Adaptive Non-Parametric Regression
With the $K$-NN Fused Lasso

Oscar Hernan Madrid Padilla
omadrid@berkeley.edu

James Sharpnack
jsharpna@ucdavis.edu

Yanzhen Chen
imyanzhen@ust.hk

Daniela Witten
dwitten@uw.edu

1 Department of Statistics, UC Berkeley
2 Department of Statistics, UC Davis
3 Department of Statistics, University of Washington
4 Department of Biostatistics, University of Washington
5 Department of ISOM, Hong Kong University of Science and Technology

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Abstract

The fused lasso, also known as total-variation denoising, is a locally-adaptive function estimator over a regular grid of design points. In this paper, we extend the fused lasso to settings in which the points do not occur on a regular grid, leading to a new approach for non-parametric regression. This approach, which we call the $K$-nearest neighbors ($K$-NN) fused lasso, involves (i) computing the $K$-NN graph of the design points; and (ii) performing the fused lasso over this $K$-NN graph. We show that this procedure has a number of theoretical advantages over competing approaches: specifically, it inherits local adaptivity from its connection to the fused lasso, and it inherits manifold adaptivity from its connection to the $K$-NN approach. We show that excellent results are obtained in a simulation study and on an application to flu data. For completeness, we also study an estimator that makes use of an $\epsilon$-graph rather than a $K$-NN graph, and contrast this with the $K$-NN fused lasso.

Keywords: non-parametric regression, local adaptivity, manifold adaptivity, total variation, fused lasso

1 Introduction

In this paper, we consider the non-parametric regression setting in which we have $n$ observations, $(x_1, y_1), \ldots, (x_n, y_n)$, of the pair of random variables $(X, Y) \in \mathcal{X} \times \mathbb{R}$, where $\mathcal{X}$ is a metric space with metric $d_X$. We suppose that the model

$$y_i = f_0(x_i) + \varepsilon_i$$

holds, where $f_0 : \mathcal{X} \to \mathbb{R}$ is an unknown function that we wish to estimate. This problem arises in many settings, including demographic applications (Petersen et al., 2016a; Sadhanala and Tibshirani, 2017), environmental data analysis (Hengl et al., 2007), image processing (Rudin et al., 1992), and causal inference (Wager and Athey, 2017).

A substantial body of work has considered estimating the function $f_0$ in (1) at the observations $X = x_1, \ldots, x_n$ (i.e. denoising) as well as at other values of the random variable $X$ (i.e. prediction). This includes
the seminal papers by Breiman et al. (1984), Duchon (1977), and Friedman (1991), as well as more recent work by Petersen et al. (2016b), Petersen et al. (2016a), and Sadhanala and Tibshirani (2017). We refer the reader to Györfi et al. (2006) for a very detailed survey of classical non-parametric regression methods. The vast majority of existing work assumes that the true regression function $f_0$ is homogeneous, in the sense that it has the same smoothness level throughout its domain. For instance, a typical assumption is that $f_0$ is Lipschitz continuous. In this paper, we propose and analyze simple estimators that are locally adaptive, in that they can estimate $f_0$ when it is piecewise constant, piecewise Lipschitz, or satisfies a more general notion of bounded variation, as well as manifold adaptive, in the sense that they adapt to the intrinsic dimensionality of the data.

Recently, interest has focused on so-called trend filtering (Kim et al., 2009), which seeks to estimate $f_0(\cdot)$ under the assumption that its discrete derivatives are sparse, in a setting in which we have access to an unweighted graph that quantifies the pairwise relationships between the $n$ observations. In particular, the fused lasso, also known as zeroth-order trend filtering or total variation denoising (Mammen and van de Geer, 1997; Rudin et al., 1992; Tibshirani et al., 2005; Tibshirani, 2014; Sadhanala et al., 2017; Wang et al., 2016), solves the optimization problem

$$
\minimize_{\theta \in \mathbb{R}^n} \left\{ \frac{1}{2} \sum_{i=1}^{n} (y_i - \theta_i)^2 + \lambda \sum_{(i,j) \in E} |\theta_i - \theta_j| \right\},
$$

where $\lambda$ is a non-negative tuning parameter, and where $(i,j) \in E$ if and only if there is an edge between the $i$th and $j$th observations in the underlying graph. Then, $\hat{\theta}_i = \hat{f}(x_i)$. Computational aspects of the fused lasso have been studied extensively in the case of chain graphs (Johnson, 2013; Barbero and Sra, 2014; Davies and Kovac, 2001) as well as general graphs (Chambolle and Darbon, 2009; Chambolle and Pock, 2011; Tansey and Scott, 2015; Landrieu and Obozinski, 2015; Hoefling, 2010; Tibshirani and Taylor, 2011; Chambolle and Darbon, 2009). Furthermore, the fused lasso is known to have excellent theoretical properties. In one dimension, Mammen and van de Geer (1997) and Tibshirani (2014) characterized rates under the assumption that $f_0$ has bounded variation, whereas Lin et al. (2017) and Guntuboyina et al. (2017) studied the performance of the fused lasso under the assumption that $f_0$ is piecewise constant. Hutter and Rigollet (2016), Sadhanala et al. (2016), and Sadhanala et al. (2017) considered grid graphs. Padilla et al. (2018) and Wang et al. (2016) provide results that hold for general graphs. Importantly, trend filtering is locally adaptive, which means that it can adapt to inhomogeneity in the level of smoothness of the underlying signal; this is discussed in Tibshirani (2014) in the context of a chain graph, and in Wang et al. (2016) in the context of a general graph. However, trend filtering and the fused lasso are only applicable when we have access to a graph underlying the observations (or when the covariate, $X$, is one-dimensional, thereby leading to a chain graph); thus, these approaches are not applicable to the general non-parametric regression setting of (1), in which no graph is available.

In this paper, we extend the utility of the fused lasso approach by combining it with the $K$-nearest neighbors ($K$-NN) procedure. $K$-NN has been well-studied from a theoretical (Stone, 1977; Chaudhuri and Dasgupta, 2014; Von Luxburg et al., 2014; Alamgir et al., 2014), methodological (Dasgupta, 2012; Kontorovich et al., 2016; Singh and Póczos, 2016; Dasgupta and Kpotufe, 2014), and algorithmic (Friedman et al., 1977; Dasgupta and Sinha, 2013; Zhang et al., 2012) perspective. We exploit these ideas in order to generalize the class of problems to which the fused lasso can be applied, thereby yielding a single procedure that inherits the computational and theoretical advantages of both $K$-NN and the fused lasso.

In greater detail, in this paper we extend the fused lasso to the general non-parametric setting of (1), by performing a two-step procedure.

**Step 1.** We construct a $K$-nearest-neighbor ($K$-NN) graph, by placing an edge between each observation and the $K$ observations to which it is closest, in terms of the metric $d_X$. 

Step 2. We apply the fused lasso to this $K$-NN graph.

The resulting $K$-NN fused lasso ($K$-NN-FL) estimator appeared as an application of graph trend filtering in Wang et al. (2016), but was not studied in detail. In this paper, we study this estimator in detail. We also consider a variant obtained by replacing the $K$-NN graph in Step 1 with an $\epsilon$-nearest-neighbor ($\epsilon$-NN) graph, which contains an edge between $x_i$ and $x_j$ only if $d_X(x_i, x_j) < \epsilon$.

