\psi(x) = \begin{cases} 
\log(1 + x + x^2/2), & x \geq 0, \\
-\log(1 - x + x^2/2), & x \leq 0
\end{cases}
\]

and put

\[
\tilde{f}(\theta, W) = f(\theta, W) - \frac{a + b}{2}.
\]

The function \( \psi \) is chosen to be symmetric and to satisfy

\[
\psi(x) \leq \log(1 + x + x^2/2), \quad x \in \mathbb{R},
\]

since we can check that

\[
\log(1 + x + x^2/2) + \log(1 - x + x^2/2) = \log \left[ \left(1 + x^2/2\right)^2 - x^2 \right] = \log(1 + x^4/4) \geq 0.
\]

Decompose (14) into

\[
(P_W - \mathbb{P}_W)\rho_{\theta' | \theta}f(\theta', W) = \rho_{\theta' | \theta}(P_W - \mathbb{P}_W)\tilde{f}(\theta', W)
\]

(17)

\[
= \rho_{\theta' | \theta}(P_W\tilde{f}(\theta', W) - \mathbb{P}_W[\lambda^{-1}\psi[\lambda\tilde{f}(\theta', W)]]]
\]

(18)

\[
+ \rho_{\theta' | \theta}\mathbb{P}_W[\lambda^{-1}\psi[\lambda\tilde{f}(\theta', W)] - \tilde{f}(\theta', W)].
\]

In order to bound (18), note that from lemma 7.2 in [10]

\[
|x - \psi(x)| \leq \frac{x^2}{4(1 + \sqrt{2})}, \quad x \in \mathbb{R}.
\]

Therefore, from the inequalities \((a + b)^2 \leq 2a^2 + 2b^2\) and \(\min_j a_j - \min_j b_j \leq \max_j (a_j - b_j)\), so that \((\min_j a_j - \min_j b_j)^2 \leq \max_j (a_j - b_j)^2\), for any \(\theta \in (\ell^2)^k\), \(P_W\) almost surely,

\[
\rho_{\theta' | \theta}\left[\lambda^{-1}\psi[\lambda\tilde{f}(\theta', W)] - \tilde{f}(\theta', W)\right] \leq \frac{\lambda}{4(1 + \sqrt{2})}\rho_{\theta' | \theta}[\tilde{f}(\theta', W)^2]
\]

\[
\leq \frac{\lambda}{2(1 + \sqrt{2})}\left[\left(\min_j(\theta_j, W) - (a + b)/2\right)^2 + \rho_{\theta' | \theta}(\max_j(\theta_j' - \theta_j, W)^2)\right].
\]

At this point, it remains to bound the variance term \(\rho_{\theta' | \theta}(\max_j(\theta_j' - \theta_j, W)^2)\). Let us remark that

\[
\rho_{\theta' | \theta} \circ (\theta' \mapsto \langle \theta_j' - \theta_j, W \rangle_{j=1}^k) = \mathcal{N}(0, ||W||^2/\beta)^{\otimes k}.
\]

In other words, under \(\rho_{\theta' | \theta}\), the sequence \(\langle \langle \theta_j' - \theta_j, W \rangle, 1 \leq j \leq k \rangle\) is made of \(k\) independent centered normal random variables with variance \(||W||^2/\beta\). Therefore, we need the following maximal inequality.

**Lemma 17.** Let \((\varepsilon_1, \ldots, \varepsilon_k)\) be a sequence of Gaussian random variables such that \(\varepsilon_j \sim \mathcal{N}(0, \sigma^2)\). We have

\[
\mathbb{E}(\max_{1 \leq j \leq k} \varepsilon_j^2) \leq 2\sigma^2 \log(ek).
\]
PROOF.

\[ E\left( \max_{1 \leq j \leq k} \epsilon_j^2 \right) = \int_{\mathbb{R}_+} \mathbb{P}\left( \max_{1 \leq j \leq k} \epsilon_j^2 > t \right) dt \]

\[ \leq \int_{\mathbb{R}_+} \min\left\{ \sum_{j=1}^k \mathbb{P}(\epsilon_j^2 > t), 1 \right\} dt \leq \int_{\mathbb{R}_+} \min\left\{ 2k \mathbb{P}(\epsilon_1 > \sqrt{t}), 1 \right\} dt \]

\[ \leq \int_{\mathbb{R}_+} \min\left\{ k \exp\left( -\frac{t}{2\sigma^2} \right), 1 \right\} dt \leq 2\sigma^2 \log(k) + \int_{2\sigma^2 \log(k)}^{+\infty} k \exp\left( -\frac{t}{2\sigma^2} \right) dt \]

\[ \leq 2\sigma^2 \log(k) + 2\sigma^2 = 2\sigma^2 \log(ek). \]

