A PERTURBATION RESILIENT FRAMEWORK FOR UNSUPERVISED LEARNING

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ABSTRACT

Designing learning algorithms that are resistant to perturbations of the underlying data distribution is a problem of wide practical and theoretical importance. We present a general approach to this problem focusing on unsupervised learning. The key assumption is that the perturbing distribution is characterized by larger losses relative to a given class of admissible models. This is exploited by a general descent algorithm which minimizes an $L$-statistic criterion over the model class, weighting more small losses. We characterize the robustness of the method in terms of bounds on the reconstruction error for the assumed unperturbed distribution. Numerical experiments with KMEANS clustering and principal subspace analysis demonstrate the effectiveness of our method.

1 Introduction

This work proposes an approach to unsupervised learning which is resistant to unstructured contamination of the underlying data distribution. As noted by Hampel [6], “outliers” are an ill-defined concept, and an approach to robust learning, which relies on rules for the rejection of outliers (as in [1]) prior to processing may be problematic, since the hypothesis class of the learning process itself may determine which data is to be regarded as structured or unstructured. Instead of the elimination of outliers – quoting Hampel “data that don’t fit the pattern set by the majority of the data” - in this paper we suggest to restrict attention to “a sufficient portion $\zeta$ of the data in good agreement with one of the hypothesized models”.

To implement the above idea, we propose to minimize an objective function, which averages only the fraction $\zeta$ of the smallest losses for each candidate model. We apply this approach to unsupervised learning, where our analysis includes the search for the mean, KMEANS clustering, principal subspace analysis and sparse coding, among others.

Contributions. This paper makes the following contributions:

- A theoretical analysis of the robustness of the proposed method (Theorem 1). Under the assumption that the data-distribution is a mixture of an unperturbed distribution adapted to our model class and a perturbing distribution, we identify conditions under which we can bound the reconstruction error, when the minimizer of the proposed objective trained from the perturbed distribution is tested on the unperturbed distribution.

- An analysis of generalization (Theorems 4–6). We give dimension-free uniform bounds in terms of Rademacher averages as well as a dimension- and variance-dependent uniform bounds in terms of covering numbers which can outperform the dimension-free bounds under favorable conditions.
**Previous work.** Some elements of our approach have a long tradition. For fixed models the proposed empirical objectives are called $L$-statistics or $L$-estimators. They have been used in robust statistics since the middle of the last century [10] and their asymptotic properties have been studied by many authors (see [16] and references therein). Although influence functions play a certain role, our approach is somewhat different from the traditions of robust statistics. Similar techniques to ours have been experimentally explored in the context of classification [7] or latent variable selection [8]. Finite sample bounds, uniform bounds, the minimization of $L$-statistics over model classes and the so called risk based-objectives however are more recent developments ([14], [15], [9]), and we are not aware of any other general bounds on the reconstruction error of models trained from perturbed data.

**Organization.** In Section 2 we give a brief overview of unsupervised (representation) learning. In Section 3 we present and analyze our method. In Section 4 we discuss an algorithm optimizing the proposed objective and in Section 5 we present numerical experiments with this algorithm. Proofs can be found in the supplementary material.

## 2 Unsupervised learning

Let $S$ be a class of subsets of $\mathbb{R}^d$. This could be the class of singletons, a class of subsets of cardinality $k$, or the class of subspaces of dimension $k$, or a class of compact convex polytopes with $k$ vertices. We call $S$ the model class. For $S \in S$ define the distortion function $d_S : \mathbb{R}^d \to [0, \infty)$ by

$$
 d_S (x) = \min_{y \in S} \| x - y \|^2 \quad \text{for } x \in \mathbb{R}^d.
$$

In most parts our analysis applies also to other distortion measures, for example omitting the square in (1). The chosen form is important for generalization bounds, when we want to bound the complexity of the class $\{ x \mapsto d_S (x) : S \in S \}$ for specific cases. The members of $S$ are either compact sets or subspaces, so the minimum in (1) is always attained.

We write $P (X)$ for the set of Borel probability measures on a locally compact Hausdorff space $X$. If $\mu \in P (\mathbb{R}^d)$, define the probability measure $\mu_S \in P ([0, \infty))$ as the push-forward of $\mu$ under $d_S$, so $\mu_S (A) = \mu \{ x : d_S (x) \in A \}$ for $A \subseteq [0, \infty)$. Now consider the functional $\Phi : P ([0, \infty)) \to [0, \infty)$ defined by

$$
 \Phi (\rho) = \int_0^\infty r d\rho (r) \quad \text{for } \rho \in P.
$$

Then $\Phi (\mu_S) = \mathbb{E}_{X \sim \mu} [d_S (X)]$ is the expected reconstruction error, incurred when coding points by the nearest neighbors in $S$. The measures $\mu_S \in P ([0, \infty))$ and the functional $\Phi$ allow the compact and general description of several problems of unsupervised learning as

$$
 \min_{S \in S} \Phi (\mu_S) = \mathbb{E}_{X \sim \mu} [d_S (X)].
$$

Denote with $S^* = S^* (\mu)$ a global minimizer of (3). If $S$ is the class of singleton sets, then $S^* (\mu)$ is the mean of $\mu$. If it is the class of subsets of cardinality $k$, then $S^* (\mu)$ is the optimal set of centers for KMEANS clustering. If $S$ is the class of $k$-dimensional subspaces, then $S^* (\mu)$ is the principal $k$-dimensional subspace.

The functional $\Phi$ is very sensitive to perturbing masses at large distortions $R$. In the tradition of robust statistics (see e.g. [5] or [16]) this can be expressed in terms of influence functions: let $\delta_R$ be the unit mass at $R > 0$. Then the influence function

$$
 \text{IF} (R; \rho, \Phi) := \frac{d}{dt} \Phi \left( (1 - t) \rho + t \delta_R \right) \bigg|_{t = 0} = R - \Phi (\rho),
$$

can be arbitrarily large, so a single datapoint could already corrupt $S^* (\mu)$.

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1In these cases the set $S$ is the image of a linear operator on a prescribed set of code vectors, see [13]. Our setting is more general, e.g. it includes non-linear manifolds.
3 The proposed method

We now assume that the only available data is from a perturbed distribution $\mu$, where $\mu$ is the mixture of an unperturbed distribution $\mu^*$, which is locally concentrated on the minimizer $S^* = S^*(\mu^*)$, and a perturbing distribution $\nu$ which is unstructured in the sense that it does not concentrate on any of our models. Figure 1 depicts such a situation, when $S$ is the set of singletons and $d = 1$.

We wish to train from the available, perturbed data a model $\hat{S} \in S$, which nearly minimizes the reconstruction error on the unperturbed distribution $\mu^*$. To this end we exploit the assumption that the unperturbed distribution $\mu^*$ is much more strongly concentrated at $S^*$ than the mixture $\mu = (1 - \lambda) \mu^* + \lambda \nu^*$ is at models $S$ away from $S^*$.

If the mixture parameter $\lambda$ is not too large, the concentration of $\mu^*$ causes the cumulative distribution function $F_{\mu^*} : r \mapsto \mu^*[0, r]$ to increase rapidly for small values of $r$, until it reaches the value $\zeta = F_{\mu^*}(r^*)$, where $r^*$ is a critical distortion radius depending on $S^*$. We will consider as irrelevant the remaining mass $1 - \zeta = \mu^*[r^*, \infty)$, which can be attributed to $\nu$ and may arise from outliers or other contaminating effects. We accordingly modify the functional (2) so as to consider only the relevant portion of data, replacing $\Phi(\mu_S)$ by

$$\zeta^{-1} \int_0^{F_{\mu_S}^{-1}(\zeta)} r d\mu_S(r).$$

Since the choice of the hard quantile-thresholding at $\zeta$ is in many ways an ad hoc decision, we might want a more gentle transition of the boundary between relevant and irrelevant data. Let $W : [0, 1] \to [0, \infty)$ be a bounded weight function and define

$$\Phi_W(\rho) = \int_0^\infty r W(F_{\rho}(r)) d\rho(r) \text{ for } \rho \in \mathcal{P}[0, \infty).$$

If $W$ is identically 1 then $\Phi_1 = \Phi$ in (2). If $W = \zeta^{-1} 1_{[0, \zeta]}$ then $\Phi_W$ is the above hard thresholding functional

$$\Phi_W(\rho) = \zeta^{-1} \int_0^{F_{\mu_S}^{-1}(\zeta)} r d\rho(r).$$

We now propose to "robustify" unsupervised learning by replacing the original problem (3) by

$$\min_{S \in S} \Phi_W(\mu_S),$$

and denote a global minimizer by $S^\dagger = S^\dagger(\mu)$. The weight function $W$ is required to be non-increasing and zero on $[\zeta, 1]$ for some critical mass $\zeta < 1$. The parameter $\zeta$ must be chosen on the basis of an estimate of the amount $\lambda$ of perturbing data.