The main contributions of this paper are as follows:

1. **Local adaptivity.** We show that provided that $f_0$ has bounded variation, along with an additional condition that generalizes piecewise Lipschitz continuity (Assumption 5), then the mean squared errors (MSE) of both the $K$-NN-FL estimator and the $\epsilon$-NN-FL estimator are $n^{-1/d}$, ignoring logarithmic factors; here, $d > 1$ is the dimension of $\mathcal{X}$. In fact, this matches the minimax rate for estimating a two-dimensional Lipschitz function (Gy"orfi et al., 2006), but over a much wider function class.

2. **Manifold adaptivity.** Suppose that the covariates are i.i.d. samples from a mixture of $\ell$ unknown bounded densities $p_1, \ldots, p_\ell$. Suppose further that for $l = 1, \ldots, \ell$, the support $\mathcal{X}_l$ of $p_l$ is homeomorphic (see Assumption 3) to $[0,1]^{d_l} = [0,1] \times [0,1] \times \cdots \times [0,1]$, where $d_l > 1$ is the intrinsic dimension of $\mathcal{X}_l$. We show that under mild conditions, if the restriction of $f_0$ to $\mathcal{X}_l$ is a function of bounded variation, then the $K$-NN-FL estimator attains the rate $(\sum_{l=1}^{\ell} n_l 1^{-1/d_l})n^{-1}$, where $n_l$ is the number of samples associated with the $l$th component. This, in turn, is the rate that we would obtain by running the $K$-NN-FL estimator separately on the samples associated with each mixture component.

The rest of this paper is organized as follows. In Section 2, we propose the $K$-NN-FL and $\epsilon$-NN-FL estimators. In Section 3, we show that these estimators are locally adaptive. In Section 4, we show that the $K$-NN-FL estimator is manifold adaptive. We discuss the use of $K$-NN-FL to predict a response at a new observation in Section 5. A simulation study and a data application are presented in Section 6, and we close with a Discussion in Section 7. Proofs are provided in the Appendix.

## 2 Methodology

### 2.1 The $K$-Nearest-Neighbor and $\epsilon$-Nearest-Neighbor Fused Lasso

Both the $K$-NN-FL and $\epsilon$-NN-FL approaches are simple two-step procedures. The first step involves constructing a graph on the $n$ observations. The $K$-NN graph, $G_K = (V, E_K)$, has vertex set $V = \{1, \ldots, n\}$, and its edge set $E_K$ contains the pair $(i, j)$ if and only if $x_i$ is among the $K$-nearest neighbors (with respect to the metric $d_X$) of $x_j$, or vice versa. By contrast, the $\epsilon$-graph, $G_\epsilon = (V, E_\epsilon)$, contains the edge $(i, j)$ in $E_\epsilon$ if and only if $d_X(x_i, x_j) < \epsilon$.

After constructing the graph, we apply the fused lasso to $y = (y_1 \ldots y_n)^T$ over the graph $G$ (either $G_K$ or $G_\epsilon$). We can re-write the fused lasso optimization problem (2) as

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^n} \left\{ \frac{1}{2} \| y - \theta \|_2^2 + \lambda \| \nabla G \theta \|_1 \right\},$$

where $\lambda > 0$ is a tuning parameter, and $\nabla G$ is an oriented incidence matrix of $G$; each row of $\nabla G$ corresponds to an edge in $G$. For instance, if the $k$th edge in $G$ connects the $i$th and $j$th observations, then

$$(\nabla G)_{k,i} = \begin{cases} 1 & \text{if } l = i \\ -1 & \text{if } l = j \\ 0 & \text{otherwise} \end{cases}.$$
In this paper, we mostly focus on the setting where $G = G_K$ is the $K$-NN graph. We also include an analysis of the $\epsilon$-graph, which results from using $G = G_\epsilon$, as a point of contrast.

Given the estimator $\hat{\theta}$ defined in (3), we can predict the response at a new observation $x \in X \backslash \{x_1, \ldots, x_n\}$ according to

$$\hat{f}(x) = \frac{1}{\sum_{j=1}^n k(x_j, x)} \sum_{i=1}^n \hat{\theta}_i k(x_i, x). \quad (4)$$

In the case of $K$-NN-FL, we take $k(x_i, x) = 1_{\{i \in N_K(x)\}}$, where $N_K(x)$ is the set of $K$ nearest neighbors of $x$ in the training data. In the case of $\epsilon$-NN-FL, we take $k(x_i, x) = 1_{\{d_A(x, x) < \epsilon\}}$. (Given a set $A$, $1_A(x)$ is the indicator function that takes on a value of 1 if $x \in A$, and 0 otherwise.)

We construct the $K$-NN and $\epsilon$-NN graphs using standard Matlab functions such as knnsearch and bssxfun; this results in a computational complexity of $O(n^2)$. We solve the fused lasso with the parametric max-flow algorithm from Chambolle and Darbon (2009), for which software is available from the authors’ website, http://www.cmap.polytechnique.fr/~antonin/software/; it is in practice much faster than its worst-case complexity of $O(mn^2)$, where $m$ is the number of edges in the graph (Boykov and Kolmogorov, 2004; Chambolle and Darbon, 2009).

In $\epsilon$-NN and $K$-NN, the values of $\epsilon$ and $K$ directly affect the sparsity of the graphs, and hence the computational performance of the $\epsilon$-NN-FL and $K$-NN-FL estimators. Corollary 3.23 in Miller et al. (1997) provides an upper bound on the maximum degree of arbitrary $K$-NN graphs in $\mathbb{R}^d$.

### 2.2 Example

We now illustrate the performance of $K$-NN-FL in a small example. We generate $X \in \mathbb{R}^2$ according to the probability density function

$$p(x) = \frac{1}{5} 1_{\{(0,1)^2 \cap [0.4,0.6]^2\}}(x) + \frac{16}{25} 1_{\{(0.45,0.55)^2\}}(x) + \frac{4}{25} 1_{\{(0.4,0.6)^2 \cap [0.45,0.55]^2\}}(x). \quad (5)$$

Thus, $p$ concentrates 64% of its mass in the small interval $[0.45, 0.55]^2$, and 80% in $[0.4, 0.6]^2$. The left-hand panel of Figure 1 displays a heatmap of $n = 5000$ observations drawn from (5).

We define $f_0 : \mathbb{R}^2 \rightarrow \mathbb{R}$ in (1) to be the piecewise constant function

$$f_0(x) = 1_{\{\|x - \frac{1}{2} 1_2\|_2^2 \leq \frac{2}{1000} \}}(x). \quad (6)$$

We then generate $\{(x_i, y_i)\}_{i=1}^n$ with $n = 5000$ from (1); the data are displayed in the right-hand panel of Figure 1. This simulation study has the following characteristics:

1. The function $f_0$ in (6) is not Lipschitz, but does have low total variation. This suggests that $K$-NN-FL should exhibit local adaptivity, and should outperform approaches that rely on Lipschitz continuity.

2. The probability density function $p$ in (5) is highly non-uniform. This should not pose a problem for $K$-NN-FL, given that it is has manifold adaptivity.

We compared the following methods:

1. $K$-NN-FL, with the number of neighbors set to $K = 5$, and the tuning parameter $\lambda$ chosen to minimize the average MSE over 100 Monte Carlo replicates.