Accordingly, we obtain \( \mathbb{P}_W \) almost surely,

\[ (20) \quad \rho_{\theta' | \theta}\left[ \lambda^{-1} \psi [\lambda \tilde{f}(\theta', W)] - \tilde{f}(\theta', W) \right] \]

\[ \leq \frac{\lambda}{2(1 + \sqrt{2})} \left[ (\min_j \langle \theta_j, W \rangle - (a + b)/2)^2 + \rho_{\theta' | \theta}\left( \max_j \langle \theta_j' - \theta_j, W \rangle^2 \right) \right] \]

\[ \leq \frac{\lambda}{2(1 + \sqrt{2})} \left[ (b - a)^2/4 + 2 \log(ek) \| W \|_{\infty}^2 / \beta \right]. \]

The right-hand side of this inequality provides an almost sure upper bound for (18). To bound (17), or rather the expectation of an exponential moment of (17), we can write a PAC-Bayesian bound using the influence function \( \psi \). According to Lemma 14 on page 17,

\[ \mathbb{P}_{W_1, \ldots, W_n} \left\{ \exp \sup_{\theta \in \Theta} \left[ -n \lambda \rho_{\theta' | \theta} \mathbb{P}_W \left( \lambda^{-1} \psi [\lambda \tilde{f}(\theta', W)] \right) \right. \right. \]

\[ \left. \left. - n \rho_{\theta' | \theta} \left[ \log \left( \mathbb{P}_W \left[ \exp \left( \psi [\lambda \tilde{f}(\theta', W)] \right) \right] \right) \right] - \frac{\beta \| \theta \|^2}{2} \right\} \leq 1. \]

Indeed, it is easy to check that the integrand of \( \rho_{\theta' | \theta} \) is integrable, so that we can apply the monotone convergence theorem to remove \( \eta \) from the equation produced by Lemma 14. Using the bound (16) on page 23 and removing the exponential according to Jensen’s inequality, we obtain

\[ \mathbb{P}_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \rho_{\theta' | \theta} \left[ \mathbb{P}_W \left( \tilde{f}(\theta', W) \right) - \mathbb{P}_W \left( \lambda^{-1} \psi [\lambda \tilde{f}(\theta', W)] \right) \right] \right] \]

\[ - \frac{\lambda}{2} \rho_{\theta' | \theta} \left[ \mathbb{P}_W \left( \tilde{f}(\theta', W)^2 \right) \right] \right\} \leq \frac{\beta \| \theta \|^2}{2}. \]

Using the maximal inequality stated in Lemma 17 on the previous page to bound the variance term, we get

\[ \mathbb{P}_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} \rho_{\theta' | \theta} \left[ \mathbb{P}_W \left( \tilde{f}(\theta', W) \right) - \mathbb{P}_W \left( \lambda^{-1} \psi [\lambda \tilde{f}(\theta', W)] \right) \right] \right) \]

\[ \leq \lambda \left[ (b - a)^2/4 + 2 \log(ek) \| W \|_{\infty}^2 / \beta \right] + \frac{\beta \| \theta \|^2}{2n \lambda}. \]
This provides an upper bound for (17). Combining it with the upper bound for (18) gives an upper bound for (14) that reads

\[
P_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} (P_W - \overline{P}_W) \rho_{\theta'} | \theta [ f(\theta', W) ] \right\}
\leq \frac{(\sqrt{2} + 1)\lambda}{2} \left[ (b - a)^2 / 4 + 2 \log(ek) \| W \|_\infty^2 / \beta \right] + \beta \| \Theta \|^2 / 2n\lambda.
\]

Choosing

\[
\lambda = \sqrt{\frac{4\beta \| \Theta \|^2}{(\sqrt{2} + 1) \left[ (b - a)^2 + 8 \log(ek) \| W \|_\infty^2 / \beta \right] n}}
\]

gives

\[
P_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} (P_W - \overline{P}_W) \rho_{\theta'} | \theta [ f(\theta', W) ] \right\}
\leq \tilde{F}(\beta)^{\text{def}} \sqrt{\frac{(\sqrt{2} + 1) \left( k(b - a)^2 + 8 \log(ek) \| W \|_\infty^2 \| \Theta \|^2 \right)}{4n}}.
\]

Putting everything together, we obtain

\[
P_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} (P_W - \overline{P}_W) f(\theta, W) \right\} \leq 2 \sqrt{2 \log(k) / \beta} \| W \|_\infty + \tilde{F}(2^{-p}\beta) + pF,
\]

where \( F \) is defined by equation (11) on page 22.