The search for $S^\dagger$ has to rely on finite data. If $\hat{\mu}(X)$ is the empirical measure induced by an i.i.d. sample $X = (X_1, ..., X_n) \sim \mu^*$,
We denote a minimizer of the empirical problem by $\hat{\mu} (X) = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$, then the empirical objective is the plug-in estimate

$$\Phi_W (\hat{\mu} (X)_S) = \frac{1}{n} \sum_{i=1}^{n} d_S (X_i) W \left( \frac{1}{n} \left\{ X_j : d_S (X_j) \leq d_S (X_i) \right\} \right)$$

$$= \frac{1}{n} \sum_{i=1}^{n} d_S (X)_j W \left( \frac{i}{n} \right), \quad (6)$$

where $d_S (X)_j$ is the $i$-th smallest member of $\{d_S (X_1), \ldots, d_S (X_n)\}$. The estimate $\Phi_W (\hat{\mu} (X)_S)$ is an L-statistic $\mathbb{T}$.

We denote a minimizer of the empirical problem by

$$\hat{S} (X) = \arg \min_{S \in \mathcal{S}} \Phi_W (\hat{\mu} (X)_S) \quad (7)$$

In the sequel we study three questions.

1. If the underlying probability measure is a mixture $\mu = (1 - \lambda) \mu^* + \lambda \nu$ of an unperturbed measure $\mu^*$ and a perturbing measure $\nu$, and $S^\dagger = S^\dagger (\mu)$ is the minimizer of (5), under which assumptions will the reconstruction error $\Phi (\mu^*_S)$ incurred by $S^\dagger$ on the unperturbed distribution approximate the minimal reconstruction error $\Phi (\mu^*_S)$?

2. When solving (5) for a finite amount of data $X$, under which conditions can we reproduce the behavior of $S^\dagger$ by the empirical minimizer $\hat{S} (X)$ in (7)?

3. How can the method be implemented and how does it perform in practice?

### 3.1 Resilience to perturbations

Before we address the first question above we make a preliminary observation in the tradition of robust statistics and compare the influence functions of the functional $\Phi_0$ to the proposed $\Phi_W$ with bounded $W$, and $W (t) = 0$ for $\zeta \leq t < 1$. While we saw in (1) that for any $\rho \in \mathcal{P} (0, \infty)$ the influence function $IF (R; \rho, \Phi) = R - \Phi (\rho)$ is unbounded in $R$, we now have for any $R \in \mathbb{R}^{d}$

$$IF (R; \rho, \Phi_W) \leq IF_{\max} (\rho, W) := \int_{0}^{\rho^{-1} (\zeta)} W (F_\rho (r)) F'_\rho (r) dr.$$  

If $W$ is bounded and $\zeta < 1$ the right hand side above is always bounded, which already indicates the improved robustness of $\Phi_W$. The upper bound $IF_{\max}$ on the influence function plays an important role in the subsequent analysis. We also have $IF_{\max} (\rho, \zeta^{-1} [0, \zeta]) = F^{-1} (\zeta) - \Phi_W (\rho)$; see Lemma 2 in the supplement.

Returning now to the data generating mixture $\mu = (1 - \lambda) \mu^* + \lambda \nu$, where $\mu^* \in \mathcal{P} (\mathbb{R}^{d})$ is the the ideal, unperturbed distribution and $\nu \in \mathcal{P} (\mathbb{R}^{d})$ the perturbation, we make the following assumption.

**Assumption A.** There exists $S_0 \in \mathcal{S}, \delta > 0, \beta \in (0, 1 - \lambda)$ and a scale parameter $r^* \in (0, 1)$ (in units of squared euclidean distance), such that for every model $S \in \mathcal{S}$ satisfying $\Phi (\mu^*_S) > \Phi (\mu^*_S_0) + \delta$ we have $F_{\mu^*_S} (r) < \beta F_{\mu^*_S_0} (r)$ for all $r \leq r^*$.

Loosely speaking: on scales up to $r^*$ the perturbed mixture is on no model nearly as concentrated as the unperturbed distribution is on $S_0$, except for models with comparably low reconstruction error to $S_0$. Normally we require $S_0 = S^* (\mu^*)$. For motivating intuition please consult Figure 1 and Figure 2.

**Theorem 1.** Let $\mu^*, \nu \in \mathcal{P} (\mathbb{R}^{d}), \mu = (1 - \lambda) \mu^* + \lambda \nu$, and $\lambda \in (0, 1)$ and suppose there are $S_0, r^*, \delta > 0$ and $\beta \in (0, 1 - \lambda)$, satisfying Assumption A. Suppose that $W$ is nonzero on a set of positive Lebesgue measure, nonincreasing and $W (t) = 0$ for $t \geq \zeta = F_{\mu^*_S_0} (r^*)$. 
Then $\text{IF}_{\max} (\mu_{S_0}, W) > 0$, and if any $S \in \mathcal{S}$ satisfies

$$\Phi_W (\mu_S) - \Phi_W (\mu_{S_0}) \leq \left( 1 - \frac{\beta}{1 - \lambda} \right) \text{IF}_{\max} (\mu_{S_0}, W)$$

then we have that $\Phi (\mu^*_S) \leq \Phi (\mu^*_{S_0}) + \delta$. In particular we always have that $\Phi (\mu^*_{S^1}) \leq \Phi (\mu^*_{S_0}) + \delta$.

Figure 2: Illustration of Theorem 1 for $d = 2$ and $k = 1$ in the case of PSA. The target distribution (dark gray) is concentrated on the subspace $S^*$, while the perturbing distribution (light gray) does not concentrate well on any individual subspace.

Remark 2. We state some important conclusions of the above theorem.

1. A simplifying illustration of Theorem 1 for principal subspace analysis with $d = 2$ and $k = 1$ is provided by Figure 2. The distributions $\mu^*$ and $\nu$ are assumed to have uniform densities $\rho (\mu^*)$ and $\rho (\nu)$ supported on dark gray and light gray areas of the unit disk respectively. Suppose $\beta = \rho (\nu) / \rho (\mu^*) < 1 - \lambda$, let $r^* = \sin^2 (\pi/\rho (\mu^*))$ and $\delta = 4r^*$. If $\Phi (\mu^*_{S^0}) > \Phi (\mu^*_{S^1}) + \delta$ then the direction of the subspace $S$ does not intersect the black part of the unit circle and therefore $F_{\mu_S} (r) \leq \beta F_{\mu^*_{S^0}} (r)$ for all $r \leq r^*$. Thus Assumption A is satisfied and consequently, if $W (t) = 0$ for $t \geq F_{\mu^*_{S^1}} (r^*)$, then $S^1$ must intersect the black part of the unit circle and $\Phi (\mu^*_{S^1}) \leq \Phi (\mu^*_{S^0}) + \delta$.

2. The generic application of this result assumes that $S_0 = S^* (\mu^*)$, but this is not required. Suppose $S$ is the set of singletons and $\mu^*$ is bimodal, say the mixture of distant standard normal distributions, and $\lambda = 0$ for simplicity. Clearly there is no local concentration on the midpoint $S^* (\mu^*)$, but there is on each of the modes. If $S_0$ is the mean of the first mode and $\zeta$ is sufficiently small, then $S^1$ can be near the mean of the other mode, because it has comparable reconstruction error. In this way the result also explains the astonishing behavior of our algorithm in clustering experiments with mis-specified number of clusters.

3. The conditions on $W$ prescribe an upper bound on the cutoff parameter $\zeta$. If the cutoff parameter $\zeta$ is chosen smaller (so that $W (t) = 0$ for $t \geq \zeta \ll F_{\mu^*_{S^1}} (r^*)$), the required upper bound in (8) decreases and it becomes more difficult to find $S$ satisfying the upper bound. This problem becomes even worse in practice, because the bounds on the estimation error also increase with $\zeta$, as we will see in the next section.

3.2 Generalization

Up to this point we were working with distributions and essentially infinite data. Now we address the question to which extent we can obtain the conclusion of Theorem 1 when $S$ is the minimizer $S (X)$ of the plug-in estimate $\hat{\Phi}_W (\hat{X} (X) \mid S)$ for a finite sample $X \sim \mu^n$ (see (7)). This can be settled by a uniform bound on the estimation error for $\Phi_W$.

Proposition 3. Under the conditions of Theorem 1 with $X \sim \mu^n$ we have that

$$\Pr \left\{ \Phi (\mu^*_{S (X)}) \leq \Phi (\mu^*_{S^*}) + \delta \right\} \geq \Pr \left\{ 2 \sup_{S \in \mathcal{S}} \left| \Phi_W (\mu_S) - \Phi_W (\hat{X} (X) \mid S) \right| \leq \left( 1 - \frac{\beta}{1 - \lambda} \right) IC_{\max} (\mu_{S^*}, W) \right\} .$$
In the sequel we give three uniform bounds, which decrease at least as quickly as \( n^{-1/2} \ln n \). The first two are dimension-free and rely on Rademacher and Gaussian averages of the function class \( \{ x \mapsto d(x, S) : S \in S \} \). Bounds for these complexity measures in the practical cases considered can be found in [13]. Our last bound is dimension dependent but may outperform the other two if the variance of the robust objective is small under its minimizer. All three bounds require special properties of the weight function \( W \).

