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Declutter and Resample: Towards Parameter Free Denoising*†

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Abstract

In many data analysis applications the following scenario is commonplace: we are given a point set that is supposed to sample a hidden ground truth K in a metric space, but it got corrupted with noise so that some of the data points lie far away from K creating outliers also termed as *ambient noise*. One of the main goals of denoising algorithms is to eliminate such noise so that the curated data lie within a bounded Hausdorff distance of K. Popular denoising approaches such as deconvolution and thresholding often require the user to set several parameters and/or to choose an appropriate noise model while guaranteeing only asymptotic convergence. Our goal is to lighten this burden as much as possible while ensuring theoretical guarantees in all cases.

Specifically, first, we propose a simple denoising algorithm that requires only a single parameter but provides a theoretical guarantee on the quality of the output on general input points. We argue that this single parameter cannot be avoided. We next present a simple algorithm that avoids even this parameter by paying for it with a slight strengthening of the sampling condition on the input points which is not unrealistic. We also provide some preliminary empirical evidence that our algorithms are effective in practice.

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1 Introduction

Real life data are almost always corrupted by noise. Of course, when we talk about noise, we implicitly assume that the data sample a hidden space called the *ground truth* with respect to which we measure the extent and type of noise. Some data can lie far away from the ground truth leading to ambient noise. Clearly, the data density needs to be higher near the ground truth if signal has to prevail over noise. Therefore, a worthwhile goal of a denoising

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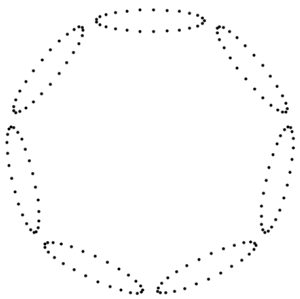


Figure 1 Scale ambiguity.

algorithm is to curate the data, eliminating the ambient noise while retaining most of the subset that lies within a bounded distance from the ground truth.

In this paper we are interested removing "outlier"-type of noise from input data. Numerous algorithms have been developed for this problem in many different application fields; see e.g [16, 21]. There are two popular families of denoising/outlier detection approaches: Deconvolution and Thresholding. Deconvolution methods rely on the knowledge of a generative noise model for the data. For example, the algorithm may assume that the input data has been sampled according to a probability measure obtained by convolving a distribution such as a Gaussian [18] with a measure whose support is the ground truth. Alternatively, it may assume that the data is generated according to a probability measure with a small Wasserstein distance to a measure supported by the ground truth [7]. The denoising algorithm attempts to cancel the noise by deconvolving the data with the assumed model.

A deconvolution algorithm requires the knowledge of the generative model and at least a bound on the parameter(s) involved, such as the standard deviation of the Gaussian convolution or the Wasserstein distance. Therefore, it requires at least one parameter as well as the knowledge of the noise type. The results obtained in this setting are often asymptotic, that is, theoretical guarantees hold in the limit when the number of points tends to infinity.

The method of thresholding relies on a density estimation procedure [20] by which it estimates the density of the input locally. The data is cleaned, either by removing points where density is lower than a threshold [14], or moving them from such areas toward higher densities using gradient-like methods such as mean-shift [11, 19]. It has been recently used for uncovering geometric information such as one dimensional features [15]. In [5], the *distance to a measure* [10] that can also be seen as a density estimator [2] has been exploited for thresholding. Other than selecting a threshold, these methods require the choice of a density estimator. This estimation requires at least one additional parameter, either to define a kernel, or a mass to define the distance to a measure. In the case of a gradient based movement of the points, the nature of the movement also has to be defined by fixing the length of a step and by determining the terminating condition of the algorithm.

New work. In above classical methods, the user is burdened with making several choices such as fixing an appropriate noise model, selecting a threshold and/or other parameters. Our main goal is to lighten this burden as much as possible. First, we show that denoising with a single parameter is possible and this parameter is in some sense unavoidable unless a stronger sampling condition on the input points is assumed. This leads to our main algorithm that is completely free of any parameter when the input satisfies a stronger sampling condition which is not unrealistic.

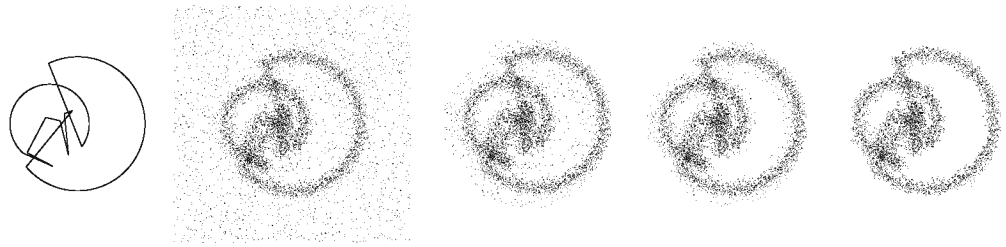


Figure 2 From left to right: the ground truth, the noisy input samples ($\sim$ 7000 points around the ground truth and 2000 ambient noise points), two intermediate steps of our iterative parameter-free denoising algorithm and the final output.

Our first algorithm *Declutter algorithm* uses a single parameter (presented in Section 3) and assumes a very general sampling condition which is not stricter than those for the classical noise models mentioned previously because it holds with high probability for those models as well. Additionally, our sampling condition also allows ambient noise and locally adaptive samplings. Interestingly, we note that our Declutter algorithm is in fact a variant of the approach proposed in [8] to construct the so-called *ε-density net*. Indeed, as we point out in Appendix D of the full version [6], the procedure of [8] can also be directly used for denoising purpose and one can obtain an analog of Theorems 9 and 13 in this paper for the resulting density net.

Use of a parameter in the denoising process is unavoidable in some sense, unless there are other assumptions about the hidden space. This is illustrated by the example in Figure 1. Does the sample here represent a set of small loops or one big circle? The answer depends on the scale at which we examine the data; see the full version [6] for the results of applying our denoising algorithms on this data set. The choice of a parameter may represent this choice of the scale [3, 13]. To remove this parameter, one needs other conditions for either the hidden space itself or for the sample, say by assuming that the data has some uniformity. Aiming to keep the sampling restrictions as minimal as possible, we show that it is sufficient to assume the homogeneity in data *only on or close to* the ground truth for our second algorithm which requires no input parameter.