Let us choose \( \beta = 2n\| \Theta \|^{-2} \) and \( p = \left\lfloor \log(n/k) / \log(2) \right\rfloor \), so that

\[2^{-p}\beta \leq 4k\| \Theta \|^{-2}.
\]

We get

\[
P_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} (P_W - \overline{P}_W) f(\theta, W) \right\}
\leq \left( \frac{\log(n/k)}{\log(2)} \right) \sqrt{\frac{8 \log(k)}{n}} + 2 \sqrt{\frac{\log(k)}{n}} \| \Theta \| \| W \|_\infty
\]

\[+ \frac{\sqrt{2 + 1} \left( k(b - a)^2 + 2 \log(ek) \| W \|_\infty^2 \| \Theta \|^2 \right)}{n}.
\]

The upper deviations from this mean are contloled by the extension of Hoeffding’s bound called the bounded difference inequality (see section 6.1 and theorem 6.2 in [7]). It gives with probability at least \( 1 - \delta \)

\[
\sup_{\theta \in \Theta} (P_W - \overline{P}_W) f(\theta, W) \leq P_{W_1, \ldots, W_n} \left\{ \sup_{\theta \in \Theta} (P_W - \overline{P}_W) f(\theta, W) \right\} + \frac{2 \log(\delta^{-1})}{n} (b - a).
\]

This proves the first statement of the lemma. To get the second one, add to the previous inequality

\[
P_{W_1, \ldots, W_n} \left\{ \left( \overline{P}_W - P_W \right) f(\theta^*, W) \right\} = 0
\]
to get

\[
\mathbb{P}_{W_1,\ldots,W_n}\left\{ \sup_{\theta \in \Theta} (P_W - \mathbb{P}_W) \left( f(\theta, W) - f(\theta^*, W) \right) \right\}
\leq \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8 \log(k)}{n} + 2 \frac{\log(k)}{n}} \right) \|\Theta\| \|W\|_{\infty}
\]

\[
+ \sqrt{\frac{(\sqrt{2} + 1) \left( k(b-a)^2 + 2 \log(ek) \|W\|_{\infty}^2 \|\Theta\|^2 \right)}{n}},
\]

and apply the bounded difference inequality to get the deviations. To prove the end of the proposition concerning an estimator \( \hat{\theta} \), apply what is already proved to the weak closure \( \bar{\Theta} \) of \( \Theta \) and to

\[
\theta^* \in \arg\min_{\theta \in \bar{\Theta}} \mathbb{P}_W \left( \min_{j \in [1,k]} \langle \theta, W_i \rangle \right)
\]

that exists due to Proposition 13 on page 16.

6. Generalization bounds for the quadratic \( k \)-means criterion. The most obvious application of the previous lemma is to get a dimension free bound for the usual quadratic \( k \)-means criterion.

**Proposition 18.** Consider a random vector \( X \) in a separable Hilbert space \( H \). Let \((X_1, \ldots, X_n)\) be a sample made of \( n \) independent copies of \( X \). Consider the ball of radius \( B \)

\[
\mathcal{B} = \left\{ x \in H : \|x\| \leq B \right\}
\]

and assume that \( \mathbb{P}(X \in \mathcal{B}) = 1 \) and that \( n \geq 2k \) and \( k \geq 2 \). For any \( \delta \in (0, 1] \), with probability at least \( 1 - \delta \),

\[
\sup_{c \in \mathcal{B}} \left( \mathbb{P}_X - \mathbb{P}_X \right) \left( \min_{j \in [1,k]} \|c_j\|^2 - 2 \langle c_j, X \rangle \right)
\leq B^2 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n} \left( \frac{6\sqrt{2}}{\log(2)} + \frac{6}{\log(n/k)} \right)}
\leq 12.3
\]

\[
+ \frac{1}{\log(n/k)} \sqrt{\frac{2(\sqrt{2} + 1)(17 + 9 \log(k))}{\log(k)}} + 2B^2 \sqrt{\frac{2 \log(\delta^{-1})}{n}}
\leq 16B^2 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n} \left( \frac{2 \log(\delta^{-1})}{n} \right)}.
\]

Concerning the excess risk, for any \( c^* \in \mathcal{B}^k \), with probability at least \( 1 - \delta \),