For this section we assume \( \mu \in \mathcal{P}(\mathbb{R}^d) \) to have compact support, write \( \mathcal{X} = \text{support}(\mu) \) and let \( \mathcal{F} \) be the function class

\[
\mathcal{F} = \{ x \mapsto d(x, S) : S \in S \}.
\]

We also set \( \max R = \sup_{f \in \mathcal{F}} \| f \|_{\infty} \).

The first bound is tailored to the weight function \( \zeta^{-1}_{[0,1]} \). It follows directly from the elegant recent results of [9]. For the benefit of the reader we give a proof in the appendix, without any claim of originality and slightly improved constants.

**Theorem 4.** Let \( W = \zeta^{-1}_{[0,1]} \) and \( \eta > 0 \). With probability at least \( 1 - \eta \) in \( X \sim \mu^n \) we have that

\[
\sup_{S \in S} | \Phi_W(\mu_S) - \Phi_W(\hat{\mu}_S(X)) | \leq \frac{2}{\zeta \eta} \mathbb{E}_X R(\mathcal{F}, X) + \frac{R_{\max}}{\zeta \sqrt{n}} \left( 2 + \sqrt{\frac{\ln(2/\eta)}{2}} \right),
\]

where \( \mathbb{E}_X R(\mathcal{F}, X) \) is the Rademacher average

\[
\mathbb{E}_X R(\mathcal{F}, X) = \mathbb{E}_\varepsilon \left[ \sup_{S \in S} \sum_{i=1}^n \varepsilon_i d(X_i, S) \right]
\]

with independent Rademacher variables \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n) \).

The next bound requires boundedness and a Lipschitz property for the weight function \( W \) which can otherwise be arbitrary. We define the norm \( \| W \|_{\infty} = \sup_{t \in [0,1]} | W(t) | \) and seminorm \( \| W \|_{\text{Lip}} = \inf \{ L : \forall t, s \in [0,1], W(t) - W(s) \leq L | t - s | \} \).

**Theorem 5.** For any \( \eta > 0 \)

\[
\sup_{S \in S} | \Phi_W(\mu_S) - \Phi_W(\hat{\mu}_S(X)) | \leq \frac{2\sqrt{\pi} (R_{\max} \| W \|_{\infty} + \| W \|_{\text{Lip}})}{n} \mathbb{E}_X G(\mathcal{F}, X) + R_{\max} \| W \|_{\infty} \sqrt{\frac{2 \ln(2/\eta)}{n}}
\]

where \( G(\mathcal{F}, X) \) is the Gaussian average

\[
G(\mathcal{F}, X) = \mathbb{E}_\gamma \left[ \sup_{S \in S} \sum_{i=1}^n \gamma_i d(X_i, S) \right],
\]

with independent standard normal variables \( \gamma_1, \ldots, \gamma_n \).

Our last result also requires a Lipschitz property for \( W \) and uses a classical counting argument with covering numbers for a variance-dependent bound.

**Theorem 6.** Under the conditions of the previous theorem, with probability at least \( 1 - \eta \) in \( X \sim \mu^n \) we have that for all \( S \in S \)

\[
| \Phi_W(\mu_S) - \Phi_W(\hat{\mu}_S(X)) | \leq \sqrt{2V_S C} + \frac{6R_{\max} (\| W \|_{\infty} + \| W \|_{\text{Lip}}) C + \| W \|_{\infty} R_{\max}}{\sqrt{n}},
\]

where \( V_S \) is the variance of the random variable \( \Phi_W(\hat{\mu}_S(X)) \), and \( C \) is the complexity term

\[
C = kd \ln \left( 16n \| S \|^2 / \eta \right)
\]

if \( S \) is the set of sets with \( k \) elements, or convex polytopes with \( k \) vertices and \( \| S \| = \sup_{x \in \mathcal{S} \in S} \| x \| \), or
Algorithm 1

1: Pick any $S_0 \in \mathcal{S}$
2: $\pi_0 \leftarrow \arg \min_{p \in \text{Sym}_n} \phi_{S_0}(x, p)$
3: for $t = 1, \ldots, T$ do
4: $S_t \leftarrow \mathcal{D}(S_{t-1}, \pi_{t-1})$
5: $\pi_t \leftarrow \arg \min_{p \in S_n} \phi_{S_t}(x, p)$
6: end for
7: return $S_T$

\[ C = kd \ln \left( 16nR_{\max}^2/\eta \right) \]

if $\mathcal{S}$ is the set of set of $k$-dimensional subspaces.

The bound in the last theorem may be considerably smaller than the previous two if $n$ is large and the unperturbed distribution is very concentrated. The last term, which is of order $n^{-1/2}$ does not carry the burden of the complexity measure and decays quickly. The second term contains the complexity, but it decreases as $n^{-1}$. It can be shown from the Efron-Stein inequality that $V_S$ is at most of order $n^{-1}$, so the entire bound is at most of order $n^{-1/2} \ln n$. On the other hand $V_\zeta$ can be very small. For example, if the unperturbed distribution is completely concentrated at $S^*$ and $\zeta$ is chosen appropriately $V_{S^*} = 0$ and, apart from the complexity-free last term the decay is as $n^{-1} \ln n$.

4 Algorithms

In this section we present our algorithm for (approximately) minimizing the robust $L$-statistic $\Phi_W(\tilde{\mu}(X)_S)$ w.r.t. model $S \in \mathcal{S}$. Throughout this section we assume $W$ non-increasing and fixed, and to simplify the notation we remove any reference to it. We abbreviate $\Phi_W(\tilde{\mu}(X)_S)$ with $\hat{\Phi}_S(X)$.

4.1 General Algorithm

Let $x = (x_1, \ldots, x_n)$ be a realization of $X \sim \mu^n$, consider the following function of $S \in \mathcal{S}$

\[ \hat{\Phi}_S(x) = \frac{1}{n} \sum_{i=1}^n W\left( \frac{\pi(i)}{n} \right) d_S(x_i) \]  \hspace{1cm} (9)

where $\pi$ is the ascending ordering of the $d_S(x_i)$ and notice that minimizing (9) is equivalent to minimize (6). Let $p$ any fixed element in $\text{Sym}_n$ and let

\[ \phi_S(x, p) = \frac{1}{n} \sum_{i=1}^n W\left( \frac{p(i)}{n} \right) d_S(x_i). \]

In the following we will leverage the following property of $\phi_S$.

Lemma 7. For any $S \in \mathcal{S}$ and any $p \in \text{Sym}_n$, if $\pi$ is the ascending ordering of the $d_S(x_i)$, then $\phi_S(x, p) \geq \phi_S(x, \pi) = \hat{\Phi}_S(x)$.

We need also the following definition.

Definition 8. A mapping $\mathcal{D} : \mathcal{S} \times \text{Sym}_n \rightarrow \mathcal{S}$ is a Descent Oracle for $\phi_S$ iff for any $S \in \mathcal{S}$ and any $p \in \text{Sym}_n$, $\phi_{\mathcal{D}(S, p)}(x, p) \leq \phi_S(x, p)$.

The algorithm attempt to minimize (9) via alternating minimization of $\phi_S$. At the beginning, it picks an initial model $S_0$ and sort the induced losses in ascending order, i.e. pick the optimal permutation $\pi_0$. Then it starts iterating this two steps by first calling the descent oracle $\mathcal{D}(S_t, \pi_t)$ and then sorting the induced losses. At each step either the permutation $\pi_t$ or the model $S_t$ are fixed. Pseudocode is given in Algorithm 1.

Indeed, at each step the algorithm first finds a descending iteration $S_{t+1}$ of $\phi_{S_t}(x, \pi_t)$ and then sort the losses according to $\pi_{t+1}$, an operation that by Lemma 7 cannot increase the value of $\phi_{S_{t+1}}$. Thus the following holds.

\footnote{Here $\text{Sym}_n$ denotes the set of all $n!$ permutations over $n$ objects.}
Theorem 9. Algorithm 1 is a descent algorithm for the problem of minimizing (9), i.e. for any \( t, \hat{\Phi}_{S_t+1}(x) \leq \hat{\Phi}_{S_t}(x) \).

This algorithm is general and to apply it to a specific learning problem an implementation of the descent oracle is needed. The efficiency of Algorithm 1 depends upon such oracle. In the following we show 2 descent oracles for the cases of KMEANS and PSA. We complement this results with a relative computational lower bound showing that, in general, minimizing (9) is NP-Hard.

Theorem 10. Minimizing (9) for the case of KMEANS when \( k = 1 \) and \( W \) is the hard threshold is NP-Hard.

Notice that in the case of KMEANS when \( W \) is the identity, the problem reduces to finding the optimal KMEANS solution, a problem which is known to be hard. However, KMEANS admits a very simple closed form solution when \( k = 1 \); in some sense minimizing the robust objective is even harder than standard KMEANS.

**k-Means Clustering (KMEANS).** In this case \( S \) is the set of all possible \( k \)-tuples of centers in \( \mathbb{R}^d \) and \( d_S(x) = \min_{c \in S} \| x - c \|_2^2 \). Keeping fixed the permutation \( p \), we consider as descent oracle the following Lloyd-like update for the centers. Each center \( c \in S \) induces a cluster formed by a subset of training points \( x_i, i \in I \) which are closer to \( c \) than every other center (breaking ties arbitrarily). The overall loss of representing point in \( I \) with \( c \) is

\[
\sum_{i \in I} W \left( \frac{p(i)}{n} \right) \| x_i - c \|_2^2
\]

This loss is minimized at

\[
\hat{c} = \frac{1}{\sum_{i \in I} W \left( \frac{p(i)}{n} \right)} \sum_{i \in I} W \left( \frac{p(i)}{n} \right) x_i,
\]

so the following holds.