2. CART (Breiman et al., 1984), with the complexity parameter chosen to minimize the average MSE over 100 Monte Carlo replicates.
3. K-NN regression (see e.g. Stone, 1977), with the number of neighbors K set to minimize the average MSE over 100 Monte Carlo replicates.

The estimated regression functions resulting from these three approaches are displayed in Figure 2. We see that K-NN-FL can adapt to low-density and high-density regions of the distribution of covariates, as well as to the local structure of the regression function. By contrast, CART has some artifacts due to the binary splits that make up the decision tree, and K-NN regression undersmoothes in large areas of the domain.

3 Local Adaptivity of K-NN-FL and ε-NN-FL

3.1 Assumptions

We assume that, in (1), the elements of \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^T \) are independent and identically-distributed mean-zero sub-Gaussian random variables,

\[
\mathbb{E}(\varepsilon_i) = 0, \quad \mathbb{P}(|\varepsilon_i| > t) \leq C \exp\left(-t^2/(2\sigma^2)\right), \quad i = 1, \ldots, n, \forall t > 0,
\]

for some positive constants \( \sigma \) and \( C \). Furthermore, we assume that \( \varepsilon \) is independent of \( X \).

In addition, for a set \( A \subset \mathcal{A} \) with \((\mathcal{A}, d_\mathcal{A})\) a metric space, we write \( B_\varepsilon(A) = \{a : \exists a' \in A, \text{ with } d_\mathcal{A}(a, a') \leq \varepsilon\} \). We let \( \partial A \) denote the boundary of the set \( A \). Moreover, we define \( \|x\|_n^2 = n^{-1} \sum_{i=1}^n x_i^2 \).

In the covariate space \( \mathcal{X} \), we consider the Borel sigma algebra, \( \mathcal{B}(\mathcal{X}) \), induced by the metric \( d_\mathcal{X} \). We let \( \mu \) be a measure on \( \mathcal{B}(\mathcal{X}) \). We complement the model in (1) by assuming that the covariates satisfy \( x_i \overset{i.i.d.}{\sim} p(x) \).

We begin by stating assumptions on the distribution of the covariates \( p(\cdot) \), and on the metric space \((\mathcal{X}, d_\mathcal{X})\). In the theoretical results in Section 3 from Györfi et al. (2006), it is assumed that \( p \) is the probability
density function of the uniform distribution in $[0, 1]^d$. In this section, we will require only that $p$ is bounded above and below. This condition appeared in the framework for studying $K$-NN graphs in Von Luxburg et al. (2014), and in the work on density quantization by Alamgir et al. (2014).

**Assumption 1.** The density $p$ satisfies $0 < p_{\min} < p(x) < p_{\max}$, for all $x \in \mathcal{X}$, where $p_{\min}, p_{\max} \in \mathbb{R}$.

Although we do not require that $\mathcal{X}$ be a Euclidean space, we do require that the balls in $\mathcal{X}$ have volume (with respect to $\mu$) that behaves similarly to the Lebesgue measure of balls in $\mathbb{R}^d$. This is expressed in the next assumption, which appeared as part of the definition of a valid region (Definition 2) in Von Luxburg et al. (2014).

**Assumption 2.** The base measure $\mu$ in $\mathcal{X}$ satisfies

$$r^d c_{1,d} \leq \mu(B_r(x)) \leq c_{2,d} r^d, \quad \forall x \in \mathcal{X},$$

for all $0 < r < r_0$, where $r_0, c_{1,d},$ and $c_{2,d}$ are positive constants, and $d \in \mathbb{N}$ is the intrinsic dimension of $\mathcal{X}$.
Next, we make an assumption about the topology of the space $\mathcal{X}$. We require that the space has no holes, and is topologically equivalent to $[0, 1]^d$, in the sense that there exists a continuous bijection between $\mathcal{X}$ and $[0, 1]^d$.

**Assumption 3.** There exists a homeomorphism (a continuous bijection with a continuous inverse) \( h : \mathcal{X} \to [0, 1]^d \), such that

\[
L_{\min} d_{\mathcal{X}}(x, x') \leq \|h(x) - h(x')\|_2 \leq L_{\max} d_{\mathcal{X}}(x, x'), \quad \forall x, x' \in \mathcal{X},
\]

for some positive constants \( L_{\min}, L_{\max} \).

In particular, Assumptions 2 and 3 immediately hold if $\mathcal{X} = [0, 1]^d$, with $d_{\mathcal{X}}$ as the Euclidean distance, $h$ as the identity mapping in $[0, 1]^d$, and $\mu$ as the Lebesgue measure in $[0, 1]^d$. A metric space $(\mathcal{X}, d_{\mathcal{X}})$ that satisfies Assumption 3 is a special case of a differential manifold; the intuition is that the space $\mathcal{X}$ is a chart of the atlas for said differential manifold.

We now proceed to state conditions on the regression function $f_0$. The first assumption simply requires bounded variation of the composition of the regression function with the homeomorphism $h$ from Assumption 3.

**Assumption 4.** The function $g_0 := f_0 \circ h^{-1}$ has bounded variation, i.e. $g_0 \in BV((0, 1)^d)$. Here $(0, 1)^d$ is the interior of $[0, 1]^d$, and $BV((0, 1)^d)$ is the class of functions in $(0, 1)^d$ with bounded variation.

A discussion of bounded variation can be found in Appendix A.1. It is worth mentioning that if $\mathcal{X} = [0, 1]^d$ and $h(\cdot)$ is the identity function in $[0, 1]^d$, then Assumption 4 simply states that $f_0$ has bounded variation. However, in order to allow for more general scenarios, the condition is stated in terms of the function $g_0$ which has domain in the unit box, whereas the domain of $f_0$ is the more general set $\mathcal{X}$.

We now recall the definition of a piecewise Lipschitz function, which induces a much larger class than the set of Lipschitz functions, as it allows for discontinuities.

**Definition 1.** Let $\Omega_{\epsilon} := [0, 1]^d \setminus B_\epsilon(\partial[0, 1]^d)$. We say that a function $g : [0, 1]^d \to \mathbb{R}$ is piecewise Lipschitz if there exists a set $S \subset (0, 1)^d$ that has the following properties:

1. $S$ has Lebesgue measure zero.
2. $\mu(h^{-1}(B_\epsilon(S) \cup ([0, 1]^d \setminus \Omega_{\epsilon}))) \leq C_S \epsilon$ for some constants $C_S, \epsilon_0 > 0$, for all $0 < \epsilon < \epsilon_0$.
3. There exists a positive constant $L_0$ such that if $z$ and $z'$ belong to the same connected component of $\Omega_{\epsilon} \setminus B_\epsilon(S)$, then $|g(z) - g(z')| \leq L_0 \|z - z'\|_2$.

Roughly speaking, Definition 1 says that $g$ is piecewise Lipschitz if there exists a small set $S$ that partitions $[0, 1]^d$ in such a way that $g$ is Lipschitz within each connected component of the partition. Theorem 2.2.1 in Ziemer (2012) implies that if $g$ is piecewise Lipschitz, then $g$ has bounded variation on any open set within a connected component.