\[
\sup_{c \in \mathcal{B}^k} \left( \mathbb{P}_X - \mathbb{P}_X \right) \left\{ \left( \min_{j \in [1,k]} \|X - c_j\|^2 \right) - \left( \min_{j \in [1,k]} \|X - c^*_j\|^2 \right) \right\}
\leq 16B^2 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n}} + 4B^2 \sqrt{\frac{2 \log(\delta^{-1})}{n}}.
\]
Consequently, for any $\varepsilon \geq 0$, for any $\varepsilon$-minimizer $\widehat{c}$, that is for any $\widehat{c} \in \mathcal{B}^k$ depending on the observed sample and satisfying
\[
\Pr_X \left( \min_{j \in [1,k]} \|X - \widehat{c}_j\|^2 \right) \leq \inf_{c \in \mathcal{H}^k} \Pr_X \left( \min_{j \in [1,k]} \|X - c_j\|^2 \right) + \varepsilon,
\]
for any $\delta \in ]0,1[$, with probability at least $1 - \delta$,
\[
\Pr_X \left( \min_{j \in [1,k]} \|X - \widehat{c}_j\|^2 \right) \leq \inf_{c \in \mathcal{H}^k} \Pr_X \left( \|X - c_j\|^2 \right)
+ 16 B^2 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n}} + 4 B^2 \sqrt{\frac{2 \log(\delta^{-1})}{n}} + \varepsilon.
\]
Moreover, we also have a bound in expectation with respect to the statistical sample distribution:
\[
\mathbb{E}_{X_1,\ldots,X_n} \left[ \Pr_X \left( \min_{j \in [1,k]} \|X - \widehat{c}_j\|^2 \right) \right] \leq \inf_{c \in \mathcal{H}^k} \Pr_X \left( \|X - c_j\|^2 \right)
+ 16 B^2 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n}} + \varepsilon.
\]

The general meaning of this proposition is that a chaining argument yields a dimension free non asymptotic generalization bound that decreases as $\sqrt{k/n}$ up to logarithmic factors.

**Proof.** We choose to work with the risk function
\[
\min_{j \in [1,k]} \left( \|c_j\|^2 - 2\langle c_j, X \rangle \right) = \min_{j \in [1,k]} \left( \|X - c_j\|^2 \right) - \|X\|^2
\]
because this provides slightly better constants. Introduce $W = (-2X, \gamma B) \in \mathcal{H} \times \mathbb{R}$ and $	heta_j = (c_j, \gamma^{-1}\|c_j\|^2B^{-1})$, where the parameter $\gamma > 0$ will be optimized later on. Remark that
\[
\|c_j\|^2 - 2\langle c_j, X \rangle = \langle \theta_j, W \rangle \in [-B^2, 3B^2].
\]

Note also that
\[
\|W\|^2 \|\theta_j\|^2 \leq B^4 \left(4 + \gamma^2\right) \left(1 + \gamma^{-2}\right) = B^4 \left(5 + \gamma^2 + 4\gamma^{-2}\right)
\]
and optimize the right-hand size, choosing $\gamma = \sqrt{2}$, to get
\[
\|W\|^2 \|\Theta\|^2 \leq 9kB^4,
\]
where
\[
\Theta = \left\{ \left( c_j, 2^{-1/2}B^{-1}\|c_j\|^2 \right)_{j=1}^k \in (\mathcal{H} \times \mathbb{R})^k : c \in \mathcal{B}^k \right\}.
\]
The proposition is then a transcription of Lemma 15 on page 19 together with the simplification
\[
(21) \quad \min \left\{ 4, \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n}} \left( \frac{6\sqrt{2}}{\log(2)} + \frac{6}{\log(n/k)} \right) \right\}
+ \frac{1}{\log(n/k)} \left[ \frac{2\left(2\sqrt{2} + 1\right) \left(17 + 9 \log(k)\right)}{\log(k)} \right]
\]
\[
\leq 16 \log \left( \frac{n}{k} \right) \sqrt{\frac{k \log(k)}{n}}
\]
that holds for any \( k \geq 2 \) and any \( n \geq 2k \) and can be used since \( 4B^2 \) is a trivial bound. Remark that in the three last inequalities of the proposition we can take the infimum on \( c \in H^k \) instead of \( c \in B^k \), since it is in fact reached on \( B^k \).

Thus, all that remains to prove is (21).

Putting \( a = \frac{6\sqrt{2}}{\log(2)} \), \( b = 16 \), \( \rho = n/k \),

\[
\eta = 6 + \sqrt{\frac{2(\sqrt{2} + 1)(17 + 9 \log(k))}{\log(k)}},
\]

\[
f(\rho, k) = \sqrt{\log(k)/\rho \left( a \log(\rho) + \eta(k) \right)},
\]

and \( g(\rho, k) = b \sqrt{\log(k)/\rho \log(\rho)} \),

we have to prove that

\[
\min\{4, f(\rho, k)\} \leq g(\rho, k), \quad \rho \geq 2, k \geq 2.
\]

In other words, we have to prove that, when \( g(\rho, k) < f(\rho, k) \), then \( g(\rho, k) \geq 4 \). This can also be written as

\[
g(\rho, k) \geq 4, \quad \min\{\rho, k\} \geq 2, g(\rho, k) < f(\rho, k).
\]

According to the definitions, this is also equivalent to

\[
\log(\rho) - 2\log(\log(\rho)) \leq 2\log(b/4) + \log(\log(k)), \quad \min\{\rho, k\} \geq 2, (b - a) \log(\rho) \leq \eta(k).
\]