**Proposition 11.** Given \( S \) and \( p \), the mapping that for every \( c \in S \) returns the \( \hat{c} \) defined above is a descent oracle for KMEANS and its runtime is \( O(nkd) \).

The resulting algorithm can is a generalization of the method proposed in [2].

**Principal Subspace Analysis (PSA).** In this case \( S \) is the set of all possible \( d \times k \) matrices \( U \) such that \( U^T U = I_d \), \( d_S(x) = \| x - U U^T x \|_2^2 \) and

\[
\phi_U(x, p) = \sum_{i=1}^n W \left( \frac{p(i)}{n} \right) \| x - U U^T x_i \|_2^2.
\]

Given \( p \), it is easy to see that the above function is minimized at the matrix \( \hat{U} \) formed by stacking as columns the \( k \) eigenvectors of \( \sum_{i}^n W \left( \frac{p(i)}{n} \right) x_i x_i^T \) associated to the top \( k \) eigenvalues, so the following holds.

**Proposition 12.** Given \( U \) and \( p \), the mapping that returns the \( \hat{U} \) defined above is a descent oracle for PSA and its runtime is \( O(\min\{d^3 + nd^2, n^3 + n^2d\}) \).

5 Experiments

This section presents our experimental results. The purpose of the numerical experiments is to show that:

- Our algorithms for PSA and KMEANS outperform standard SVD, KMEANS++ and the Spherical Depth method (SD) in presence of outliers, while obtain the similar performances on clean data.
- Our algorithms on real data are not too sensitive to the parameters of the weight function. In particular, we show that there exist a wide-range of \( \zeta \) values such that using the hard-threshold function leads to good results.
- In the case of KMEANS our method is able to accurately reconstruct some of the true centers even when the value of \( k \) is miss-specified. This matches the second remark after Theorem 1.
 Implemented Algorithms. For KMEANS++ we used the sklearn implementation fed with the same parameters for the maximum number of iterations $T$ and the initializations $r$ we used for our method. Notice that $T$ is only an upper bound to the number of iterations, the algorithms stop when the difference between the current objective value and the previous one is smaller than $10^{-7}$. To set $r$ we used the largest value before diminishing returns were observed. For standard PSA we compute the SVD of $\sum_i x_i x_i^\top$. The SD method is a general purpose pre-processing technique that is applied on the data before performing KMEANS and PSA (e.g. [3,4]). This method computes a score for each point in the dataset by counting in how many balls, whose antipodes are pairs of points in the data, it is contained. The $1 - \zeta n$ points with the smallest scores are discarded. If the data contain $n$ points, the methods needs to check $O(n^2)$ balls for each of the $n$ point resulting in a runtime of $O(n^3)$. For scalability on real data, we implemented a randomized version of this method that for each point only check $M$ balls picked uniformly at random from the set of all possible balls and used $M = O(n)$; the resulting runtime is $O(n^2)$. All experiments have been run on an standard laptop equipped with an Intel i9 with 8 cores each working at 2.4 GHz and 16 GB of RAM DDR4 working at 2.6 GHz.
5.1 KMEANS Clustering

This subsection presents our experiments for the case of KMEANS clustering on both synthetic and real data and we refer to our method as RKM.

**Synthetic Data.** We run two experiments with artificial data in $\mathbb{R}^2$. In the first experiment, we generated 300 inliers from 3 isotropic Gaussians (100 points each) with variance 0.1 along both axis and mean $(-3, 0)$, $(0, 1)$ and $(3, 0)$ respectively. We then corrupt the data adding 100 points from a fourth isotropic Gaussian centered at $(-1, -5)$ with variance 5 along both axis. For both RKM and KMEANS++ we $T = 10$ and $r = 30$. We initialized RKM with uniform centers and set $\zeta = 0.75$, the same $\zeta$ is used for SD. Results are shown in Figure 3 top left, where it is possible to see that while RKM recovers the true centers, SD and KMEANS++ both fail badly placing one centers in the middle of the two clusters and the other close to the mean of the perturbing distribution. In the second experiment, we generated 300 points from the same 3 inliers Gaussians and set the algorithms with $k = 2$ and $\zeta = 0.6$, while $T$ and $r$ are as above. Results are shown in the top right of Figure 3 where it is possible to see that KMEANS++ and SD – although to a lesser extend – wasted a center to merge 2 clusters, while RKM correctly recovers 2 out of the 3 centers.

**Real Data.** In the synthetic experiments, we choose $\zeta$ according to the exact fraction of outliers, a quantity which is usually unknown in practice. Here we show that there is a wide range of values for $\zeta$ such that RKM performs better than KMEANS++. We used the EMNIST dataset which consists of about 814000 $28 \times 28$ images of digits, lowercase and uppercase letters from the English alphabet arranged in 62 classes. The training data were generated by sampling 1000 0s and 1000 1s as inliers and sampling 33 points from each other class as outliers. The resulting fraction of outliers is about 0.5. The test data consist of all the 0s and 1s in the test set and has a size of about 2000. We run the algorithms with $T = 50$, $r = 30$, $M = 4000$ and $\zeta$ in the range $[0.4, 1]$. For each value of $\zeta$, we measure the reconstruction error of the learned centers on the unperturbed test data. Results are shown in the bottom row of Figure 3. In the lower left, it is possible to see that the centers learned by RKM and SD at the optimal threshold value $\zeta = 0.6$ look good, while the centers found by KMEANS++ are affected by the outliers as the marked grey background reveals. As for the reconstruction error, $\zeta = 0.6$ is the minimizer for both RKM and SD the latter achieves a slightly smaller minimum.

5.2 Principal Subspace Analysis

In this subsection presents our experiments for the case of PSA on both synthetic and real data and refer to our method as DPSA.

**Synthetic Data.** We run a synthetic experiment with artificial data in $\mathbb{R}^2$. We generate 50 points from the uniform distribution over $[-1, 1] \times [-0.1, 0.1]$ as inliers and 50 points for the uniform distribution over $\mathbb{R}_{++} \cup \mathbb{R}_{--} \cap B(0, 1)^2$ as outliers. We run RPSA with $T = 50$, $r = 30$, $\zeta = 0.5$ and initialize $U$ as a normalized Gaussian matrix. We set $k = 1$ for all algorithms. Results are shown in the left plot of Figure 4 where it is possible to see that the principal subspace learned by RPSA is not affected by the outliers, as opposed to SD and PSA.

**Real Data.** Similarly to the case of KMEANS, we tested our method on real data for a range of values of $\zeta$. We used the fashion MNIST dataset which consists of about 70000 $28 \times 28$ images of clothes arranged in 9 classes: tops, trousers, pullovers, coats, dresses, shirts, bags, sneakers, sandals and boots. The training data were generated by sampling 1000 points from each of the shoes class as inliers, and 140 points from each other class as outliers. The resulting fraction of outliers is about 0.2. The test data consist of all the shoes in the test set and has size of about 3000. We run the algorithms we $T = 50$, $r = 5$, $M = 4000$, $k = 2$ and $\zeta$ in the range $[0.5, 1]$. Results are shown in the right plot of Figure 4 where it is possible our algorithm outperforms both PSA and does better than SD.

6 Conclusions and Future Works

We proposed a general framework to design algorithms that are resilient to the presence of outliers and/or to model miss-specification. Our method has strong statistical guarantees, is flexible enough to incorporate many problems in unsupervised learning and is effective in practice as the experiments reveal. On the other hand, several extension can be considered. First, here we studied in details KMEANS and PSA, but our theory also covers the cases of KMEDIAN, sparse coding or non-negative matrix factorization. Second, we believe that this framework can be extended to supervised learning problems such as canonical correlation analysis and partial least squares. Third, our algorithm has only a descent property, and it would be interesting to design algorithms with stronger guarantees such as provable approximation properties.

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\footnote{Here with $\mathbb{R}_{++}$ and $\mathbb{R}_{--}$ we denote the top right and the bottom left orthant of $\mathbb{R}^2$.}
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Supplementary Material

The supplementary material is organized as follows. Appendix A we prove the statistical properties of the proposed method; in particular we prove Theorem 1, 3 and 5. In Appendix B we give a proof of the hardness result described by Theorem 10. Finally, in Appendix C we present additional experiments with the proposed method for the case of K-MEANS.