Theorem 1 will require Assumption 5, which is a milder assumption on $g_0$ than piecewise Lipschitz continuity (Definition 1). We now present some notation that is needed in order to introduce Assumption 5.

For $\epsilon > 0$, we denote by $\mathcal{P}_\epsilon$ the rectangular partition of $(0, 1)^d$ whose elements all have Lebesgue measure $\epsilon^d$. We define $\Omega_{2\epsilon} := [0, 1]^d \setminus B_{2\epsilon}(\partial[0, 1]^d)$. Then, for a set $S \subset (0, 1)^d$, we define

\[
\mathcal{P}_{\epsilon, S} := \{ A \cap (\Omega_{2\epsilon} \setminus B_{2\epsilon}(S)) : A \in \mathcal{P}_\epsilon, A \cap (\Omega_{2\epsilon} \setminus B_{2\epsilon}(S)) \neq \emptyset \};
\]

this is the partition induced in $\Omega_{2\epsilon} \setminus B_{2\epsilon}(S)$ by the grid $\mathcal{P}_\epsilon$. 

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For a function \( g \) with domain \([0, 1]^d\), we define
\[
S_1(g, \mathcal{P}_\epsilon, \mathcal{S}) := \sum_{A \in \mathcal{P}_\epsilon, \mathcal{S}} \left[ \sup_{z_A \in A} \frac{1}{\epsilon} \int_{B_\epsilon(z_A)} |g(z_A) - g(z)| \, dz \right].
\]
(8)

If \( g \) is piecewise Lipschitz, then \( S_1(g, \mathcal{P}_\epsilon, \mathcal{S}) \) will be bounded. To see this, assume that Definition 1 holds with \( \mathcal{S} \) the set above. Then
\[
S_1(g, \mathcal{P}_\epsilon, \mathcal{S}) \leq \sum_{A \in \mathcal{P}_\epsilon, \mathcal{S}} \left[ \sup_{z_A \in A} \int_{B_\epsilon(z_A)} \frac{|g(z_A) - g(z)|}{\|z_A - z\|^2} \, dz \right] \leq \frac{L_0 \pi^{d/2}}{\Gamma\left(\frac{d}{2} + 1\right)} < \infty,
\]
where the second-to-last inequality follows from the fact that the volume of a \( d \)-dimensional ball of radius \( \epsilon \) is \( \pi^{d/2} \epsilon^d / \Gamma(d/2 + 1) \), as well as the fact that there are at most in the order of \( \epsilon^{-d} \) elements of \( \mathcal{P}_\epsilon, \mathcal{S} \). To better understand (8), notice that we can view \( S_1(g, \mathcal{P}_\epsilon, \mathcal{S}) \) as a discretization over the set \( \Omega_{2\epsilon} \setminus B_{2\epsilon}(\mathcal{S}) \) of the integral of the function
\[
m(z_A, \epsilon) = \frac{1}{\epsilon^{d+1}} \int_{B_\epsilon(z_A)} |g(z_A) - g(z)| \, dz.
\]
(10)

Recall that \( z_A \) is a Lebesgue point of \( g \) if \( \lim_{\epsilon \to 0} \epsilon m(z_A, \epsilon) = 0 \) (see Definition 2.18 in Giaquinta and Modica, 2010). Furthermore, if \( g \in L_1(\mathbb{R}^d) \) (see Appendix A.1 for this notation) then almost all points are Lebesgue points (this follows from the Lebesgue differentiation theorem; see Theorem 2.16 in Giaquinta and Modica, 2010). Thus, if \( g \in L_1(\mathbb{R}^d) \), then loosely speaking each term in (8) is \( O(\epsilon^{-d}) \), for any configuration of points \( z_A \). In Assumption 5, we will further require \( S_1(f_0 \circ h^{-1}, \mathcal{P}_\epsilon, \mathcal{S}) \) to be bounded, which as mentioned before holds if \( f_0 \circ h^{-1} \) is piecewise Lipschitz.

Next, we define
\[
S_2(g, \mathcal{P}_\epsilon, \mathcal{S}) := \sum_{A \in \mathcal{P}_\epsilon, \mathcal{S}} \left[ \sup_{z_A \in A} T(g, z_A) \epsilon^d \right].
\]
(11)

where
\[
T(g, z_A) = \sup_{z \in B_\epsilon(z_A)} \sum_{l=1}^{d} \left[ \int_{\|z'\|_2 \leq \epsilon} \frac{\partial \psi(z'/\epsilon)}{\partial z_l} \left( \frac{g(z_A - z') - g(z - z')}{\|z_A - z\|_2 \epsilon^d} \right) \, dz' \right],
\]
(12)
and \( \psi \) is a test function (see (21) in the Appendix). Thus, (11) is the summation, over evenly-sized rectangles of volume \( \epsilon \) that intersect \( \Omega_{2\epsilon} \setminus B_{2\epsilon}(\mathcal{S}) \), of the supremum of the function in (12). The latter, for a function \( g \), can be thought as the average “Lipschitz constant” near \( z_A \) — see the expression inside parenthesis in (12) — weighted by the derivative of a test function. The scaling factor \( \epsilon^d \) in (12) arises because the integral is taken over a set of measure proportional to \( \epsilon^d \).

As with \( S_1(g, \mathcal{P}_\epsilon, \mathcal{S}) \), one can verify that if \( g \) is a piecewise Lipschitz function, then \( S_2(g, \mathcal{P}_\epsilon, \mathcal{S}) \) is bounded. The argument is similar to that in (9).

We now make use of (8) and (11) in order to state our next condition on \( g_0 = f_0 \circ h^{-1} \). This next condition is milder than a piecewise Lipschitz assumption (see Definition 1), and is independent of Assumption 4.

**Assumption 5.** Let \( \Omega_\epsilon := [0, 1]^d \setminus B_\epsilon(\partial[0, 1]^d) \). There exists a set \( \mathcal{S} \subset (0, 1)^d \) that satisfies the following:

1. \( \mathcal{S} \) has Lebesgue measure zero.
2. \( \mu(h^{-1}(B_\epsilon(\mathcal{S}) \cup ((0, 1)^d \setminus \Omega_\epsilon))) \leq C_\mathcal{S} \epsilon \) for some constants \( C_\mathcal{S}, \epsilon_0 > 0 \), and for all \( 0 < \epsilon < \epsilon_0 \).
3. \( \sup_{0 < \epsilon < \epsilon_0} \max\{S_1(g_0, \mathcal{P}_\epsilon, \mathcal{S}), S_2(g_0, \mathcal{P}_\epsilon, \mathcal{S})\} < \infty. \)
3.2 Results

Letting $\theta^*_i = f_0(x_i)$, we express the MSEs of $K$-NN-FL and $\epsilon$-NN-FL in terms of the total variation of $\theta^*$ with respect to the $K$-NN and $\epsilon$-NN graphs.

**Theorem 1.** Let $K \asymp \log^{1+2r} n$ for some $r > 0$. Then under Assumptions 1–3, with an appropriate choice of the tuning parameter $\lambda$, the $K$-NN-FL estimator $\hat{\theta}$ satisfies

$$
\|\hat{\theta} - \theta^*\|^2_n = O_p \left( \frac{\log^{1+2r} n}{n} + \frac{\log^{1.5+r} n}{n} \|\nabla G_K \theta^*\|_1 \right).
$$

This upper bound also holds for $\epsilon$-NN-FL if we replace $\|\nabla G_K \theta^*\|_1$ with $\|\nabla G, \theta^*\|_1$, for an appropriate choice of $\lambda$.