Specifically, the parameter-free algorithm presented in Section 4 relies on an iteration that intertwines our decluttering algorithm with a novel resampling procedure. Assuming that the sample is sufficiently dense and somewhat uniform near the ground truth at scales beyond a particular scale s, our algorithm selects a subset of the input point set that is close to the ground truth without requiring any input from the user. The output maintains the quality at scale s even though the algorithm has no explicit knowledge of this parameter. See Figure 2 for an example.

All missing details from this extended abstract can be found in the full version [6]. In addition, in Appendix C of the full version [6], we show how the denoised data set can be used for homology inference. In Appendix E of the full version [6] , we provide various preliminary experimental results of our denoising algorithms.

▶ Remark. Very recently, Jiang and Kpotufe proposed a consistent algorithm for estimating the so-called modal-sets with also only one parameter [17]. The problem setup and goals are very different: In their work, they assume that input points are sampled from a density field that is locally maximal and constant on a compact domain. The goal is to show that as the number of samples n tends to infinity, such domains (referred to as modal-sets in their paper) can be recovered, and the recovered set converges to the true modal-sets under the Hausdorff distance. We also note that our Declutter algorithm allows adaptive sampling as well.

2 Preliminaries

We assume that the input is a set of points P sampled around a hidden compact set K, the ground truth, in a metric space $(\mathbb{X}, d_{\mathbb{X}})$. For simplicity, in what follows the reader can assume $\mathbb{X} = \mathbb{R}^d$ with $P, K \subset \mathbb{X} = \mathbb{R}^d$, and the metric $d_{\mathbb{X}}$ of $\mathbb{X}$ is simply the Euclidean distance. Our goal is to process P into another point set Q guaranteed to be Hausdorff close to K and hence to be a better sample of the hidden space K for further applications. By Hausdorff close, we mean that the (standard) *Hausdorff distance* $\delta_H(Q, K)$ between Q and K, defined as the infimum of δ such that $\forall p \in Q, d_{\mathbb{X}}(p, K) \leq \delta$ and $\forall x \in K, d_{\mathbb{X}}(x, Q) \leq \delta$, is bounded. Note that ambient noise/outliers can incur a very large Hausdorff distance.

The quality of the output point set Q obviously depends on the "quality" of input points P, which we formalize via the language of *sampling conditions*. We wish to produce good quality output for inputs satisfying much weaker sampling conditions than a bounded Hausdorff distance. Our sampling condition is based on the sampling condition introduced and studied in [4, 5]; see Chapter 6 of [4] for discussions on the relation of their sampling condition with some of the common noise models such as Gaussian. Below, we first introduce a basic sampling condition deduced from the one in [4, 5], and then introduce its extensions incorporating adaptivity and uniformity.

Basic sampling condition. Our sampling condition is built upon the concept of k-distance, which is a specific instance of a broader concept called *distance to a measure* introduced in [10]. The k-distance $d_{P,k}(x)$ is simply the root mean of square distance from x to its k-nearest neighbors in P. The averaging makes it robust to outliers. One can view $d_{P,k}(x)$ as capturing the inverse of the density of points in P around x [2]. As we show in Appendix D [6], this specific form of k-distance is not essential – Indeed, several of its variants can replace its role in the definition of sampling conditions below, and our Declutter algorithm will achieve similar denoising guarantees.

▶ **Definition 1** ([10]). Given a point $x \in \mathbb{X}$, let $p_i(x) \in P$ denote the i-th nearest neighbor of x in P. The *k-distance* to a point set $P \subseteq \mathbb{X}$ is $d_{P,k}(x) = \sqrt{\frac{1}{k}\sum_{i=1}^{k} d_{\mathbb{X}}(x, p_i(x))^2}$.

▶ **Claim 2** ([10]). *$d_{P,k}(\cdot)$ is 1-Lipschitz, i.e. $|d_{P,k}(x) - d_{P,k}(y)| \leq d_{\mathbb{X}}(x, y)$ for $\forall (x, y) \in \mathbb{X} \times \mathbb{X}$.*

All our sampling conditions are dependent on the choice of k in the k-distance, which we reflect by writing ϵ_k instead of ϵ in the sampling conditions below. The following definition is related to the sampling condition proposed in [5].

▶ **Definition 3.** Given a compact set $K \subseteq \mathbb{X}$ and a parameter k, a point set P is an *ϵ_k-noisy sample* of K if

1. $\forall x \in K,\ d_{P,k}(x) \leq \epsilon_k$
2. $\forall x \in \mathbb{X},\ d_{\mathbb{X}}(x, K) \leq d_{P,k}(x) + \epsilon_k$

Condition 1 in Definition 3 means that the density of P on the compact set K is bounded from below, that is, K is well-sampled by P. Note, we only require P to be a dense enough sample of K – there is no uniformity requirement in the sampling here.

Condition 2 implies that a point with low k-distance, i.e. lying in high density region, has to be close to K. Intuitively, P can contain outliers which can form small clusters but their density can not be significant compared to the density of points near the compact set K.

Note that the choice of ϵ_k always exists for a bounded point set P, no matter what value of k is – For example, one can set ϵ_k to be the diameter of point set P. However, the smallest

possible choice of ϵ_k to make P an ϵ_k-noisy sample of K depends on the value of k. We thus use ϵ_k in the sampling condition to reflect this dependency.

In Section 4, we develop a parameter-free denoising algorithm. As Figure 1 illustrates, it is necessary to have a mechanism to remove potential ambiguity about the ground truth. We do so by using a stronger sampling condition to enforce some degree of uniformity:

▶ **Definition 4.** Given a compact set $K \subseteq \mathbb{X}$ and a parameter k, a point set P is a uniform (ϵ_k, c)-noisy sample of K if P is an ϵ_k-noisy sample of K (i.e, conditions of Def. 3 hold) and
3. $\forall p \in P,\ d_{P,k}(p) \geq \frac{\epsilon_k}{c}$.

It is important to note that the lower bound in Condition 3 enforces that the sampling needs to be homogeneous – i.e, $d_{P,k}(x)$ is bounded both from above and from below by some constant factor of ϵ_k – *only for points on and around* the ground truth K. This is because condition 1 in Def. 3 is only for points from K, and condition 1 together with the 1-Lipschitz property of $d_{P,k}$ (Claim 2) leads to an upper bound of $O(\epsilon_k)$ for $d_{P,k}(y)$ only for points y within $O(\epsilon_k)$ distance to K. There is no such upper bound on $d_{P,k}$ for noisy points far away from K and *thus no homogeneity/uniformity requirements for them.*

Adaptive sampling conditions. The sampling conditions given above are global, meaning that they do not respect the "feature" of the ground truth. We now introduce an adaptive version of the sampling conditions with respect to a feature size function.