Since \( \eta \) is decreasing and since \( k \mapsto \log(\log(k)) \) is increasing, if the statement is true for \( k = 2 \), it is true for any \( k \geq 2 \). Thus we have to prove that

\[
\log(\rho) - 2\log(\log(\rho)) \leq 2\log(b/4) + \log(\log(2)), \quad \log(2) \leq \log(\rho) \leq \eta(2)/(b - a).
\]

Putting \( \xi = \log(\rho) \), we have to prove that

\[
\xi - 2\log(\xi) \leq 2\log(b/4) + \log(\log(2)), \quad \log(2) \leq \xi \leq \eta(2)/(b - a).
\]

Since \( \xi \mapsto \xi - 2\log(\xi) \) is convex, it is enough to check the inequality at the two ends of the interval, that is when \( \xi \in \{\log(2), \eta(2)/(b - a)\} \), which can be done numerically. More precisely, we have to check that

\[
2\log(b/4) + \log(\log(2)) - \max\{\log(2) - 2\log(\log(2)), \eta(2)/(b - a) - 2\log[\eta(2)/(b - a)]\} \geq 0,
\]

and we get numerically that the left-hand side is larger than the minimum of 0.9 and 0.6. \( \square \)

7. Generalization bounds for the robust \( k \)-means criterion.

**Proposition 19.** Let \( X \) be a random vector in a separable Hilbert space \( H \) and let \( (X_1, \ldots, X_n) \) be a statistical sample made of \( n \) independent copies of \( X \). Consider for some scale parameter \( \sigma > 0 \) the criterion \( R_2 \) of equation (5) on page 7 and its empirical counterpart

\[
\overline{R}_2(c) = 2\sigma^2 \overline{F}_X \left[ 1 - \exp\left( -\frac{1}{2\sigma^2} \min_{j \in [1, k]} \|X - c_j\|^2 \right) \right], \quad c \in H^k.
\]
Consider any \( k \geq 2 \) and any \( n \geq 2k \). For any \( \delta \in ]0, 1[ \), with probability at least \( 1 - \delta \), for any \( c \in H^k \),

\[
\mathcal{R}_2(c) \leq \mathcal{R}_2(c) + 2\sigma^2 \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k \log(k)}{n}} + 2\sqrt{\frac{k \log(k)}{n}} \right.
\]

\[
+ \sqrt{\left( \frac{\sqrt{2} + 1}{n} \right) k \left( 3 + 2\log(k) \right)} + \sqrt{\frac{\log(\delta^{-1})}{2n}} \bigg). 
\]

For any non random family of centers \( c^* \in H^k \), with probability at least \( 1 - \delta \), for any \( c \in H^k \),

\[
\mathcal{R}_2(c) - \mathcal{R}_2(c^*) \leq \mathcal{R}_2(c) - \mathcal{R}_2(c^*) + 2\sigma^2 \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k \log(k)}{n}} + 2\sqrt{\frac{k \log(k)}{n}} \right.
\]

\[
+ \sqrt{\left( \frac{\sqrt{2} + 1}{n} \right) k \left( 3 + 2\log(k) \right)} + \sqrt{\frac{2\log(\delta^{-1})}{n}} \bigg). 
\]

Consequently, for any \( \varepsilon \geq 0 \), if \( \hat{c} \) is an \( \varepsilon \)-minimizer satisfying

\[
\mathcal{R}_2(\hat{c}) \leq \inf_{c \in \mathbb{R}^d \times k} \mathcal{R}_2(c) + \varepsilon,
\]

with probability at least \( 1 - \delta \),

\[
\mathcal{R}_2(\hat{c}) \leq \inf_{c \in \mathbb{R}^d \times k} \mathcal{R}_2(c) + 2\sigma^2 \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k \log(k)}{n}} + 2\sqrt{\frac{k \log(k)}{n}} \right.
\]

\[
+ \sqrt{\left( \frac{\sqrt{2} + 1}{n} \right) k \left( 3 + 2\log(k) \right)} + \sqrt{\frac{2\log(\delta^{-1})}{n}} \bigg) + \varepsilon. 
\]

In the same way, in expectation,

\[
\mathbb{P}_{X_1, \ldots, X_n} \left( \mathcal{R}_2(\hat{c}) \right) \leq \inf_{c \in \mathbb{R}^d \times k} \mathcal{R}_2(c) + 2\sigma^2 \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k \log(k)}{n}} + 2\sqrt{\frac{k \log(k)}{n}} \right.
\]

\[
+ \sqrt{\left( \frac{\sqrt{2} + 1}{n} \right) k \left( 3 + 2\log(k) \right)} + \sqrt{\frac{2\log(\delta^{-1})}{n}} \bigg) + \varepsilon. 
\]

As we can see, the robust criterion has a scale parameter \( \sigma \), that allows to remove all integrability conditions on the sample distribution or boundedness assumptions on the centers.