Clearly, this rate is a function of $\|\nabla G \theta^*\|_1$ (where $G$ equals $G_K$ or $G_E$). For the grid graph considered in Sadhanala et al. (2016), $\|\nabla G \theta^*\|_1 \asymp n^{-1/d}$, leading to the rate $n^{-1/d}$. In fact, when $d = 2$, this is the minimax rate for estimation of a Lipschitz continuous function (Györfi et al., 2006). However, for a general graph, there is no prior reason to expect that $\|\nabla G \theta^*\|_1 \asymp n^{-1/d}$. Our next result shows that this is actually the case under the assumptions discussed in Section 3.1.

**Theorem 2.** Under Assumptions 1–5, if $K \asymp \log^{1+2r} n$ for some $r > 0$, then for an appropriate choice of the tuning parameter $\lambda$, the $K$-NN-FL estimator defined in (3) satisfies

$$
\|\hat{\theta} - \theta^*\|^2_n = O_p \left( \frac{\log^\alpha n}{n^{1/d}} \right),
$$

with $\alpha = 3r + 5/2 + (2r + 1)/d$. In addition, under the same assumptions, the same upper bound holds for the $\epsilon$-NN-FL estimator with $\epsilon \asymp \log^{1+2r} n/n^{1/d}$.

Theorem 2 indicates that under Assumptions 1–5, both the $K$-NN-FL and $\epsilon$-NN-FL estimators attain the convergence rate $n^{-1/d}$, ignoring logarithmic terms. Importantly, Theorem 3.2 from Györfi et al. (2006) shows that in the two-dimensional setting, this rate is actually minimax for estimation of a Lipschitz continuous function, when the design points are uniformly drawn from $[0, 1]^2$. This is of course a much smaller class than that implied by Assumptions 1–5. In addition, the upper bounds in Theorem 2 hold if Assumptions 1–3 are met and $f_0$ satisfies Definition 1 (replacing Assumptions 4–5), i.e. if $f_0$ is piecewise Lipschitz. The proof of this fact is included in Appendix A.9.

We see from Theorem 2 that both $\epsilon$-NN-FL and $K$-NN-FL are locally adaptive, in the sense that they can adapt to the form of the function $f_0$. Specifically, if $f_0$ satisfies Assumptions 4–5 (or, instead, Definition 1), then these estimators do not require knowledge of the set $S$. This is similar in spirit to the one-dimensional fused lasso, which does not require knowledge of the breakpoints when estimating a piecewise Lipschitz function.

However, there is an important difference between the applicability of Theorem 2 for $K$-NN-FL and $\epsilon$-NN-FL. In order to attain the rate in Theorem 2, $\epsilon$-NN-FL requires knowledge of the dimension $d$, since this quantity appears in the rate of decay of $\epsilon$. But in practice, the value of $d$ might not be clear: for instance, suppose that $X' = [0, 1]^2 \times \{0\}$; this is a subset of $[0, 1]^3$, but it is homeomorphic to $[0, 1]^2$, so that $d = 2$. If $d$ is unknown, then it can be challenging to choose $\epsilon$ for $\epsilon$-NN-FL. By contrast, the choice of $K$ in $K$-NN-FL only involves the sample size $n$. Consequently, local adaptivity of $K$-NN-FL may be much easier to achieve in practice.
4 Manifold Adaptivity of $K$-NN-FL

In this section, we show that under a much milder set of assumptions than those posed in Section 3, the $K$-NN-FL estimator can still achieve a desirable rate. In particular, we now allow the observations $\{(x_i, y_i)\}_{i=1}^n$ to be drawn from a mixture distribution, in which each mixture component satisfies the assumptions in Section 3.

We assume that there exists a partition $\{A_l\}_{l=1,\ldots,\ell}$ of $[n]$ such that $n_l = |A_l|$, where $n = n_1 + \ldots + n_{\ell}$, and

$$
\begin{align*}
y_i &= \theta_i^* + \varepsilon_i, \\
\theta_i^* &= f_{0,l}(x_i) \text{ if } i \in A_l, \\
x_i &\overset{\text{i.i.d.}}{\sim} p_l(x) \text{ if } i \in A_l,
\end{align*}
$$

where $\varepsilon$ satisfies (7), $p_l$ is a density with support $\mathcal{X}_l \subset \mathcal{X}$, $f_{0,l} : \mathcal{X}_l \to \mathbb{R}$, and $\{\mathcal{X}_l\}_{l=1,\ldots,\ell}$ is a collection of subsets of $\mathcal{X}$. For simplicity, we will assume that $\mathcal{X} \subset \mathbb{R}^d$ for some $d > 1$, and $d_\mathcal{X}$ is the Euclidean distance.

We further assume that each set $\mathcal{X}_l$ is homeomorphic to a Euclidean box of dimension depending on $l$, as follows:

**Assumption 6.** For $l = 1, \ldots, \ell$, the set $\mathcal{X}_l$ satisfies Assumptions 1–3 with metric given by $d_\mathcal{X}$, with dimension $d_l \in \mathbb{N} \setminus \{0, 1\}$, and with $\mu$ equal to some measure $\mu_l$. In addition:

1. There exists a positive constant $\tilde{c}_l$ such that the set

$$
\partial \mathcal{X}_l := \bigcup_{l' \neq l} \mathcal{X}_{l'} \cap \mathcal{X}_l
$$

satisfies

$$
\mu_l (B_{\varepsilon} (\partial \mathcal{X}_l) \cap \mathcal{X}_l) \leq \tilde{c}_l \varepsilon,
$$

for any small enough $\varepsilon > 0$.

2. There exists a positive constant $r_l$ such that for any $x \in \mathcal{X}_l$, either

$$
\inf_{x'' \in \partial \mathcal{X}_l} d_\mathcal{X}(x, x'') < d_\mathcal{X}(x, x') \text{ for all } x' \in \mathcal{X} \setminus \mathcal{X}_l,
$$

or

$$
B_{r_l}(x) \subset \mathcal{X}_l \text{ for all } \varepsilon < r_l.
$$

The constraints implied by Assumption 6 are very natural. Inequality (15) states that the intersections of the different manifolds $\mathcal{X}_1, \ldots, \mathcal{X}_\ell$ are small. To put it in perspective, if the extrinsic space $(\mathcal{X})$ were $[0, 1]^d$ with the Lebesgue measure, then balls of radius of $\varepsilon$ would have measure $\varepsilon^d$ which is less than $\varepsilon$ for all $d > 1$, and the set $B_{\varepsilon}(\partial [0, 1]^d) \cap [0, 1]^d$ has measure that scales like $\varepsilon$, the same scaling appearing (15). On the other hand (15) and (16) hold if $\mathcal{X}_1, \ldots, \mathcal{X}_\ell$ are compact and convex subsets of $\mathbb{R}^d$ whose interiors are disjoint.

We are now ready to extend Theorem 2 to the framework described in this section. The following theorem indicates that the $K$-NN-FL estimator can adapt to the “dimension” of the data in multiple regions of the domain.