▶ **Definition 5.** Given a compact set $K \subseteq \mathbb{X}$, a feature size function $f : K \to \mathbb{R}^+ \cup \{0\}$ is a 1-Lipschitz non-negative real function on K.

Several feature sizes exist in the literature of manifold reconstruction and topology inference, including the *local feature size* [1], *local weak feature size*, *μ-local weak feature size* [9] or *lean set feature size* [12]. All of these functions describe how complicated a compact set is locally, and therefore indicate how dense a sample should be locally so that information can be inferred faithfully. Any of these functions can be used as a feature size function to define the adaptive sampling below. Let $\bar{p}$ denote any one of the nearest points of p in K. Observe that, in general, a point p can have multiple such nearest points.

▶ **Definition 6.** Given a compact set $K \subseteq \mathbb{X}$, a feature size function f of K, and a parameter k, a point set P is a *uniform (ϵ_k, c)-adaptive noisy sample of K* if
1. $\forall x \in K,\ d_{P,k}(x) \leq \epsilon_k f(x)$,
2. $\forall y \in \mathbb{X},\ d_{\mathbb{X}}(y, K) \leq d_{P,k}(y) + \epsilon_k f(\bar{y})$,
3. $\forall p \in P,\ d_{P,k}(p) \geq \frac{\epsilon_k}{c} f(\bar{p})$.
We say that P is *an ϵ_k-adaptive noisy sample of K* if only conditions 1 and 2 above hold.

We require that the feature size is *positive everywhere* as otherwise, the sampling condition may require infinite samples in some cases. We also note that the requirement of the feature size function being 1-Lipschitz is only needed to provide the theoretical guarantee for our second parameter-free algorithm.

3 Decluttering

We now present a simple yet effective denoising algorithm which takes as input a set of points P and a parameter k, and outputs a set of points $Q \subseteq P$ with the following guarantees: If P is an ϵ_k-noisy sample of a hidden compact set $K \subseteq \mathbb{X}$, then the output Q lies close to K in the *Hausdorff distance* (i.e, within a small tubular neighborhood of K and outliers are all

Algorithm 1: Declutter(P,k).

Data: Point set P, parameter k
Result: Denoised point set Q

```
begin
    sort P such that d_{P,k}(p_1) ≤ ··· ≤ d_{P,k}(p_{|P|}).
    Q_0 ⟵ ∅
    for i ⟵ 1 to |P| do
        if Q_{i−1} ∩ B(p_i, 2d_{P,k}(p_i)) = ∅ then
            Q_i = Q_{i−1} ∪ {p_i}
        end
        else  Q_i = Q_{i−1}
    end
    Q ⟵ Q_n
end
```

eliminated). The theoretical guarantee holds for both the non-adaptive and the adaptive cases, as stated in Theorems 9 and 13.

As the k-distance behaves like the inverse of density, points with a low k-distance are expected to lie close to the ground truth K. A possible approach is to fix a threshold α and only keep the points with a k-distance less than α. This thresholding solution requires an additional parameter α. Furthermore, very importantly, such a thresholding approach does not easily work for adaptive samples, where the density in an area with large feature size can be lower than the density of noise close to an area with small feature size.

Our algorithm Declutter(P,k), presented in **Algorithm 1**, works around these problems by considering the points in the order of increasing values of their k-distances and using a pruning step: Given a point p_i, if there exists a point q deemed better in its vicinity, i.e., q has smaller k-distance and has been previously selected ($q \in Q_{i-1}$), then p_i is not necessary to describe the ground truth and we throw it away. Conversely, if no point close to p_i has already been selected, then p_i is meaningful and we keep it. The notion of "closeness" or "vicinity" is defined using the k-distance, so k is the only parameter. In particular, the "vicinity" of a point p_i is defined as the metric ball $B(p_i, 2d_{P,k}(p_i))$; observe that this radius is different for different points, and the radius of the ball is larger for outliers. Intuitively, the radius $2d_{P,k}(p_i)$ of the "vicinity" around p_i can be viewed as the length we have to go over to reach the hidden domain with certainty. So, bad points have a larger "vicinity". We remark that this process is related to the construction of the "density net" introduced in [8], which we discuss more in Appendix D [6].

See Figure 3 on the right for an artificial example, where the black points are input points, and red crosses are in the current output Q_{i-1}. Now, at the ith iteration, suppose we are processing the point p_i (the green point). Since within the vicinity of p_i there is already a good point p, we consider p_i to be not useful, and remove it. Intuitively, for an outlier p_i, it has a large k-distance and hence a large vicinity. As we show later, our ϵ_k-noisy sampling condition ensures that this vicinity of p_i reaches the hidden compact set which the input points presumably sample. Since points around the hidden compact set should have higher density, there should be a good point already chosen in Q_{i-1}. Finally, it is also important to note that, contrary to many common sparsification procedures, our Declutter algorithm removes a noisy point because it has a good point within its vicinity, and *not because* it is within the vicinity of a good point. For example, in Figure 3, the red points such as p have small vicinity, and p_i is not in the vicinity of any of the red point.

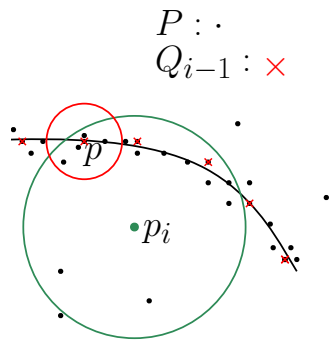


Figure 3 Declutter.

In what follows, we will make this intuition more concrete. We first consider the simpler non-adaptive case where P is an ϵ_k-noisy sample of K. We establish that Q and the ground truth K are Hausdorff close in the following two lemmas. The first lemma says that the ground truth K is well-sampled (w.r.t. ϵ_k) by the output Q of Declutter.