A The proposed method

We first analyze some basic properties of the functional $\Phi_W$. The following is easily seen to be an alternative definition of $\Phi_W$.

$$K_W(t) = \int_0^t W(u) \, du \quad \text{and} \quad \Phi_W(\rho) = \int_0^\infty r dK_W(F_\rho(r)) \text{ for } \rho \in \mathcal{P}([0, \infty)).$$

From this we find

**Lemma 13.** For $\rho_1, \rho_2 \in \mathcal{P}$ and $W$ bounded

$$\Phi_W(\rho_1) - \Phi_W(\rho_2) = -\int_0^\infty (K_W(F_{\rho_1}(r)) - K_W(F_{\rho_2}(r))) \, dr,$$

and

$$\frac{d}{dt} \Phi_W((1-t)\rho_1 + t\rho_2) = \int_0^\infty W((1-t)F_{\rho_1}(r) + tF_{\rho_2}(r)) (F_{\rho_1}(r) - F_{\rho_2}(r)) \, dr.$$

**Proof.** Since members of $\mathcal{P}$ have finite first moments we have for any $\rho \in \mathcal{P}$ that $r\rho(r, \infty) \to 0$ as $r \to \infty$, so

$$\lim_{r \to \infty} r (K_W(F_{\rho_1}(r)) - K_W(F_{\rho_2}(r))) \leq ||W||_\infty \lim_{r \to \infty} r |\rho_2(r, \infty) - \rho_1(r, \infty)| = 0,$$

and the formula (10) follows from integration by parts. Thus for arbitrary $\rho \in \mathcal{P}$

$$\Phi_W((1-t)\rho_1 + t\rho_2) - \Phi_W(\rho) = -\int_0^\infty (K_W((1-t)F_{\rho_1}(r) + tF_{\rho_2}(r)) - K_W(F_{\rho}(r))) \, dr.$$

Taking the derivative w.r.t. $t$ and using the chain rule and $K_W' = W$ gives the second identity. \qed

We now analyze the influence function of the functional $\Phi_W$.

**Lemma 14.** Let $R \in [0, \infty)$, $\rho \in \mathcal{P}([0, \infty))$

(i) If $W$ is nonnegative, bounded and $W(t) = 0$ for $t \geq \zeta$ and $\zeta < 1$ then

$$IF(R; \rho, \Phi_W) \leq IF_{\text{max}}(\rho, W) := \int_0^{F_\rho^{-1}(\zeta)} W(F_\rho(r)) F_\rho(r) \, dr.$$  

(ii) If $\zeta > 0$, $W = \zeta^{-1}1_{[0, \zeta]}$, $\rho$ is non-atomic and $F_\rho^{-1}(\zeta) = F_\rho^{-1}(\zeta) = F_\rho^{-1}(\zeta)$. Then

$$IC(R; \rho, \Phi_W) = \begin{cases} \zeta^{-1}(R + (\zeta - 1)F_\rho^{-1}(\zeta)) - \Phi_W(\rho) & \text{if } 0 \leq R \leq F_\rho^{-1}(\zeta) \\ F_\rho^{-1}(\zeta) - \Phi_W(\rho) & \text{if } F_\rho^{-1}(\zeta) < R \end{cases}.$$  

**Proof.** (i) In the second conclusion of Lemma 13, letting $\rho_2 = \delta_R$ and taking the limit $t \to 0$ we obtain the influence function

$$IF(R; \rho, \Phi_W) = \int_0^\infty W(F_\rho(r)) (F_\rho(r) - F_{\delta_R}(r)) \, dr.$$  

Part (i) follows.
We prove Theorem 1.

Let \( \Phi \) nonincreasing and \( W \)

Proof. From integration by parts the first term in parenthesis is \( \zeta (F^{-1}_\rho (\zeta) - \Phi_W (\rho)) \). The second term is zero if \( F^{-1}_\rho (\zeta) < R \), otherwise it is \( F^{-1}_\rho (\zeta) - R \). This gives the identity. For the inequality observe that \( R \leq F^{-1}_\rho (\zeta) \) implies \( \zeta (R + (\zeta - 1) F^{-1}_\rho (\zeta)) \leq F^{-1}_\rho (\zeta) \).

\[ \Box \]

A.1 Resilience to perturbations

We prove Theorem 1.

Lemma 15. Let \( S, S^* \in S, \mu \in \mathcal{P}(\mathbb{R}^d) \), and suppose that there exists \( r^* > 0 \) and \( \alpha \in (0, 1) \) such that

\[ \forall r \in (0, r^*) , F_{\mu^*} (r) \leq \alpha F_{\mu^{S*}} (r). \tag{11} \]

If \( W \) is nonzero on a set of positive Lebesgue measure, nonincreasing and \( W (t) = 0 \) for all \( t \geq F_{\mu^{S*}} (r^*) \) then

\[ \Phi_W (\mu_S) - \Phi_W (\mu_{S^*}) \geq (1 - \alpha) \int_0^{r^*} W (F_{\mu^{S*}} (r)) F_{\mu^{S^*}} (r) \, dr = (1 - \alpha) IF_{\mu S^*}, W > 0. \]

Proof. By Lemma 13 and the fundamental theorem of calculus

\[ \Phi_W (\mu_S) - \Phi_W (\mu_{S^*}) = \int_0^\infty \left( \int_{[0,1]} W (sF_{\mu^*} (r) + (1 - s) F_{\mu^{S^*}} (r)) \, ds \right) (F_{\mu^{S^*}} (r) - F_{\mu_S} (r)) \, dr. \]

Suppose first \( r^* \leq r \). If \( W > 0 \) then \( sF_{\mu^*} (r) + (1 - s) F_{\mu^{S^*}} (r) < F_{\mu^{S^*}} (r^*) \leq F_{\mu^{S^*}} (r) \) and therefore \( F_{\mu^*} (r) < F_{\mu^{S^*}} (r^*) \), so the integrand is positive, or else \( W = 0 \). For a lower bound we can therefore restrict the integration in \( r \) to the interval \([0, r^*]\).

If \( r < r^* \) then by (11) \( sF_{\mu^*} (r) + (1 - s) F_{\mu^{S^*}} (r) < F_{\mu^{S^*}} (r^*) \) so \( W (sF_{\mu^*} (r) + (1 - s) F_{\mu^{S^*}} (r)) \geq W (F_{\mu^{S^*}} (r)) \), since \( W \) is nonincreasing. The conclusion follows from (11). \( \Box \)

We restate Assumption A and Theorem 1.

Assumption A. There exists \( S_0 \in S, \delta > 0, \beta \in (0, 1 - \lambda) \) and a scale parameter \( r^* \in (0, 1) \) (in units of squared Euclidean distance), such that for every model \( S \in S \) satisfying \( \Phi (\mu_{S^*}) > \Phi (\mu_{S_0^*}) + \delta \) we have \( F_{\mu_S} (r) < \beta F_{\mu_{S_0}} (r) \) for all \( r \leq r^* \).

Theorem 16. Let \( \mu^*, \nu \in \mathcal{P}(\mathbb{R}^d), \mu = (1 - \lambda) \mu^* + \lambda \nu, \alpha \in (0, 1) \) and suppose there are \( S_0, r^*, \beta > 0 \) and \( 0 < \beta < 1 - \lambda \), satisfying Assumption A. Suppose that \( W \) is nonzero on a set of positive Lebesgue measure, nonincreasing and \( W (t) = 0 \) for \( t \geq \zeta = F_{\mu_{S_0}} (r^*) \).

Proof. Let \( S, S_0 \in S \) and assume that \( \Phi (\mu_{S^*}) > \Phi (\mu_{S_0^*}) + \delta \). Then for \( r \leq r^* \) Assumption A implies \( F_{\mu_S} (r) \leq \beta F_{\mu_{S_0}} (r) \), and the conditions on \( W \) also imply that \( W = 0 \) on \([F_{\mu^{S^*}} (r^*), 1]\). Thus Lemma 15 with \( a = \beta / (1 - \lambda) < 1 \) gives

\[ \Phi_W (\mu_S) - \Phi_W (\mu_{S_0}) \geq \left( 1 - \frac{\beta}{1 - \lambda} \right) IF_{\mu S_0}, W > 0. \]

Thus, if \( \Phi_W (\mu_S) - \Phi_W (\mu_{S_0}) < \left( 1 - \frac{\beta}{1 - \lambda} \right) IF_{\mu S_0}, W \), we must have \( \Phi (\mu_{S^*}) \leq \Phi (\mu_{S_0^*}) + \delta \). The condition (11) is clearly always satisfied by the minimizer \( S^* (\mu) \) of \( \Phi_W (\mu_S) \). \( \Box \)
A.2 Generalization

A second application of Lemma 13 gives a Lipschitz property of \( \Phi_W \) relative to the Wasserstein and Kolmogorov metrics for distributions with bounded support.

**Lemma 17.** For \( \rho_1, \rho_2 \in \mathcal{P} \) with support in \([0, R_{\text{max}}]\) and \( \|W\|_\infty < \infty \)

\[
\Phi_W (\rho_2) - \Phi_W (\rho_1) \leq \|W\|_\infty d_W (\rho_1, \rho_2) \quad \text{and} \quad \Phi_W (\rho_2) - \Phi_W (\rho_1) \leq R_{\text{max}} \|W\|_\infty d_K (\rho_1, \rho_2).
\]

Here \( d_W (\rho_1, \rho_2) = \|F_{\rho_1} - F_{\rho_2}\|_1 \) is the 1-Wasserstein distance and \( d_K (\rho_1, \rho_2) = \|F_{\rho_1} - F_{\rho_2}\|_\infty \) the Kolmogorov-Smirnov distance.