**Theorem 3.** Suppose that the data are generated as in (13), and Assumption 6 holds. Suppose also that the functions $f_{0,1}, \ldots, f_{0,\ell}$ satisfy Assumptions 4–5 in the domain $\mathcal{X}_l$. If $\log n \asymp \log n_l$ for all $l \in [\ell]$, then for an appropriate choice of the tuning parameter $\lambda$, the $K$-NN-FL estimator defined in (3) satisfies

$$
\|\hat{\theta} - \theta^*\|_n^2 = O_p \left( \left( \frac{\log n}{\sum_{l=1}^{\ell} n_l^{-1/d_l}} \right) \right),
$$

provided that $K \asymp \log^{1+2r} n$ for some positive constant $r$, where $\text{poly}(\cdots)$ is a polynomial function.
The following example suggests that the $\epsilon$-NN-FL estimator may not be manifold adaptive.

**Example 1.** For $\mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2 \subset \mathbb{R}^3$, suppose that $\mathcal{X}_1 = [0, 1] \times \{c\}$ for some $c < 0$, and $\mathcal{X}_2 = [0, 1]^3$. Note that the sets $\mathcal{X}_1$ and $\mathcal{X}_2$ satisfy Assumption 6. Let us assume that all of the conditions of Theorem 3 are met with $n_1 \ll n$, and $n_2 \ll n^{3/4}$. Motivated by the scaling of $\epsilon$ in Theorem 2, we let $\epsilon \asymp \text{poly}(\log n)/n^{1/4}$. We now consider two possibilities for $t$: $t \in (0, 2]$, and $t > 2$.

- For any $t \in (0, 2]$, and for any positive constant $a \in (0, 3/4)$, there exists a positive constant $c(a)$ such that

$$
\mathbb{E}\|\hat{\theta}_\epsilon - \theta^*\|_n^2 \geq \frac{c(a)}{n^{4+a}},
$$

for large enough $n$, where $\hat{\theta}_\epsilon$ is the $\epsilon$-NN-FL estimator. (This is shown in Appendix A.11.) In other words, if $t < 2$, then $\epsilon$-NN-FL does not achieve a desirable rate. By contrast, with an appropriate choice of $\lambda$ and $K$, the $K$-NN-FL estimator attains the rate $n^{-1/2} \ll n_1^{-1/2}/n + n_2^{-1/3}/n$ (ignoring logarithmic terms) by Theorem 3.

- If $t > 2$, then the minimum degree in the $\epsilon$-graph of the observations in $\mathcal{X}_1$ will be at least $c(t)n^{1-2/t}$, with high probability, for some positive constant $c(t)$. (This can be seen as in Lemma 8.) This has two consequences:

1. Recall that the algorithm from Chambolle and Darbon (2009) has worst-case complexity $O(mn^2)$, where $m$ is the number of edges in the graph (although empirically the algorithm is typically much faster. Wang et al., 2016). Therefore, if $t$ is too large, then the computations involved in applying the fused lasso to the $\epsilon$-NN graph may be too demanding.

2. The choice of $\epsilon$ in Theorem 2 leads to an $\epsilon$-NN graph with degree $\text{poly}(\log n)$ (This follows from Proposition 27 in Von Luxburg et al. (2014)). In a different context, El Alaoui et al. (2016) argues that it is desirable for geometric graphs (which generalize $\epsilon$-NN graphs) to have degree $\text{poly}(\log n)$. This suggests that using $t > 2$ leads to an $\epsilon$-NN graph that is too dense.

## 5 Prediction for $K$-NN-FL

Recall from Section 2 that we estimate $f_0(x)$ for $x \in \mathcal{X}\setminus\{x_1, \ldots, x_n\}$ using (4); this amounts to averaging the predictions for the training observations that are near $x$. We now provide an upper bound for the mean integrated squared error (MISE) of this estimator.

**Theorem 4.** Suppose that Assumptions 1–3 hold, and choose $K \asymp \log^{1+2r} n$ for some $r > 0$. With $\hat{f}(x)$ the prediction function for the $K$-NN-FL estimator as defined in (4), and for an appropriate choice of $\lambda$, it follows that

$$
\mathbb{E}_{X \sim p} \left| f_0(X) - \hat{f}(X) \right|^2 = O_p \left( \frac{\log^{1+2r} n}{n} + \frac{\log^{1.5+r} n}{n} \|\nabla_{G_K} \theta^*\|_1 + \text{AErr} \right),
$$

where $\text{AErr}$ is the approximation error, defined as

$$
\text{AErr} = \int \left( f_0(x) - \frac{1}{K} \sum_{i \in \mathcal{X}(x)} f_0(x_i) \right)^2 p(x) \mu(dx).
$$

The right-hand side of (17) involves the penalty $\|\nabla_{G_K} \theta^*\|_1$ and the approximation error $\text{AErr}$. We saw in Section 3.2 that the former can be characterized under Assumptions 4–5, or if $f_0$ satisfies Definition 1. We will now show that the piecewise Lipschitz condition (Definition 1) is sufficient to ensure an upper bound on the approximation error.
Theorem 5. Assume that \( g_0 := f_0 \circ h^{-1} \) satisfies Definition 1, i.e. \( g_0 \) is piecewise Lipschitz. Then, under Assumptions 1–3,

\[
AErr = O_p \left( \frac{K^{1/d}}{n^{1/d}} \right),
\]

provided that \( K/ \log n \to \infty \). Consequently, with \( K \asymp \log^{1+2r} n \) for some \( r > 0 \), and for an appropriate choice of \( \lambda \), we have that

\[
E_{X \sim p} \left| f_0(X) - \hat{f}(X) \right|^2 = O_p \left( \frac{\log^{2.5+3r+(1+2r)/d} n}{n^{1/d}} \right). \tag{18}
\]

This implies that the rate \( n^{-1/d} \) from Theorem 2 is also attained for the prediction error. This implies that in two dimensions, \( K \)-NN-FL together with interpolation exhibits the minimax rate at unobserved locations drawn from \( p \).

6 Experiments

Throughout this section, we take \( d_X \) to be Euclidean distance.

6.1 Simulated Data

In this section, we compare the following approaches:

- \( \epsilon \)-NN-FL, with \( \epsilon \) held fixed, and \( \lambda \) treated as a tuning parameter.
- \( K \)-NN-FL, with \( K \) held fixed, and \( \lambda \) treated as a tuning parameter.
- CART (Breiman et al., 1984), implemented in the \( R \) package \texttt{rpart}, with the complexity parameter treated as a tuning parameter.
- MARS (Friedman, 1991), implemented in the \( R \) package \texttt{earth}, with the penalty parameter treated as a tuning parameter.
- Random forests (Breiman, 2001), implemented in the \( R \) package \texttt{randomForest}, with the number of trees fixed at 800, and with the minimum size of each terminal node treated as a tuning parameter.
- \( K \)-NN regression (e.g. Stone, 1977), implemented in Matlab using the function \texttt{knnsearch}, with \( K \) treated as a tuning parameter.

We evaluate each method’s performance using mean squared error (MSE; defined as \( \| \theta^* - \hat{\theta} \|^2_n \)). Specifically, we apply each method to 150 Monte Carlo data sets with a range of tuning parameter values. For each method, we then identify the tuning parameter value that leads to the smallest average MSE (where the average is taken over the 150 data sets). We refer to this smallest average MSE as the optimized MSE in what follows.