▶ **Lemma 7.** *Let $Q \subseteq P$ be the output of Declutter(P,k) where P is an ϵ_k-noisy sample of a compact set $K \subseteq \mathbb{X}$. Then, for any $x \in K$, there exists $q \in Q$ such that $d_{\mathbb{X}}(x, q) \leq 5\epsilon_k$.*

Proof. Let $x \in K$. By Condition 1 of Def. 3, we have $d_{P,k}(x) \leq \epsilon_k$. This means that the nearest neighbor p_i of x in P satisfies $d_{\mathbb{X}}(p_i, x) \leq d_{P,k}(x) \leq \epsilon_k$. If $p_i \in Q$, then the claim holds by setting $q = p_i$. If $p_i \notin Q$, there must exist $j < i$ with $p_j \in Q_{i-1}$ such that $d_{\mathbb{X}}(p_i, p_j) \leq 2d_{P,k}(p_i)$. In other words, p_i was removed by our algorithm because $p_j \in Q_{i-1} \cap B(p_i, 2d_{P,k}(p_i))$. Combining triangle inequality with the 1-Lipschitz property of $d_{P,k}$ (Claim 2), we then have

$$d_{\mathbb{X}}(x, p_j) \leq d_{\mathbb{X}}(x, p_i) + d_{\mathbb{X}}(p_i, p_j) \leq d_{\mathbb{X}}(x, p_i) + 2d_{P,k}(p_i) \leq 2d_{P,k}(x) + 3d_{\mathbb{X}}(p_i, x) \leq 5\epsilon_k,$$

which proves the claim. ◀

The next lemma implies that all outliers are removed by our denoising algorithm.

▶ **Lemma 8.** *Let $Q \subseteq P$ be the output of Declutter(P,k) where P is an ϵ_k-noisy sample of a compact set $K \subseteq \mathbb{X}$. Then, for any $q \in Q$, there exists $x \in K$ such that $d_{\mathbb{X}}(q, x) \leq 7\epsilon_k$.*

Proof. Consider any $p_i \in P$ and let $\bar{p}_i$ be one of its nearest points in K. It is sufficient to show that if $d_{\mathbb{X}}(p_i, \bar{p}_i) > 7\epsilon_k$, then $p_i \notin Q$.

Indeed, by Condition 2 of Def. 3, $d_{P,k}(p_i) \geq d_{\mathbb{X}}(p_i, \bar{p}_i) - \epsilon_k > 6\epsilon_k$. By Lemma 7, there exists $q \in Q$ such that $d_{\mathbb{X}}(\bar{p}_i, q) \leq 5\epsilon_k$. Thus,

$$d_{P,k}(q) \leq d_{P,k}(\bar{p}_i) + d_{\mathbb{X}}(\bar{p}_i, q) \leq 6\epsilon_k.$$

Therefore, $d_{P,k}(p_i) > 6\epsilon_k \geq d_{P,k}(q)$ implying that $q \in Q_{i-1}$. Combining triangle inequality and Condition 2 of Def. 3, we have

$$d_{\mathbb{X}}(p_i, q) \leq d_{\mathbb{X}}(p_i, \bar{p}_i) + d_{\mathbb{X}}(\bar{p}_i, q) \leq d_{P,k}(p_i) + \epsilon_k + 5\epsilon_k < 2d_{P,k}(p_i).$$

Therefore, $q \in Q_{i-1} \cap B(p_i, 2d_{P,k}(p_i))$, meaning that $p_i \notin Q$. ◀

▶ **Theorem 9.** *Given a point set P which is an ϵ_k-noisy sample of a compact set $K \subseteq \mathbb{X}$, Algorithm Declutter returns a set $Q \subseteq P$ such that $\delta_H(K, Q) \leq 7\epsilon_k$.*

Interestingly, if the input point set is uniform then the denoised set is also uniform, a fact that turns out to be useful for our parameter-free algorithm later.

▶ **Proposition 10.** *If P is a uniform (ϵ_k, c)-noisy sample of a compact set $K \subseteq \mathbb{X}$, then the distance between any pair of points of Q is at least $2\frac{\epsilon_k}{c}$.*

Proof. Let p and q be in Q with $p \neq q$ and, assume without loss of generality that $d_{P,k}(p) \leq d_{P,k}(q)$. Then, $p \notin B(q, 2d_{P,k}(q))$ and $d_{P,k}(q) \geq \frac{\epsilon_k}{c}$. Therefore, $d_{\mathbb{X}}(p,q) \geq 2\frac{\epsilon_k}{c}$. ◀

Adaptive case

Assume the input is an adaptive sample $P \subseteq \mathbb{X}$ with respect to a feature size function f. The denoised point set Q may also be adaptive. We hence need an adaptive version of the Hausdorff distance denoted $\delta_H^f(Q,K)$ and defined as the infimum of δ such that (i) $\forall p \in Q$, $d_{\mathbb{X}}(p,K) \leq \delta f(\bar{p})$, and (ii) $\forall x \in K, d_{\mathbb{X}}(x,Q) \leq \delta f(x)$, where $\bar{p}$ is a nearest point of p in K. Similar to the non-adaptive case, we establish that P and output Q are Hausdorff close via Lemmas 11 and 12 whose proofs are same as those for Lemmas 7 and 8 respectively, but using an adaptive distance w.r.t. the feature size function. Note that the algorithm does not need to know what the feature size function f is, hence only one parameter (k) remains.

▶ **Lemma 11.** *Let $Q \subseteq P$ be the output of Declutter(P,k) where P is an ϵ_k-adaptive noisy sample of a compact set $K \subseteq \mathbb{X}$. Then, $\forall x \in K, \exists q \in Q,\ d_{\mathbb{X}}(x,q) \leq 5\epsilon_k f(x)$.*

▶ **Lemma 12.** *Let $Q \subseteq P$ be the output of Declutter(P,k) where P is an ϵ_k-adaptive noisy sample of a compact set $K \subseteq \mathbb{X}$. Then, for $\forall q \in Q,\ d_{\mathbb{X}}(q,\bar{q}) \leq 7\epsilon_k f(\bar{q})$.*

▶ **Theorem 13.** *Given an ϵ_k-adaptive noisy sample P of a compact set $K \subseteq \mathbb{X}$ with feature size f, Algorithm Declutter returns a sample $Q \subseteq P$ of K where $\delta_H^f(Q,K) \leq 7\epsilon_k$.*

Again, if the input set is uniform, the output remains uniform as stated below.

▶ **Proposition 14.** *Given an input point set P which is an uniform (ϵ_k, c)-adaptive noisy sample of a compact set $K \subseteq \mathbb{X}$, the output $Q \subseteq P$ of Declutter satisfies*

$$\forall (q_i, q_j) \in Q,\ i \neq j \implies d_{\mathbb{X}}(q_i, q_j) \geq 2\frac{\epsilon_k}{c} f(\bar{q}_i)\,.$$

Proof. Let q_i and q_j be two points of Q with $i < j$. Then q_i is not in the ball of center q_j and radius $2d_{P,k}(q_j)$. Hence $d_{\mathbb{X}}(q_i,q_j) \geq 2d_{P,k}(q_j) \geq 2\frac{\epsilon_k}{c} f(\bar{q}_j)$. Since $i < j$, it also follows that $d_{\mathbb{X}}(q_i,q_j) \geq 2d_{P,k}(q_j) \geq 2d_{P,k}(q_i) \geq 2\frac{\epsilon_k}{c} f(\bar{q}_i)$. ◀

The algorithm Declutter removes outliers from the input point set P. As a result, we obtain a point set which lies close to the ground truth with respect to the Hausdorff distance. Such point sets can be used for inference about the ground truth with further processing. For example, in topological data analysis, our result can be used to perform topology inference from noisy input points in the non-adaptive setting; see Appendix C [6] for more details.