**Proof.** From (10) and Hölder’s inequality we get

\[
\Phi_W (\rho_1) - \Phi_W (\rho_2) = - \int_0^{\infty} \left( \int_{F_{\rho_1}(r)}^{F_{\rho_2}(r)} W(u) \, du \right) \, dr \leq 2 \|W\|_\infty \int_0^{\infty} |F_{\rho_1}(r) - F_{\rho_2}(r)| \, dr.
\]

We can bound the integral either by \( \|F_{\rho_1} - F_{\rho_2}\|_1 = d_W (\rho_1, \rho_2) \), which gives the first inequality, or by

\[
\int_0^{R_{\text{max}}} |F_{\rho_1}(r) - F_{\rho_2}(r)| \, dr \leq \|F_{\rho_1} - F_{\rho_2}\|_\infty \int_0^{R_{\text{max}}} - d_K (\rho_1, \rho_2),
\]

which gives the second inequality. \( \square \)

The Lipschitz properties imply estimation and bias bounds for the plug-in estimator.

**Corollary 18.** Let \( \rho \in \mathcal{P} \) with support in \([0, R_{\text{max}}]\) and \( \|W\|_\infty < \infty \) and suppose that \( \hat{\rho} \) is the empirical measure generated from \( n \) iid observations \( R = (R_1, ..., R_n) \sim \rho^n \)

\[
\hat{\rho}(R) = \frac{1}{n} \sum_{i=1}^{n} \delta_{R_i}.
\]

Then (i)

\[
\Pr \{ |\Phi_W (\rho) - \Phi_W (\hat{\rho}(R))| > t \} \leq 2 \exp \left( -\frac{2nt^2}{R_{\text{max}} \|W\|_\infty^2} \right).
\]

and (ii)

\[
\Phi_W (\rho) - \mathbb{E} [\Phi_W (\hat{\rho}(R))] \leq \frac{R_{\text{max}} \|W\|_\infty}{\sqrt{2nt}}.
\]

**Proof.** (i) By Lemma 17 and the Dvoretzky-Kiefer-Wolfowitz Theorem in the version of Massart [9]

\[
\Pr \{ |\Phi_W (\rho) - \Phi_W (\hat{\rho}(R))| > t \} \leq \Pr \left\{ d_K (\rho, \hat{\rho}(R)) > \frac{t}{R_{\text{max}} \|W\|_\infty} \right\} \leq 2 \exp \left( -\frac{2nt^2}{R_{\text{max}}^2 \|W\|_\infty^2} \right).
\]

(ii) Let \( R' = (R_1, ..., R_n) \) be iid to \( R \). Then
\[ \Phi_W (\rho) - E [ \Phi_W (\hat{\rho} (R))] \leq \| W \|_\infty E [d_W (\rho_1, \hat{\rho} (R))] \]

\[ = \| W \|_\infty E_R \int_0^{R_{\max}} \left| \frac{1}{n} \sum_{i=1}^{\lambda n} 1_{[r_1, \infty)} (t) \right| dt \]

\[ \leq \| W \|_\infty \frac{n}{\sqrt{n}} \int_0^{R_{\max}} \left| \sum_{i=1}^{\lambda n} (1_{[r_1, \infty)} (t) - 1_{[r_1, \infty)} (t)) \right|^2 dt \]

\[ = \| W \|_\infty \int_0^{R_{\max}} \left( \sum_{i=1}^{\lambda n} (1_{[r_1, \infty)} (t) - 1_{[r_1, \infty)} (t)) \right)^2 dt \]

by Jensens inequality and independence. But the expectation is just twice the variance of the Bernoulli variable \( 1_{[r_1, \infty)} (t) \), and therefore at most 1/2. The result follows. \( \square \)

Rephrasing part (i) of this corollary in terms of confidence windows we have, for any \( \delta > 0 \) with probability at least \( 1 - \delta \) that

\[ | \Phi_W (\rho) - \Phi_W (\hat{\rho} (R)) | \leq R_{\max} \| W \|_\infty \sqrt{\frac{\ln (2/\delta)}{2n}}. \]

For the weight function \( W = \zeta^{-1} 1_{[0, \zeta]} \) the bound on the estimation error scales with \( \zeta^{-1} \), which is not surprising, since we only consider a fraction \( \zeta \) of the data. So for decreasing \( \zeta \) the functional becomes more robust (because the influence \( R_\zeta \) decreases) but it becomes more difficult to estimate.

Restatement of Proposition 2.

**Proposition 19.** Assume the conditions of Theorem 1. Then

\[ \Pr \left\{ \Phi \left( \mu_{\hat{S}(X)}^* \right) \leq \Phi (\mu_{S^*}) + \delta \right\} \geq \Pr \left\{ 2 \sup_{S \in S} | \Phi_W (\mu_S) - \Phi_W (\hat{\mu}_S (X)) | \leq \left( 1 - \frac{\beta}{1 - \lambda} \right) IC_{\max} (\mu_{S^*}, W) \right\}. \]

**Proof.**

\[ \Phi_W (\mu_{\hat{S}(X)}) - \Phi_W (\mu_{S^*}) \leq \left( \Phi_W (\mu_{\hat{S}(X)}) - \Phi_W (\hat{\mu}_{\hat{S}(X)} (X)) \right) + \left( \Phi_W (\hat{\mu}_{\hat{S}(X)} (X)) - \Phi_W (\hat{\mu}_{S^*} (X)) \right) + \left( \Phi_W (\hat{\mu}_{S^*} (X)) - \Phi_W (\mu_{S^*}) \right) + \left( \Phi_W (\mu_{S^*}) - \Phi_W (\mu_{S^*}) \right). \]

The second term and the last term are negative by the minimality properties of \( \hat{S}(X) \) and \( S^* \). The remaining terms are bounded by \( 2 \sup_{S \in S} | \Phi_W (\mu_S) - \Phi_W (\hat{\mu}_S (X)) | \). Thus

\[ \Pr \left\{ 2 \sup_{S \in S} | \Phi_W (\mu_S) - \Phi_W (\hat{\mu}_S (X)) | \leq \left( 1 - \frac{\beta}{1 - \lambda} \right) IC_{\max} (\mu_{S^*}, W) \right\} \]

\[ \leq \Pr \left\{ \Phi_W (\mu_{\hat{S}(X)}) - \Phi_W (\mu_{S^*}) \leq \left( 1 - \frac{\beta}{1 - \lambda} \right) IC_{\max} (\mu_{S^*}, W) \right\} \]

\[ \leq \Pr \left\{ \Phi \left( \mu_{\hat{S}(X)}^* \right) \leq \Phi (\mu_{S^*}) + \delta \right\}, \]

where the last inequality follows from Theorem 1. \( \square \)

**Lemma 20.** If \( W = \zeta^{-1} 1_{[0, \zeta]} \) with \( \zeta < 1 \), then for \( \rho \in P (\{0, R_{\max}\}) \)

\[ \Phi_W (\rho) = \sup_{\lambda \in [0, R_{\max}]} \left\{ \lambda - \zeta^{-1} \int_0^{\infty} \max \{ \lambda - t, 0 \} d \rho (t) \right\} \]

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Proof. Integration by parts gives
\[
\int_0^\infty \max \{\lambda - t, 0\} \, d\rho(t) = \int_0^\lambda F_\rho(t) \, dt = \lambda F_\rho(\lambda) - \int_0^\lambda t \, d\rho(t).
\]
The maximum of \(\lambda - \zeta^{-1} \int_0^\lambda F_\rho(t) \, dt\) is attained at \(\zeta = F_\rho(\lambda)\), which shows \(\lambda \leq R_{\text{max}}\), and substitution gives
\[
\sup_{\lambda \in \mathbb{R}} \left\{ \lambda - \zeta^{-1} \int_0^\infty \max \{\lambda - t, 0\} \, d\rho(t) \right\} = \lambda - \zeta^{-1} \left( \lambda F_\rho(\lambda) - \int_0^\lambda t \, d\rho(t) \right)
\]
\[
= \zeta^{-1} \int_0^\infty t \zeta^{-1} 1_{[0,\zeta]}(F_\rho(t)) \, d\rho(t)
\]
\[
= \Phi_W(\rho).
\]

\[\square\]

Restatement of Theorem 3.

**Theorem 21.** Let \(W = \zeta^{-1} 1_{[0,\zeta]}\) and \(\eta > 0\). With probability at least \(1 - \eta\) in \(X \sim \mu^n\) we have that
\[
\sup_{S \in \mathcal{S}} |\Phi_W(\mu_S) - \Phi_W(\hat{\mu}_S(X))| \leq \frac{2}{\zeta n} \mathbb{E}_X \mathcal{R}(\mathcal{F}, X) + \frac{R_{\text{max}}}{\zeta \sqrt{n}} \left( 2 + \sqrt{\frac{\ln(2/\eta)}{2}} \right),
\]
where \(\mathcal{R}(\mathcal{F}, X)\) is the Rademacher average
\[
\mathcal{R}(\mathcal{F}, X) = \mathbb{E}_\epsilon \left[ \sup_{S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i d(X_i, S) \right]
\]
with independent Rademacher variables \(\epsilon = (\epsilon_1, \ldots, \epsilon_n)\).