6.1.1 Fixed \( d \), varying \( n \)

Throughout this section, we consider two scenarios with \( d = 2 \) covariates.
Figure 3: (a): A scatterplot of data generated under Scenario 1. The vertical axis displays $f_0(x_i)$, while the other two axes display the two covariates. (b): Optimized MSE (averaged over 150 Monte Carlo simulations) of competing methods under Scenario 1. Here $(\epsilon_1, \epsilon_2) = (\frac{3}{4} \sqrt{\log n/n}, \sqrt{\log n/n})$. (c): Computational time (in seconds) for Scenario 1, averaged over 150 Monte Carlo simulations. (d): Optimized MSE (averaged over 150 Monte Carlo simulations) of competing methods under Scenario 2.

**Scenario 1.** The function $f_0 : [0, 1]^2 \rightarrow \mathbb{R}$ is piecewise constant,

$$f_0(x) = 1_{\{t \in \mathbb{R}^2 : \|t - \frac{3}{4} 1_2\|_2 < \|t - \frac{1}{2} 1_2\|_2\}}(x).$$

(19)
Figure 4: (a) Optimized MSE, averaged over 150 Monte Carlo simulations, for Scenario 3. (b): Optimized MSE, averaged over 150 Monte Carlo simulations, for Scenario 4. In both Scenario 3 and Scenario 4, $\epsilon_1$ is chosen to be the minimum value such that the total number of edges in the graph $G_{\epsilon_1}$ is at most 50000.

The covariates are drawn from a uniform distribution on $[0, 1]^2$. The data are generated as in (1) with $N(0, 1)$ errors.

**Scenario 2.** The function $f_0 : [0, 1]^2 \rightarrow \mathbb{R}$ is as in (6), with generative density for $X$ as in (5). The data are generated as in (1) with $N(0, 1)$ errors.

Data generated under Scenario 1 are displayed in Figure 3(a). Data generated under Scenario 2 are displayed in Figure 1(b).

Figure 3(b) and Figure 3(d) display the optimized MSE, as a function of the sample size, for Scenarios 1 and 2, respectively. $K$-NN-FL gives the best results in both scenarios. $\epsilon$-NN-FL performs a bit worse than $K$-NN-FL in Scenario 1, and very poorly in Scenario 2 (results not shown).

Timing results for all approaches are reported in Figure 3(c). For all methods, the times reported are averaged over a range of tuning parameter values. For instance, for $K$-NN-FL, we fix $K$ and compute the time for different choices of $\lambda$; we then report the average of those times.

### 6.1.2 Fixed $n$, varying $d$

We now consider two scenarios with $n = 8000$.

**Scenario 3.** The function $f_0 : [0, 1]^d \rightarrow \mathbb{R}$ is defined as

$$f_0(x) = \begin{cases} 
1 & \text{if } \|x - \frac{1}{4} 1_d\|_2 < \|x - \frac{3}{4} 1_d\|_2, \\
-1 & \text{otherwise}
\end{cases}$$
Figure 5: Results for the flu data. “Normalized Prediction Error” was obtained by dividing each method’s test set prediction error by the test set prediction error of $K$-NN-FL, with $K = 7$.

and the generative density for $X$ is uniform in $[0, 1]^d$. The errors in (1) have a $N(0, 0.3)$ distribution.

**Scenario 4.** The function $f_0 : [0, 1]^d \to \mathbb{R}$ is defined as

$$f_0(x) = \begin{cases} 
2 & \text{if } \|x - q_1\|_2 < \min\{\|x - q_2\|_2, \|x - q_3\|_2, \|x - q_4\|_2\} \\
1 & \text{if } \|x - q_2\|_2 < \min\{\|x - q_1\|_2, \|x - q_3\|_2, \|x - q_4\|_2\} \\
0 & \text{if } \|x - q_3\|_2 < \min\{\|x - q_1\|_2, \|x - q_2\|_2, \|x - q_4\|_2\} \\
-1 & \text{otherwise}
\end{cases},$$

where $q_1 = \left(\frac{1}{4}1_T^{T_{[d/2]}}, \frac{1}{2}1_T^{T_{d-[d/2]}}\right)^T$, $q_2 = \left(\frac{1}{2}1_T^{T_{[d/2]}}, \frac{1}{4}1_T^{T_{d-[d/2]}}\right)^T$, $q_3 = \left(\frac{3}{4}1_T^{T_{[d/2]}}, \frac{1}{2}1_T^{T_{d-[d/2]}}\right)^T$ and $q_4 = \left(\frac{1}{2}1_T^{T_{[d/2]}}, \frac{3}{4}1_T^{T_{d-[d/2]}}\right)^T$. Once again, the generative density for $X$ is uniform in $[0, 1]^d$, and the errors are i.i.d. $N(0, 0.3)$.

Optimized MSE for each approach is displayed in Figure 4. When $d$ is small, most methods perform well; however, as $d$ increases, the competing methods quickly deteriorate, whereas $K$-NN-FL continues to perform well.

**6.2 Flu Data**

We consider a data set that consists of flu activity and atmospheric conditions in Texas between January 1, 2003 and December 31, 2009 across different cities. Our data-use agreement does not permit dissemination.
of these hospital records. We also use data on temperature and air quality (particulate matter) in these cities, which can be obtained directly from CDC Wonder (http://wonder.cdc.gov/). Using the number of flu-related doctor’s office visits as the dependent variable, we fit a separate nonparametric regression model to each of 24 cities; each day was treated as a separate observation, so that the number of samples is \( n = 2556 \) in each city. Five independent variables are included in the regression: maximum and average observed concentration of particulate matter, maximum and minimum temperature, and day of the year. All variables are scaled to lie in \([0, 1]\). We performed 50 75%/25% splits of the data into a training set and a test set. All models were fit on the training data, with 5-fold cross-validation to select tuning parameter values. Then prediction performance was evaluated on the test set.

We apply \( K \)-NN-FL with \( K \in \{5, 7\} \), and \( \epsilon \)-NN-FL with \( \epsilon = j/n^{1/d} \) for \( j \in \{1, 2, 3\} \). We also fit neural networks (Hagan et al., 1996; implemented in Matlab using the functions newfit and train), thin plate splines (Duchon, 1977; implemented using the R package fields), and MARS, CART, and random forests, using software described in Section 6.1.

Average test set prediction error (across the 50 test sets) is displayed in Figure 5. We see that \( K \)-NN-FL and \( \epsilon \)-NN-FL tend to have the best performance. In particular, \( K \)-NN-FL performs best in 13 out the 24 cities, and second best in 6 cities. In 8 of the 24 cities, \( \epsilon \)-NN-FL performs best.

7 Conclusion

In this paper, we introduced a two-stage non-parametric regression estimator, by (i) constructing a nearest-neighbors graph over the observations; and (ii) performing the fused lasso over the graph. We have shown that when the \( K \)-NN or \( \epsilon \)-NN graph is used, the resulting procedure is locally adaptive; furthermore, when the \( K \)-NN graph is used, the procedure is manifold adaptive. Our theoretical results are bolstered by findings on simulated data and on a flu data set.