An example of the output of algorithm Declutter is given in Figure 4(a)–(d). More examples (including for adaptive inputs) can be found in the full version [6].

Extensions

It turns out that there are many choices that can be used for the k-distance $d_{P,k}(x)$ instead of the one introduced in Definition 1. Indeed, the goal of k-distance intuitively is to provide a more robust distance estimate – Specifically, assume P is a noisy sample of a hidden domain

(a) (b) (c) (d) (e)

Figure 4 (a)–(d) show results of the Algorithm Declutter: (a) the ground truth, (b) the noisy input with 15K points with 1000 ambient noisy points, (c) the output of Algorithm Declutter when $k = 9$, (d) the output of Algorithm Declutter when $k = 30$. In (e), we show the output of Algorithm ParfreeDeclutter. As shown in Appendix E [6], algorithm ParfreeDeclutter can remove ambient noise for much sparser input samples with more noisy points.

$K \subset \mathbb{X}$. With the presence of noisy points far away from K, the distance $d_{\mathbb{X}}(x, P)$ no longer serves as a good approximation of $d_{\mathbb{X}}(x, K)$, the distance from x to the hidden domain K. We thus need a more robust distance estimate. The k-distance $d_{P,k}(x)$ introduced in Definition 1 is one such choice, and there are many other valid choices. As we show in Appendix D [6], we only need the choice of $d_{P,k}(x)$ to be 1-Lipschitz, and is less sensitive than $d_{\mathbb{X}}(x, P)$ (that is, $d_{\mathbb{X}}(x, P) \leq d_{P,k}(x)$). We can then define the sampling condition (as in Definitions 3 and 4) using a different choice of $d_{P,k}(x)$, and Theorems 9 and 13 still hold. For example, we could replace k-distance by $d_{P,k}(x) = \frac{1}{k}\sum_{i=1}^{k} d(x, p_i(x))$ where $p_i(x)$ is the ith nearest neighbor of x in P; that is, $d_{P,k}(x)$ is the average distance to the k nearest neighbors of x in P. Alternatively, we can replace k-distance by $d_{P,k}(x) = d(x, p_k(x))$, the distance from x to its k-th nearest neighbor in P (which was used in [8] to construct the ε-density net). Declutter algorithm works for all these choices with the same denoising guarantees.

One can in fact further relax the conditions on $d_{P,k}(x)$ or even on the input metric space $(\mathbb{X}, d_{\mathbb{X}})$ such that the triangle inequality for $d_{\mathbb{X}}$ only approximately holds. The corresponding guarantees of our Declutter algorithm are provided in Appendix D of the full version [6].

4 Parameter-free decluttering

The algorithm Declutter is not entirely satisfactory. First, we need to fix the parameter k a priori. Second, while providing a Hausdorff distance guarantee, this procedure also "sparsifies" input points. Specifically, the empty-ball test also induces some degree of sparsification, as for any point q kept in Q, the ball $B(q, 2d_{P,k}(q))$ does not contain any other output points in Q. While this sparsification property is desirable for some applications, it removes too many points in some cases – See Figure 4 for an example, where the output density is dominated by ϵ_k and does not preserve the dense sampling provided by the input around the hidden compact set K. In particular, for $k = 9$, it does not completely remove ambient noise, while, for $k = 30$, the output is too sparse.

In this section, we address both of the above concerns by a novel iterative re-sampling procedure as described in Algorithm ParfreeDeclutter(P). Roughly speaking, we start with $k = |P|$ and gradually decrease it by halving each time. At iteration i, let P_i denote the set of points so far kept by the algorithm; i is initialized to be $\lfloor \log_2(|P|) \rfloor$ and is gradually decreased. We perform the denoising algorithm Declutter$(P_i, k = 2^i)$ given in the previous section to first denoise P_i and obtain a denoised output set Q. This set can be too sparse.

Algorithm 2: ParfreeDeclutter(P).

Data: Point set P
Result: Denoised point set P_0
begin
  Set $i_* = \lfloor \log_2(|P|) \rfloor$, and $P_{i_*} \longleftarrow P$
  for $i \longleftarrow i_*$ *to* 1 **do**
    $Q \longleftarrow$ Declutter(P_i,2^i)
    $P_{i-1} \longleftarrow \cup_{q \in Q} B(q, (10 + 2\sqrt{2}) d_{P_i,2^i}(q)) \cap P_i$
  end
end

We enrich it by re-introducing some points from P_i, obtaining a denser sampling $P_{i-1} \subseteq P_i$ of the ground truth. We call this a *re-sampling* process. This re-sampling step may bring some outliers back into the current set. However, it turns out that a repeated cycle of decluttering and resampling with decreasing values of k removes these outliers progressively. See Figure 2 and also more examples in the full version [6]. The entire process remains free of any user supplied parameter. In the end, we show that for an input that satisfies a uniform sampling condition, we can obtain an output set which is both dense and Hausdorff close to the hidden compact set, without the need to know the parameters of the input sampling conditions.

In order to formulate the exact statement of Theorem 15, we need to introduce a more relaxed sampling condition. We relax the notion of uniform (ϵ_k, c)-noisy sample by removing condition 2. We call it a *weak uniform* (ϵ_k, c)*-noisy sample*. Recall that condition 2 was the one forbidding the noise to be too dense. So essentially, a weak uniform (ϵ_k, c)-noisy sample only concerns points on and around the ground truth, with no conditions on outliers.