**Proof.** Using Lemma 20 we get with independent Rademacher variables \(\epsilon = (\epsilon_1, \ldots, \epsilon_n)\)
\[
\mathbb{E} \left[ \sup_{S \in \mathcal{S}} \Phi_W(\mu_S) - \Phi_W(\hat{\mu}_S(X)) \right]
\]
\[
\leq \zeta^{-1} \mathbb{E}_X \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \int_0^\infty \max \{\lambda - t, 0\} \, d\hat{\mu}_S(X)(t) - \int_0^\infty \max \{\lambda - t, 0\} \, d\mu_S(t) \right]
\]
\[
= \zeta^{-1} \mathbb{E}_X \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \frac{1}{n} \sum_{i=1}^n \max \{\lambda - d(X_i, S), 0\} - \mathbb{E}_{X \sim \mu} \left[ \max \{\lambda - d(X, S), 0\} \right] \right]
\]
\[
= \frac{1}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i \left( \max \{\lambda - d(X_i, S), 0\} - \max \{\lambda - d(X_i', S), 0\} \right) \right]
\]
\[
= \frac{1}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i \max \{\lambda - d(X_i, S), 0\} \right]
\]
\[
\leq \frac{2}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i \max \{\lambda - d(X_i, S), 0\} \right]
\]
\[
\leq \frac{2}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{\lambda \in [0, R_{\text{max}}], S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i \left( \lambda - d(X_i, S) \right) \right]
\]
\[
\leq \frac{2}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{S \in \mathcal{S}} \sum_{i=1}^n \epsilon_i d(X_i, S) \right] + \frac{2}{\zeta n} \mathbb{E}_{XX'} \left[ \sup_{\lambda \in [0, R_{\text{max}}]} \lambda \sum_{i=1}^n \epsilon_i \right]
\]
\[
\leq \frac{2}{\zeta n} \mathbb{E}_X \mathcal{R}(\mathcal{F}, X) + \frac{2 R_{\text{max}}}{\zeta \sqrt{n}}.
\]
Here the third identity is a standard symmetrization argument, the second inequality the triangle inequality, followed by the contraction inequality for Rademacher averages, since \( t \to \max\{t, 0\} \) is a contraction. Then we used the triangle inequality again. Now let \( \Psi(X) \) be the random variable \( \sup_{S \in S} \Phi_W(\mu_S) - \Phi_W(\tilde{\mu}_S(X)) \). It then follows from Lemma[17] and the bounded difference inequality that with probability at least \( 1 - \eta \) we have \( \Psi(X) \leq \mathbb{E}\Psi(X) + \zeta^{-1}R_{\max}\sqrt{\ln (1/\eta)} / (2n) \).

Combined with above bound on \( \mathbb{E}\Psi(X) \) this completes the proof.

Theorem 4 follows directly from Theorems 2 and 5 in [13] and from the bias bound, Corollary [18](ii).

Restatement of Theorem 5.

**Theorem 22.** Under the conditions of the previous theorem, with probability at least \( 1 - \eta \) in \( X \sim \mu^n \) we have that for all \( S \in \mathcal{S} \)

\[
|\Phi_W(\mu_S) - \Phi_W(\tilde{\mu}_S(X))| \leq \sqrt{2V_S C} + \frac{6R_{\max}\left(\|W\|_\infty + \frac{\|W\|_{Lip}}{n}\right)C}{n} + \frac{\|W\|_\infty R_{\max}}{\sqrt{n}},
\]

where \( V_S \) is the variance of the random variable \( \Phi_W(\tilde{\mu}_S(X)) \), and \( C \) is the complexity term

\[
C = kd \ln \left(16n\|S\|^2/\eta\right)
\]

if \( S \) is the set of sets with \( k \) elements, or convex polytopes with \( k \) vertices and \( \|S\| = \sup_{x \in S} \|x\| \), or \( C = kd \ln (16nR_{\max}^2/\eta) \)

if \( S \) is the set of set of \( k \)-dimensional subspaces.

**Proof.** For any fixed \( S \in \mathcal{S} \) the L-statistic \( x \in X^n \mapsto f_S(x) := \Phi_W(\tilde{\mu}_S(x)) \) is \( \left(R_{\max}\|W\|_\infty, R_{\max}\|W\|_{Lip}\right) \)-weakly interacting (see [12]) and therefore satisfies the following version of Bernstein’s inequality (see [12], [12]): For \( \eta \in (0, 1/\epsilon) \) with probability at least \( 1 - \eta \) in \( X \sim \mu^n \) we have

\[
\mathbb{E}[f_S] - f_S(X) \leq \sqrt{2V_S \ln (1/\eta)} + R_{\max}\left(\frac{2\|W\|_\infty}{3} + \frac{3\|W\|_{Lip}}{2}\right)\ln (1/\eta)/n,
\]

where \( \mathbb{E}[f_S] \) and \( V_S \) are expectation and variance of the random variable \( f_S(X) = \Phi_W(\tilde{\mu}_S(X)) \) respectively. We will make this bound uniform with a covering number argument.

Define a pseudo metric \( d_X \) on \( S \) by

\[
d_X(S_1, S_2) = \sup_{x \in X} |d(x, S_1) - d(x, S_2)|.
\]

It follows from Lemma[17] that for every \( x \in X^n \) we have

\[
f_{S_1}(x) - f_{S_2}(x) \leq \|W\|_\infty d_W(\tilde{\mu}_{S_1}(x), \tilde{\mu}_{S_2}(x)) \leq \|W\|_\infty d_X(S_1, S_2).
\]

In particular \( \mathbb{E}[f_{S_1}] - \mathbb{E}[f_{S_2}] \leq \|W\|_\infty d_X(S_1, S_2) \).

\[
\sqrt{V_{S_1}} - \sqrt{V_{S_2}} = \|f_{S_1} - \mathbb{E}[f_{S_1}]\|_{L_2(\mu^n)} - \|f_{S_2} - \mathbb{E}[f_{S_2}]\|_{L_2(\mu^n)} \\
\leq \|f_{S_1} - f_{S_2}\|_{L_2(\mu^n)} + \|\mathbb{E}[f_{S_1}] - \mathbb{E}[f_{S_2}]\|_2 \leq 2\|W\|_\infty d_X(S_1, S_2).
\]

Now let \( N = N(S, d_X, \epsilon) \) be the corresponding minimal covering number of \( S \) with \( d_X \)-balls of radius \( \epsilon \), and let \( S_0 \subseteq S \) be such that \( \forall S \in S, \exists S' \in S_0 \) with \( d_R(S, S') < 1/n \) and \( |S_0| \leq N \). Then, abbreviating \( R_{\max}\left(\frac{2\|W\|_\infty}{3} + \frac{3\|W\|_{Lip}}{2}\right) \) with \( C \), with probability at least \( 1 - \eta \) in \( X \) that for every \( S \in S \)
\[ \mathbb{E} [f_S] - f_S (X) \leq \mathbb{E} [f_{S'}] - f_S (X) + \frac{2 \|W\|_\infty}{n} \leq \sqrt{2V_S} \ln (N/\eta) + \frac{C \ln (N/\eta) + 2 \|W\|_\infty}{n} \]

\[ \leq \sqrt{2V_S} \ln (N/\eta) + \frac{C \ln (N/\eta) + 2 \|W\|_\infty \sqrt{2\ln (N/\eta)} + 2 \|W\|_\infty}{n} \]

In the first inequality we used uniform approximation of \( f_S \) by \( f_{S'} \), where \( S' \) is the nearest neighbour of \( S \) in \( S_0 \). The next line combines Bernstein's inequality with a union bound over \( S_0 \). Finally we again approximate \( \sqrt{V_{S'}} \) by \( \sqrt{V_S} \).

Next we bound the covering numbers \( N(S, d_X, 1/n) \), which we do separately for the case of uniformly bounded \( S \) and PSA. In case of the mean, k-means or sparse coding is easy to see that for \( S_1, S_2 \in S \) and any two respective enumerations \( x_i \) and \( y_i \) or enumerations of the extreme points

\[ d_X (S_1, S_2) \leq 2 \|S\| H (S_1, S_2) \leq 2 \|S\| \max_i \|x_i - y_i\| . \]

It follows that \( N(S, d_X, 1/n) \) can be bounded by the covering number of a ball of radius \( \|S\|^2 \) in a \( kd \)-dimensional Banach space. Use the standard result of Cucker and Smale \([2]\) we have

\[ N(S, d_X, 1/n) \leq \left( 8n \|S\|^2 \right)^{kd} . \]

For PSA we can use unit vectors spanning the subspaces and instead of \( \|S\|^2 \) we have the maximal squared norm in the support, so

\[ N(S, d_X, 1/n) \leq \left( 8n \|S\|^2 \right)^{kd} . \]

Putting it all together and adding the bias bound \( \Phi_W (\mu_S) - \mathbb{E} [\Phi_W (\hat{\mu}_S (X))] \leq \|W\|_\infty R_{\text{max}}/\sqrt{n} \) (Corollary \([18](ii)\)) we get

\[ \Phi_W (\mu_S) - \Phi_W (\hat{\mu}_S (X)) \leq \sqrt{2\sigma^2 \left( \Phi_W (\hat{\mu}_S (X)) \right)} \cdot kd \ln \left( 8n \|S\|^2 / \eta \right) + \frac{R_{\text{max}} \left( 6 \|W\|_\infty + \frac{3\|W\|_{L^p}^2}{2} \right)}{n} \cdot kd \ln \left( 8n \|S\|^2 / \eta \right) + \frac{\|W\|_\infty R_{\text{max}}}{\sqrt{n}} \]

The result follows from elementary estimates and algebraic simplifications.