**Proof.** According to the Aronszajn theorem [2], there exists a mapping \( \Psi : H \to \mathcal{H} \) such that

\[
\exp\left( -\frac{1}{2\sigma^2} \|x - y\|^2 \right) = \langle \Psi(x), \Psi(y) \rangle_{\mathcal{H}}, \quad x, y \in H.
\]

Moreover the reproducing kernel Hilbert space \( \mathcal{H} \), being based on a continuous kernel defined on a separable topological space, is separable according to [13, lemma 4.33 page 130]. We can express the risk as

\[
\mathcal{R}_2(c) = 2\sigma^2 \left[ 1 + \mathbb{P}_W \left( \min_{j \in [1,k]} \langle -\theta_j, W \rangle_{\mathcal{H}} \right) \right], 
\]
where $\theta_j = \Psi(c_j)$ and $W = \Psi(X)$. The proof then follows from Lemma 15 on page 19, taking into account that $\theta_j$ and $W$ belong to the unit ball of $\mathcal{H}$, so that $\|W\|_\infty = 1$ and $\|\Theta\| = \sqrt{k}$. □

8. Generalization bounds for the information $k$-means criterion. In order to apply Lemma 15 on page 19 and obtain a generalization bound, we are going to linearize the information $k$-means algorithm presented in section 4 on page 8, using the kernel trick.

Let us introduce the separable Hilbert space $H = \{(f, x) \in \mathbb{L}^2(\nu) \times \mathbb{R}\}$ equipped with the inner-product

$$\langle h, h' \rangle = \langle h_1, h'_1 \rangle_{\mathbb{L}^2(\nu)} + \mu h_2 h'_2, \quad h = (h_1, h_2), \ h' = (h'_1, h'_2) \in H,$$

where $\mu > 0$ is a positive real parameter to be chosen afterwards. The associated norm is

$$\|(h_1, h_2)\| = \sqrt{\langle h_1, h_1 \rangle_{\mathbb{L}^2(\nu)} + \mu h_2^2} = \sqrt{\int h_1^2 \, d\nu + \mu h_2^2}, \quad h = (h_1, h_2) \in H.$$

Define for any constant $B \in \mathbb{R}_+$

$$\Theta_B = \left\{(q, \mathcal{K}(q, 1)) : q \in \mathbb{L}^1_+(\nu) \cap \mathbb{L}^2(\nu), \int q^2 \, d\nu \leq B^2 \right\} \subset H,$$

this definition being justified by the fact that

$$\mathcal{K}(q, 1) = \int q \log(q) \, d\nu \leq \log\left(\int q^2 \, d\nu\right) < +\infty \quad \text{whenever} \int q^2 \, d\nu < +\infty.$$

**Lemma 20.** Assume that $\text{ess sup}_X \int \log(p_X)^2 \, d\mu_X < \infty$ and $\text{ess sup}_X \int p_X^2 \, d\mu_X < \infty$. Remark first that the smallest information ball containing the support of $\mathbb{P}_{p_X}$ has an information radius

$$\inf_{q \in \mathbb{L}^1_+(\nu)} \text{ess sup}_X \mathcal{K}(q, p_X) \leq \text{ess sup}_X \mathcal{K}(1, p_X)$$

$$= \text{ess sup}_X \int \log(p_X^{-1}) \, d\mu_X \leq \text{ess sup}_X \left(\int \log(p_X) \, d\mu_X\right)^{1/2} < \infty.$$

Define $B = \text{ess sup}_X \left(\int p_X^2 \, d\nu\right)^{1/2} \exp\left[\inf_{q \in \mathbb{L}^1_+(\nu)} \text{ess sup}_X \mathcal{K}(q, p_X)\right] < \infty$ and consider the random variable

$$W = (-\log(p_X), \mu^{-1}) \in H.$$

The following two minimization problems are equivalent

$$\inf_{q \in \mathbb{L}^1_+(\nu)} \mathbb{P}_X \left(\min_{j \in [1,k]} \mathcal{K}(q_j, p_X)\right) = \inf_{\theta \in \Theta_B^k} \mathbb{P}_W \left(\min_{j \in [1,k]} \langle \theta_j, W \rangle_H\right).$$

**Proof.** Let $B' = \text{ess sup}_X \left(\int p_X^2 \, d\nu\right)^{1/2}$ and $C = \text{ess sup}_X \left(\int \log(p_X) \, d\nu\right)^{1/2}$. First let us remark that under the hypothesis of the lemma, the information $k$-means criterion is finite.
Indeed,

\[
\inf_{q \in L^1_\nu} P_X \left( \min_{j \in [1,k]} K(q_j, p_X) \right) \leq P_X \left( K(1, p_X) \right)
\]

\[
= P_X \left( \int \log(p_X^{-1}) \, d\nu \right) \leq C < +\infty.
\]