▶ **Theorem 15.** *Given a point set P and i_0 such that for all $i > i_0$, P is a weak uniform $(\epsilon_{2^i}, 2)$-noisy sample of K and is also a uniform $(\epsilon_{2^{i_0}}, 2)$-noisy sample of K, Algorithm ParfreeDeclutter returns a point set $P_0 \subseteq P$ such that $d_H(P_0, K) \leq (87 + 16\sqrt{2})\epsilon_{2^{i_0}}$.*

We elaborate a little on the sampling conditions. On one hand, as illustrated by Figure 1, the uniformity on input points is somewhat necessary in order to obtain a parameter-free algorithm. So requiring a uniform $(\epsilon_{2^{i_0}}, 2)$-noisy sample of K is reasonable. Now it would have been ideal if the theorem only required that P is a uniform $(\epsilon_{2^{i_0}}, 2)$-noisy sample of K for some $k_0 = 2^{i_0}$. However, to make sure that this uniformity is not destroyed during our iterative declutter-resample process before we reach $i = i_0$, we also need to assume that, *around the compact set*, the sampling is uniform for any $k = 2^i$ with $i > i_0$ (i.e, before we reach $i = i_0$). The specific statement for this guarantee is given in Lemma 17. However, while the uniformity for points *around the compact set* is required for any $i > i_0$, the condition that noisy points cannot be arbitrarily dense is *only* required for one parameter, $k = 2^{i_0}$.

The constant for the ball radius in the resampling step is taken as $10 + 2\sqrt{2}$ which we call the resampling constant C. Our theoretical guarantees hold with this resampling constant though a value of 4 works well in practice. The algorithm reduces more noise with decreasing C. On the flip side, the risk of removing points causing loss of true signal also increases with decreasing C. Section 5 and Appendix E [6] provide several results for Algorithm ParfreeDeclutter. We also point out that while our theoretical guarantee is for non-adaptive case, in practice, the algorithm works well on adaptive sampling as well.

Proof for Theorem 15

Aside from the technical Lemma 16 on the k-distance, the proof is divided into three steps. First, Lemma 17 shows that applying the loop of the algorithm once with parameter $2k$ does not alter the existing sampling conditions for $k' \leq k$. This implies that the $\epsilon_{2^{i_0}}$-noisy sample condition on P will also hold for P_{i_0}. Then Lemma 18 guarantees that the step going from P_{i_0} to P_{i_0-1} will remove all outliers. Combined with Theorem 9, which guarantees that P_{i_0-1} samples well K, it guarantees that the Hausdorff distance between P_{i_0-1} and K is bounded. However, we do not know i_0 and we have no means to stop the algorithm at this point. Fortunately, we can prove Lemma 19 which guarantees that the remaining iterations will not remove too many points and break the theoretical guarantees – that is, no harm is done in the subsequent iterations even after $i < i_0$. Putting all three together leads to our main result Theorem 15.

▶ **Lemma 16.** *Given a point set P, $x \in \mathbb{X}$ and $0 \leq i \leq k$, the distance to the i-th nearest neighbor of x in P satisfies, $d_{\mathbb{X}}(x, p_i) \leq \sqrt{\frac{k}{k-i+1}} d_{P,k}(x)$.*

Proof. The claim is proved by the following derivation.

$$\frac{k-i+1}{k} d_{\mathbb{X}}(x,p_i)^2 \leq \frac{1}{k}\sum_{j=i}^{k} d_{\mathbb{X}}(x,p_j)^2 \leq \frac{1}{k}\sum_{j=1}^{k} d_{\mathbb{X}}(x,p_j)^2 = d_{P,k}(x)^2. \qquad \blacktriangleleft$$

▶ **Lemma 17.** *Let P be a weak uniform $(\epsilon_{2k}, 2)$-noisy sample of K. For any $k' \leq k$ such that P is a (weak) uniform $(\epsilon_{k'}, c)$-noisy sample of K for some c, applying one step of the algorithm, with parameter $2k$ and resampling constant $C = 10 + 2\sqrt{2}$ gives a point set $P' \subseteq P$ which is a (weak) uniform $(\epsilon_{k'}, c)$-noisy sample of K.*

Proof. We show that if P is a uniform $(\epsilon_{k'}, c)$-noisy sample of K, then P' will also be a uniform $(\epsilon_{k'}, c)$-noisy sample of K. The similar version for weak uniformity follows from the same argument.

First, it is easy to see that as $P' \subset P$, the second and third sampling conditions of Def. 4 hold for P' as well. What remains is to show that Condition 1 also holds.

Take an arbitrary point $x \in K$. We know that $d_{P,2k}(x) \leq \epsilon_{2k}$ as P is a weak uniform $(\epsilon_{2k}, 2)$-noisy sample of K. Hence there exists $p \in P$ such that $d_{\mathbb{X}}(p, x) \leq d_{P,2k}(x) \leq \epsilon_{2k}$ and $d_{P,2k}(p) \leq 2\epsilon_{2k}$. Writing Q the result of the decluttering step, $\exists q \in Q$ such that $d_{\mathbb{X}}(p, q) \leq 2d_{P,2k}(p) \leq 4\epsilon_{2k}$. Moreover, $d_{P,2k}(q) \geq \frac{\epsilon_{2k}}{2}$ due to the uniformity condition for P.

Using Lemma 16, for $k' \leq k$, the k' nearest neighbors of x, which are chosen from P, $NN_{k'}(x)$ satisfies:

$$NN_{k'}(x) \subset B(x, \sqrt{2}\epsilon_{2k}) \subset B(p, (1+\sqrt{2})\epsilon_{2k}) \subset B(q, (5+\sqrt{2})\epsilon_{2k}) \subset B(q, (10+2\sqrt{2})d_{P,2k}(q))$$

Hence $NN_{k'}(x) \subset P'$ and $d_{P',k'}(x) = d_{P,k'}(x) \leq \epsilon_k$. This proves the lemma. $\blacktriangleleft$

▶ **Lemma 18.** *Let P be a uniform $(\epsilon_k, 2)$-noisy sample of K. One iteration of decluttering and resampling with parameter k and resampling constant $C = 10 + 2\sqrt{2}$ provides a set $P' \subseteq P$ such that $\delta_H(P', K) \leq 8C\epsilon_k + 7\epsilon_k$.*

Proof. Let Q denote the output after the decluttering step. Using Theorem 9 we know that $\delta_H(Q, K) \leq 7\epsilon_k$. Note that $Q \subset P'$. Thus, we only need to show that for any $p \in P'$, $d_{\mathbb{X}}(p, K) \leq 8C\epsilon_k + 7\epsilon_k$. Indeed, by the way the algorithm removes points, for any $p \in P'$, there exists $q \in Q$ such that $p \in B(q, Cd_{P,k}(q))$. It then follows that

$$d_{\mathbb{X}}(p, K) \leq Cd_{P,k}(q) + d_{\mathbb{X}}(q, K) \leq C(\epsilon_k + d_{\mathbb{X}}(q, K)) + 7\epsilon_k \leq 8C\epsilon_k + 7\epsilon_k. \qquad \blacktriangleleft$$

▶ **Lemma 19.** *Given a point $y \in P_i$, there exists $p \in P_0$ such that $d_{\mathbb{X}}(y,p) \leq \kappa d_{P_i,2^i}(y)$, where $\kappa = \frac{18+17\sqrt{2}}{4}$.*

Proof. We show this lemma by induction on i. First for $i = 0$ the claim holds trivially. Assuming that the result holds for all $j < i$ and taking $y \in P_i$, we distinguish three cases.