**B Algorithms**

Restatement of Lemma 7.

**Lemma 23.** For any \( S \in S \) and any \( p \in \text{Sym}_n \), if \( \pi \) is the ascending ordering of the \( d_S(x_i)s \), then \( \phi_S(x, p) \geq \phi_S(x, \pi) = \hat{\phi}_S(x) \).

**Proof.** Writing \( w(i) = W \left( \frac{\pi(i)}{n} \right) \) and \( z_i = d_S (x_{\pi(i)}) \) it is enough to show that the identity permutation is a minimizer of \( r(p) = \sum_{i=1}^n w(p(i)) z_i \) for \( p \in \text{Sym}_n \).

This follows from the following claim, which we prove by induction:

For \( k \in \{1, ..., n\} \) there is for every \( p \in \text{Sym}_n \) some \( p' \in \text{Sym}_n \) such that \( r(p') \leq r(p) \) and \( p'(j) = j \) for all \( 1 \leq j < k \). The case \( k = 1 \) holds trivially. If the claim holds for any \( k \leq n - 1 \) then there is \( q \in \text{Sym}_n \) such that
We recall the definition of NP-hardness for optimization problems.

To show hardness of an optimization problem whether there exist an assignment to the variables \( \mu \) if the minimum exists, then

\[
\text{Lemma 25. Let } X \subseteq Y, \text{ then }
L(C) = \frac{1}{2|C|} \sum_{x,y \in C} \|x - y\|_2^2. \tag{12}
\]

**Proof.** Let \( X \) and \( Y \) two i.i.d. random variables supported on \( C \), then

\[
\mathbb{E}[\|X - Y\|_2^2] = \mathbb{E}[\|X\|_2^2] + \mathbb{E}[\|Y\|_2^2] - 2\mathbb{E}[\langle X, Y \rangle]
\]

\[
= \mathbb{E}[\|X\|_2^2] + \mathbb{E}[\|X\|_2^2] - 2\mathbb{E}[\|X\|_2^2]
\]

\[
= 2\mathbb{E}[\|X\|_2^2] - 2\mathbb{E}[\|E[X]\|_2^2] = 2\mathbb{E}[\|X - E[X]\|_2^2].
\]

Now assume \( X \) and \( Y \) are independent samples from the uniform distribution on \( C \), then

\[
\mathbb{E}[\|X - E[X]\|_2^2] = \frac{1}{|C|} \sum_{x \in C} \|x - \mu_C\|_2^2
\]

\[
= \mathbb{E}[\|X - Y\|_2^2]/2 = \frac{1}{2|C|^2} \sum_{x,y \in C} \|x - y\|_2^2
\]

from which the thesis follows. 

We recall the definition of NP-hardness for optimization problems.

**Definition 26.** A computational problem \( \Pi \) is said NP-hard (optimization) if and only if the related decision problem \( \Pi_D \) is NP-hard. Assume \( \Pi \) is defined as the problem of minimizing a function \( f_X(\mu) \) defined by an input instance \( X \) if the minimum exists, then \( \Pi_D \) is defined as the problem of determining, given in input \( X \) and a rational number \( c \), whether there exist an assignment to the variables \( \mu \) such that \( f_X(\mu) \leq c \).

In order to show hardness of an optimization problem \( \Pi \), it is enough to show hardness of the related decision problem \( \Pi_D \). For this reason, the following will be useful.

**Definition 27.** Decision Robust 1-Means

Input: Points \( X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d \), an integer \( h \) and a rational number \( c \).
Output: Yes if there exist a $C \subseteq X$ such that $|C| = h$ and $L(C) \leq c$, No otherwise.

To prove the theorem we will reduce $n^{\sqrt{2}}$-CLIQUE to the decision version ROBUST 1-MEANS via a polynomial time algorithm. Since $n^{\sqrt{2}}$-CLIQUE is NP-complete, hardness for ROBUST 1-MEANS will follow.

**Definition 28.** $n^{\sqrt{2}}$-CLIQUE

**Input:** A simple undirected connected graph $G = (V, E)$ with $|V| = n$.

**Output:** Yes if $G$ contains a clique of size $n^{\sqrt{2}}$, No otherwise.

Given an instance of $n^{\sqrt{2}}$-CLIQUE in the form of a graph $G = (V, E)$ with $n$ vertices, we create an instance of ROBUST 1-MEANS $\Pi_D(G)$ which is equivalent to $G$. Let $A$ denote the symmetric $n \times n$ adjacency matrix of $G$, i.e. $A_{ij} = 1$ iff $(i, j) \in E$ otherwise $A_{ij} = 0$. Consider the graph embedding given by the map $\phi : V \rightarrow \mathbb{R}^n$ such that $\phi(i) = A_i + ne_i$, where $A_i$ denotes the $i$-th row of $A$ and $e_i$ denotes the $i$-th vector of the canonical basis of $\mathbb{R}^n$. Given $G$ we build an instance of ROBUST 1-MEANS by setting $X = \{\phi(1), \ldots, \phi(n)\}$, $h = n^{\sqrt{2}}$ and $c = m(n^2 - 3n)$, where we set $m = \binom{n}{2}$ as a shortcut. Notice that it takes $O(n)$ to build such instance. The following lemma finishes the proof by showing the aforementioned equivalence.

**Lemma 29.** $G$ is a Yes instance iff $\Pi_D(G)$ is a Yes instance.

**Proof.** Assume that $G$ is a Yes instance, i.e. $G$ contains at least clique of size $n^{\sqrt{2}}$. Notice that for any $(i, j) \in E$ it holds that

$$\|\phi(i) - \phi(j)\|^2 \leq (n - 1)^2 + (n - 1)^2 = 2n^2 - 4n + 2 \leq 2n^2 - 3n$$

while for any $(i, j) \notin E$ it holds

$$\|\phi(i) - \phi(j)\|^2 \geq 2n^2.$$

If $\{c_1, \ldots, c_{n^{\sqrt{2}}}\}$ are the vertices in the clique, the cost $L(C)$, by Lemma 25, of the subset $C = \{\phi(c_1), \ldots, \phi(c_{n^{\sqrt{2}}}\})$ is at most $c$, since in such clique contains exactly $m$ edges.

Now suppose that $\Pi_D(G)$ admits a cost of at most $c$. Let denote by $C$ the subsets of $X$ achieving such cost, then the associated vertices must form a clique otherwise at least one of the $m$ distance will be $2n^2$ larger than $2n^2$ leading to a cost larger of $c$.

Thus if we could solve in polynomial time DECISION ROBUST 1-MEANS we could solve in polynomial time $n^{\sqrt{2}}$-CLIQUE.

**C Experiments**

In this section we present additional experimental results we obtained for our method.

**KMEANS.** We performed 3 additional experiments for the case of KMEANS. In the first experiment, we used the fashion MNIST dataset. The training data were generated by sampling 1000 points each from the sneakers and the trousers classes as inliers, and 250 points from each other class as outliers. The resulting fraction of outliers is about 0.5. The test data consist of all the sneakers and the trousers in the test set and has size of about 2000. We run the algorithms we $T = 50, r = 30, M = 4000, k = 2$ and $\zeta$ in the range $[0.4, 1]$. The results are shown in the Figure 5 top row, where it is possible to see that our method outperform both the baselines.

In the second experiment, we used the EMNIST dataset. In this case, we wanted to test our method against more aggressive outliers. The training data were generated by sampling 1000 points each from the 0s and the 1s as inliners. For the outliers we first sampled 500 points each from 0s and 1s and then we sheered such images of 90 degrees, by stretching the digits along the $x$-axis. The resulting fraction of outliers is about 0.37. The test data consist of all the 0s and 1s in the test set and has size of about 2000. We run the algorithms we $T = 50, r = 30, M = 4000, k = 2$ and $\zeta$ in the range $[0.4, 1]$. The results are shown in the Figure 5 middle row, where it is possible to see that our method outperform both the baselines.

In the third experiment, we used again the EMNIST dataset and tested our method in the very high outliers regime. The training data were generated by sampling 1000 points each from the 0s and the 1s as inliners. For the outliers we
sampled 100 points from each other class. The resulting fraction of outliers is about 0.7. The test data consist of all the 0s and 1s in the test set and has size of about 2000. We run the algorithms we $T = 50$, $r = 30$, $M = 4000$, $k = 2$ and $\zeta$ in the range $[0.3, 1]$. The results are shown in the Figure 5 lower row, where it is possible to see that our method outperform both the baselines.

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