Now, for any measurable classification function \( \ell : X \to [1,k] \) for which the criterion is finite, we know from Lemma 11 on page 15 that \( q_{\ell}^{*, \ell} \in L^2(\nu) \) and we can remark that

\[
K(q, 1) = \int q \log(q) \, d\nu \leq \log \left( \int q^2 \, d\nu \right),
\]

so that \( q_{\ell}^{*, \ell} \in L^2(\nu) \) implies that \( K(q_{\ell}^{*, \ell}, 1) < +\infty \). So, it is sufficient to conclude the proof to show that \( q_{\ell}^{*, \ell} \in \Theta_B \). As in the proof of Lemma 11 on page 15,

\[
\int (q_{\ell}^{*, \ell})^2 \, d\nu \leq Z_j^{-2} P_X |_{\ell(X) = j} \left( \int p_X^2 \, d\nu \right) \leq Z_j^{-2} B', \quad j \in [1,k].
\]

By Jensen’s inequality, for any \( j \in [1,k] \),

\[
Z_j = \sup_{q \in L^1_\nu} \int q \exp \left\{ P_X |_{\ell(X) = j} \left[ \log(p_X/q) \right] \right\} \, d\nu
\]

\[
\geq \sup_{q \in L^1_\nu} \exp \left\{ P_X |_{\ell(X) = j} \left[ \int q \log(p_X/q) \, d\nu \right] \right\}
\]

\[
= \exp \left\{ - \inf_{q \in L^1_\nu} P_X |_{\ell(X) = j} \left[ K(q, p_X) \right] \right\}.
\]

Hence

\[
Z_j^{-1} \leq \exp \left\{ \inf_{q \in L^1_\nu} \text{ess sup}_X K(q, p_X) \right\} \leq \exp(C).
\]

Therefore

\[
\left( \int (q_{\ell}^{*, \ell})^2 \, d\nu \right)^{1/2} \leq B' \exp \left[ \inf_{q \in L^1_\nu} \text{ess sup}_X K(q, p_X) \right] = B' \exp(C) < \infty,
\]

proving that \( B < \infty \) and that \( q_{\ell}^{*, \ell} \in \Theta_B \), which concludes the proof. \( \square \)

**Proposition 21.** Under the hypotheses of the previous lemma there exists an optimal quantizer \( \theta^* \in \Theta_B^k \) minimizing the \( k \)-means risk, that is such that

\[
E \left( \min_{j \in [1,k]} \langle \theta^*_j, W \rangle \right) = \inf_{\theta \in \Theta_B^k} E \left( \min_{j \in [1,k]} \langle \theta_j, W \rangle \right).
\]
PROOF. Note that

$$\|\Theta_B\| = \sup_{\theta \in \Theta_B} \|\theta\| \leq \sqrt{B^2 + \mu \log(B^2)^2} < +\infty,$$

according to equation (22) on page 30. Therefore $\Theta_B$ is bounded. Applying Proposition 13 on page 16 to $\Theta_B^k$, we find $\bar{\theta} \in \Theta_B^k$, the weak closure of $\Theta_B^k$, such that

$$\mathcal{R}(\bar{\theta}) \overset{\text{def}}{=} \mathbb{P}_W \left( \min_{j \in [1, k]} \langle \bar{\theta}_j, W \rangle \right) = \inf_{\theta \in \Theta_B^k} \mathcal{R}(\theta).$$

Remark now that, since, according to the Donsker Varadhan representation,

$$K(q, 1) = \sup_{h \in \mathbb{L}^2(\nu)} \int hq \, d\nu - \log \left( \int \exp(h) \, d\nu \right),$$

the function $q \mapsto K(q, 1)$ defined on $\mathbb{L}^2(\nu) \cap \mathbb{L}^1_{+, 1}(\nu)$ is weakly lower semicontinuous. Indeed, it is a supremum of weakly continuous function. Accordingly, its epigraph is weakly closed. As $\Theta_B$ belongs to this epigraph, its weak closer also belongs to it. This implies that for each $j \in [1, k]$, $\bar{\theta}_j$ belongs to it, so that $\bar{\theta} = (\langle q_j, y_j \rangle, j \in [1, k])$, where $y_j \geq \mathcal{K}(q_j, 1)$.