Case 1: $y \in P_{i-1}$ and $d_{P_{i-1},2^{i-1}}(y) \leq d_{P_i,2^i}(y)$. Applying the recurrence hypothesis for $j = i-1$ gives the result immediately.

Case 2: $y \notin P_{i-1}$. It means that y has been removed by decluttering and not been put back by resampling. These together imply that there exists $q \in Q_i \subseteq P_{i-1}$ such that $d_{\mathbb{X}}(y,q) \leq 2d_{P_i,2^i}(y)$ and $d_{\mathbb{X}}(y,q) > Cd_{P_i,2^i}(q)$ with $C = 10 + 2\sqrt{2}$. From the proof of Lemma 17, we know that the 2^{i-1} nearest neighbors of q in P_i are resampled and included in P_{i-1}. Therefore, $d_{P_{i-1},2^{i-1}}(q) = d_{P_i,2^{i-1}}(q) \leq d_{P_i,2^i}(q)$. Moreover, since $q \in P_{i-1}$, the inductive hypothesis implies that there exists $p \in P_0$ such that $d_{\mathbb{X}}(p,q) \leq \kappa d_{P_{i-1},2^{i-1}}(q) \leq \kappa d_{P_i,2^i}(q)$. Putting everything together, we get that there exists $p \in P_0$ such that

$$\begin{aligned} d_{\mathbb{X}}(p,y) &\leq d_{\mathbb{X}}(p,q) + d_{\mathbb{X}}(q,y) \\ &\leq \kappa d_{P_i,2^i}(q) + 2d_{P_i,2^i}(y) \\ &\leq \left(\frac{\kappa}{5+\sqrt{2}} + 2\right) d_{P_i,2^i}(y) \\ &\leq \kappa d_{P_i,2^i}(y). \end{aligned}$$

The derivation above also uses the relation that $d_{P_i,2^i}(q) < \frac{1}{C} d_{\mathbb{X}}(y,q) \leq \frac{2}{C} d_{P_i,2^i}(y)$.

Case 3: $y \in P_{i-1}$ and $d_{P_{i-1},2^{i-1}}(y) > d_{P_i,2^i}(y)$. The second part implies that at least one of the 2^{i-1} nearest neighbors of y in P_i does not belong to P_{i-1}. Let z be such a point. Note that $d_{\mathbb{X}}(y,z) \leq \sqrt{2} d_{P_i,2^i}(y)$ by Lemma 16. For point z, we can apply the second case and therefore, there exists $p \in P_0$ such that

$$\begin{aligned} d_{\mathbb{X}}(p,y) &\leq d_{\mathbb{X}}(p,z) + d_{\mathbb{X}}(z,y) \\ &\leq \left(\frac{\kappa}{5+\sqrt{2}} + 2\right) d_{P_i,2^i}(z) + \sqrt{2} d_{P_i,2^i}(y) \\ &\leq \left(\frac{\kappa}{5+\sqrt{2}} + 2\right) \left(d_{P_i,2^i}(y) + d_{\mathbb{X}}(z,y)\right) + \sqrt{2} d_{P_i,2^i}(y) \\ &\leq \left(\left(\frac{\kappa}{5+\sqrt{2}} + 2\right)(1+\sqrt{2}) + \sqrt{2}\right) d_{P_i,2^i}(y) \leq \kappa d_{P_i,2^i}(y) \end{aligned}$$

◀

Putting everything together. A repeated application of Lemma 17 (with weak uniformity) guarantees that P_{i_0+1} is a weak uniform $(\epsilon_{2^{i_0+1}}, 2)$-noisy sample of K. One more application (with uniformity) provides that P_{i_0} is a uniform $(\epsilon_{2^{i_0}}, 2)$-noisy sample of K. Thus, Lemma 18 implies that $d_H(P_{i_0-1}, K) \leq (87 + 16\sqrt{2})\epsilon_{2^{i_0}}$. Notice that $P_0 \subset P_{i_0-1}$ and thus for any $p \in P_0$, $d_{\mathbb{X}}(p,K) \leq (87+16\sqrt{2})\epsilon_{2^{i_0}}$.

To show the other direction, consider any point $x \in K$. Since P_{i_0} is a uniform $(\epsilon_{2^{i_0}}, 2)$-noisy sample of K, there exists $y \in P_{i_0}$ such that $d_{\mathbb{X}}(x,y) \leq \epsilon_{2^{i_0}}$ and $d_{P_{i_0},2^{i_0}}(y) \leq 2\epsilon_{2^{i_0}}$. Applying Lemma 19, there exists $p \in P_0$ such that $d_{\mathbb{X}}(y,p) \leq \frac{18+17\sqrt{2}}{2}\epsilon_{2^{i_0}}$. Hence $d_{\mathbb{X}}(x,p) \leq \left(\frac{18+17\sqrt{2}}{2} + 1\right)\epsilon_{2^{i_0}} \leq (87+16\sqrt{2})\epsilon_{2^{i_0}}$. The theorem then follows.

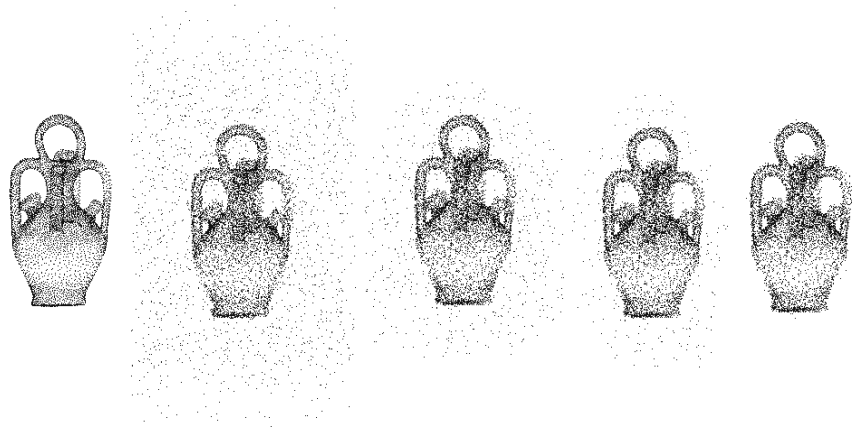


Figure 5 Experiment on a two dimensional manifold in three dimensions. From left to right, the ground truth, the noisy adaptively sampled input, output of two intermediate steps of the algorithm, and the final result.