Indeed the weak closure of $\Theta_B^k$ is the product $\Theta_B^k$ of $k$ times the weak closure of $\Theta_B$. Let us put $\theta^* = (\langle q_j, \mathcal{K}(q_j, 1) \rangle, j \in [1, k])$. By monotonicity of $\mathcal{R}$ with respect to $y_j$, the corresponding coefficient of $W$ being positive,

$$\inf_{\theta \in \Theta_B^k} \mathcal{R}(\theta) = \mathcal{R}(\bar{\theta}) \geq \mathcal{R}(\theta^*).$$

Since $\theta^* \in \Theta_B^k$, the reverse inequality also holds and $\mathcal{R}(\theta^*) = \inf_{\theta \in \Theta_B^k} \mathcal{R}(\theta)$.

The link we just made between the information $k$-means criterion and the linear $k$-means criterion allows us to apply Lemma 15 on page 19, proving the next proposition.

PROPOSITION 22. Assume that

$$\text{ess sup}_X \left( \int p_X^2 \, d\nu \right) < +\infty \quad \text{and} \quad \text{ess sup}_X \left( \int \log(p_X)^2 \, d\nu \right) < +\infty.$$

Consider the information radius

$$R = \inf_{q \in \mathbb{L}^1_{+, 1}(\nu)} \text{ess sup}_X \mathcal{K}(q, p_X)$$

and the bounds

$$B = \text{ess sup}_X \left( \int p_X^2 \, d\nu \right)^{1/2} \exp(R)$$

and $C = \text{ess sup}_X \left( \int \log(p_X)^2 \, d\nu \right)^{1/2}$.

Introduce the parameter space

$$\Omega_B = \left\{ q \in \mathbb{L}^1_{+, 1}(\nu) \cap \mathbb{L}^2(\nu) : \int q^2 \, d\nu \leq B^2 \right\}.$$
Given \((X_1, \ldots, X_n)\), a sample made of \(n\) independent copies of \(X\), with probability at least \(1 - \delta\), for any \(q \in \Omega^k_B\),

\[
(P_X - P_X) \left( \min_{j \in [1, k]} \mathcal{K}(q_j, p_X) \right) 
\leq \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k\log(k)}{n}} + 2 \sqrt{\frac{k\log(k)}{n}} 
\right.
\left. + \sqrt{\frac{(\sqrt{2} + 1)k(3 + 2\log(k))}{n}} + \sqrt{\frac{\log(\delta^{-1})}{2n}} \right) (BC + 2\log(B)).
\]

For some \(\varepsilon \geq 0\), consider an empirical \(\varepsilon\)-minimizer \(\hat{q}(X_1, \ldots, X_n) \in \Omega^k_B\) satisfying

\[
\mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(\hat{q}_j, p_X) \right) \leq \inf_{q \in \Omega^k_B} \mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(q_j, p_X) \right) + \varepsilon.
\]

For any \(\delta \in ]0, 1[\), with probability at least \(1 - \delta\),

\[
\mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(\hat{q}_j, p_X) \right) \leq \inf_{q \in (L^1_{\nu}, \nu)^k} \mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(q_j, p_X) \right) 
\]
\[
+ \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k\log(k)}{n}} + 2 \sqrt{\frac{k\log(k)}{n}} 
\right.
\left. + \sqrt{\frac{(\sqrt{2} + 1)k(3 + 2\log(k))}{n}} + \sqrt{\frac{2\log(\delta^{-1})}{n}} \right) (BC + 2\log(B)) + \varepsilon.
\]

Moreover, in expectation,

\[
\mathbb{E}_{X_1, \ldots, X_n} \left[ \mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(\hat{q}_j, p_X) \right) \right] \leq \inf_{q \in (L^1_{\nu}, \nu)^k} \mathbb{P}_X \left( \min_{j \in [1, k]} \mathcal{K}(q_j, p_X) \right) 
\]
\[
+ \left( \frac{\log(n/k)}{\log(2)} \sqrt{\frac{8k\log(k)}{n}} + 2 \sqrt{\frac{k\log(k)}{n}} 
\right.
\left. + \sqrt{\frac{(\sqrt{2} + 1)k(3 + 2\log(k))}{n}} \right) (BC + 2\log(B)) + \varepsilon.
\]

**Proof.** Apply Lemma 20 on page 30. Note that, choosing \(\mu = BC^{-1}\log(B^2)^{-1}\), we get

\[
\|\Theta_{B}\|_2^2 \|W\|_\infty^2 \leq k(B^2 + \mu \log(B^2)^2)(C^2 + \mu^{-1}) = k(BC + 2\log(B))^2.
\]

Remark also that for any \(\theta \in \Theta_{B}\), with probability one,

\[
\min_{j \in [1, k]} \langle \theta_j, W \rangle \in [0, \|\Theta_{B}\|\|W\|_\infty] \subset [0, BC + 2\log(B)].
\]

Use these bounds in Lemma 15 on page 19 to conclude the proof. \(\square\)

**Acknowledgements.** We are grateful to Nikita Zhivotovskiy for useful comments and references.
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