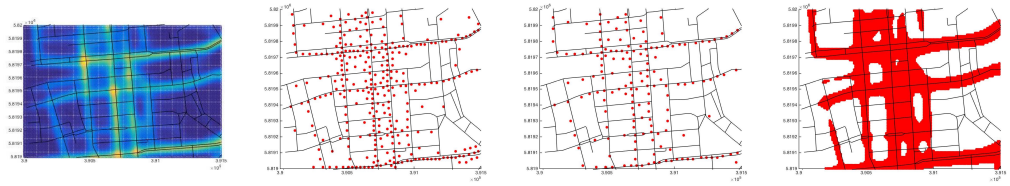
5 Preliminary experimental results

We now present some preliminary experimental results for the two denoising algorithms developed in this paper. See Appendix E of the full version [6] for more results.

In Figure 5, we show different stages of the ParfreeDeclutter algorithm on an input with *adaptively* sampled points. Even though for the parameter-free algorithm, theoretical guarantees are only provided for uniform samples, we note that it performs well on this adaptive case as well.

A second example is given in Figure 6. Here, the input data is obtained from a set of noisy GPS trajectories in the city of Berlin. In particular, given a set of trajectories (each modeled as polygonal curves), we first convert it to a density field by KDE (kernel density estimation). We then take the input as the set of grid points in 2D where every point is associated with a mass (density). Figure 6(a) shows the heat-map of the density field where light color indicates high density and blue indicates low density. In (b) and (c), we show the output of our Declutter algorithm (the ParfreeDeclutter algorithm does not provide good results as the input is highly non-uniform) for $k = 40$ and $k = 75$ respectively. In (d), we show the set of 40% points with the highest density values. The sampling of the road network is highly non-uniform. In particular, in the middle portion, even points off the roads have very high density due to noisy input trajectories. Hence a simple thresholding cannot remove these points and the output in (d) fills the space between roads in the middle portion; however more aggressive thresholding will cause loss of important roads. Our Declutter algorithm can capture the main road structures without collapsing nearby roads in the middle portion though it also sparsifies the data.

In another experiment, we apply the denoising algorithm as a pre-processing for high-dimensional data classification. Here we use MNIST data sets, which is a database of handwritten digits from '0' to '9'. Table 1 shows the experiment on digit 1 and digit 7. We take a random collection of 1352 images of digit '1' and 1279 images of digit '7' correctly labeled as a training set, and take 10816 images of digit 1 and digit 7 as a testing set. Each of the image is 28×28 pixels and thus can be viewed as a vector in $\mathbb{R}^{784}$. We use the L_1 metric to measure distance between such image-vectors. We use a linear SVM to classify the 10816 testing images. The classification error rate for the testing set is 0.6564% shown in the second row of Table 1.



(a) (b) (c) (d)

Figure 6 (a) The heat-map of a density field generated from GPS traces. There are around 15k (weighted) grid points serving as an input point set. The output of Algorithm Declutter when (b) $k = 40$ and (c) $k = 75$, (d) thresholding of 40% points with the highest density.

Table 1 Results of denoising on digit 1 and digit 7 from the MNIST.

1						Error(%)
2	Original	# Digit 1 1352		# Digit 7 1279		0.6564
3	Swap. Noise	# Mislabelled 1 270		# Mislabelled 7 266		4.0957
4		Digit 1		Digit 7		
5		# Removed	# True Noise	# Removed	# True Noise	
6	L1 Denoising	314	264	17	1	2.4500
7	Back. Noise	# Noisy 1 250		# Noisy 7 250		1.1464
8		Digit 1		Digit 7		
9		# Removed	# True Noise	# Removed	# True Noise	
10	L1 Denoising	294	250	277	250	0.7488

Next, we artificially add two types of noises to input data: the *swapping-noise* and the *background-noise*. The swapping-noise means that we randomly mislabel some images of '1' as '7', and some images of '7' as '1'. As shown in the third row of Table 1, the classification error increases to about 4.096% after such mislabeling in the training set.

Next, we apply our ParfreeDeclutter algorithm to this training set with added swapping-noise (to the set of images with label '1' and the set with label '7' separately) to first clean up the training set. As we can see in Row-6 of Table 1, we removed most images with a mislabeled '1' (which means the image is '7' but it is labeled as '1'). A discussion on why mislabeled '7's are not removed is given in the full version [6]. We then use the denoised dataset as the new training set, and improved the classification error to 2.45%.

The second type of noise is the *background noise*, where we replace the black backgrounds of a random subset of images in the training set (250 '1's and 250 '7's) with some other grey-scaled images. Under such noise, the classification error increases to 1.146%. Again, we perform our ParfreeDeclutter algorithm to denoise the training sets, and use the denoised data sets as the new training set. The classification error is then improved to 0.7488%. More results on the MNIST data sets are reported in the full version [6].

6 Discussions

Parameter selection is a notorious problem for many algorithms in practice. Our high level goal is to understand the roles of parameters in algorithms for denoising, how to reduce their use and what theoretical guarantees do they entail. While this paper presented some results

towards this direction, many interesting questions ensue. For example, how can we further relax our sampling conditions, making them allow more general inputs, and how to connect them with other classical noise models?

We also note that while the output of ParfreeDeclutter is guaranteed to be close to the ground truth w.r.t. the Hausdorff distance, this Hausdorff distance itself is not estimated. Estimating this distance appears to be difficult. We could estimate it if we knew the correct scale, i.e. i_0, to remove the ambiguity. Interestingly, even with the uniformity condition, it is not clear how to estimate this distance in a parameter free manner.

We do not provide guarantees for the parameter-free algorithm in an adaptive setting though the algorithm behaved well empirically for the adaptive case too. A partial result is presented in Appendix B of the full version [6], but the need for a small ϵ_k in the conditions defeat the attempts to obtain a complete result.

The problem of parameter-free denoising under more general sampling conditions remains open. It may be possible to obtain results by replacing uniformity with other assumptions, for example topological assumptions: say, if the ground truth is a simply connected manifold without boundaries, can this help to denoise and eventually reconstruct the manifold?

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