A Proofs

A.1 Notation

Throughout, given \( m \in \mathbb{N} \), we denote by \([m]\) the set \( \{1, \ldots, m\} \). For \( a \in A \), \( A \subset A \), with \((A, d_A)\) a metric space, we write

\[
d_A(a, A) = \inf_{b \in A} d_A(a, b),
\]

\[
B_\epsilon(A, d_A) = \{ b \in A : d_A(b, A) < \epsilon \},
\]

and when the context is clear we will simply write \( B_\epsilon(A) \) instead of \( B_\epsilon(A, d_A) \). In the case of the space \( \mathbb{R}^d \), we will use the notation \( \text{dist}(\cdot, \cdot) \) for the metric induced by the norm \( \|\cdot\|_\infty \), and we will write \( B_\epsilon(x) \) for the ball \( B_\epsilon(x, \|\cdot\|_2) \). We use the notation \( \|\cdot\|_n \) for the rescaling of the \( \|\cdot\|_2 \) norm, such that for \( x \in \mathbb{R}^n \),

\[
\|x\|_n^2 = \frac{1}{n} \sum_{i=1}^n x_i^2.
\]

On the other hand, we write

\[
\Omega_\epsilon = [0, 1]^d \setminus B_\epsilon(\partial [0, 1]^d).
\]

Thus, \( \Omega_\epsilon \) is the set of points in the interior of \([0, 1]^d\) such that balls of radius \( \epsilon \) with center in such points are also contained in \([0, 1]^d\).

Given an open set \( \Omega \subset \mathbb{R}^d \), as is usual in mathematical analysis, we denote by \( C^1_c(\Omega, \mathbb{R}^d) \) the set of functions \( \phi : \Omega \rightarrow \mathbb{R}^d \) that have compact support and continuous first derivative. We also write \( C^\infty(\Omega) \) for...
the class of functions $\phi : \Omega \to \mathbb{R}$ which have derivatives of all orders. The function $\psi : \mathbb{R}^d \to \mathbb{R}$ given as

$$\psi(z) = \begin{cases} C_1 \exp \left( -1/(1 - \|x\|_2^2) \right) & \text{if } \|x\|_2 < 1, \\ 0 & \text{otherwise}, \end{cases}$$

is called a test function if $C_1$ is chosen such that $\int \psi(z) \, dz = 1$. We also denote, for $s \in \mathbb{N}$, by $1_s := (1, \ldots, 1)^T \in \mathbb{R}^s$. Moreover, for vectors $u \in \mathbb{R}^s$ and $v \in \mathbb{R}^t$, we write $w = (u^T, v^T)^T \in \mathbb{R}^{s+t}$ for the concatenation of $u$ and $v$.

Furthermore, we denote by $L_1(\Omega)$ the set of measurable functions (with respect to the Lebesgue measure) $f : \Omega \to \mathbb{R}$ such that

$$\int_\Omega |f(x)| \mu(dx) < \infty,$$

where $\mu$ is the Lebesgue measure in $\Omega$.

**BV class.** We now review some notation regarding general spaces of functions of bounded variation. Let $\Omega \subset \mathbb{R}^d$ be an open set. Recall that the divergence of a function $g : \Omega \to \mathbb{R}$ is defined as

$$\text{div}(g)(x) = \sum_{j=1}^{d} \frac{\partial g(x)}{\partial x_j}, \quad \forall x \in \Omega,$$

provided that the partial derivatives involved exist.

A function $f : \Omega \to \mathbb{R}$ has bounded variation if

$$|f|_{BV(\Omega)} := \sup \left\{ \int_\Omega f(x) \, \text{div}(g)(x) \, dx ; \ g \in C^1_c(\Omega, \mathbb{R}^d), \ |g|_\infty \leq 1 \right\},$$

is finite. Here, we use the notation

$$\|g\|_\infty := \left\| \left( \sum_{j=1}^{d} g_j^2 \right)^{1/2} \right\|_{L_\infty(\Omega)}.$$

The space of functions of bounded variation on $\Omega$ is denoted by $BV(\Omega)$. We refer the reader to Ziemer (2012) for a full description of the class of functions of bounded variation.

**A.2 Mesh Embedding idea for $K$-NN graph**

We now highlight how to embed a mesh on a $K$-NN graph generated under Assumptions 1–3. This construction will then be used in the next subsection in order to upper bound the MSE of the $K$-NN-FL estimator.

The embedding idea that we will present appeared in the flow-based proof of Theorem 4 from Von Luxburg et al. (2014) regarding commute distance on $K$-NN-graphs. There, the authors introduced the notion of a valid grid (Definition 17). For a fixed set of design points, a grid graph $G$ is a valid grid if, among other things, $G$ satisfies the following: (i) The grid width is not too small, in the sense that each cell of the grid contains at least one of the design points. (ii) The grid width is not too large: points in the same or neighboring cells of the grid are always connected in the $K$-NN graph.

The notion of a valid grid was introduced for fixed design points, but through a minor modification, we construct a grid graph that with high probability satisfies the conditions of valid grid from Von Luxburg et al.
for all \( e \in \mathbb{R}^n \) to bound the quantity estimator. In particular, by the basic inequality argument (see Wang et al. (2016) for instance), it is of interest to bound each term in the right hand side of (25). Hence in the proof of our main theorem stated in the next subsection (see Appendix A.7), we proceed to bound each term in the right hand side of (25).

On the other hand, Lemma 6 does not require that the homeomorphism \( h \) is known. In fact, in practice it can be challenging to construct a partition of the domain, especially since the latter is typically unknown as we are considering \( \mathcal{X} \) to be the support of \( p \). Even if \( \mathcal{X} \) is known, the edges in the mesh \( I(N) \) will have different sizes, which can make the construction of \( I(N) \) impractical. In contrast, constructing the \( K \)-NN graph only requires specifying \( K \), a single parameter.

(2014). We now proceed to construct a grid embedding that for any signal will lead to a lower bound on the total variation along the \( K \)-NN graph.

Given \( N \in \mathbb{N} \), in \([0,1]^d\) we construct a \( d \)-dimensional grid graph \( G_{lat} = (V_{lat}, E_{lat}) \), i.e., a lattice graph, with equal side lengths, and total number of nodes \(|V_{lat}| = N^d\). Without loss of generality, we assume that the nodes of the grid correspond to the points

\[
P_{lat}(N) = \left\{ \left( \frac{i_1}{N} - \frac{1}{2N}, \ldots, \frac{i_d}{N} - \frac{1}{2N} \right) : i_1, \ldots, i_d \in \{1, \ldots, N\} \right\}.
\]

Moreover, we say \( z, z' \in P_{lat}(N) \) share an edge in the graph \( G_{lat}(N) \) if only if \( \|z - z'\|_2 = N^{-1} \). If the nodes corresponding to \( z, z' \) share an edge, then we will write (perhaps with an abuse of notation) \((z, z') \in E_{lat}(N)\). Note that the lattice \( G_{lat}(N) \) is constructed in \([0,1]^d\) and not in the set \( \mathcal{X} \). However, this lattice can be transformed into a mesh in the covariate space through the homeomorphism from Assumption 3, by \( I(N) = h^{-1}(P_{lat}(N)) \). We can use \( I(N) \) to perform a quantization in the domain \( \mathcal{X} \) by using the cells associated with \( I(N) \). See Alamgir et al. (2014) for more general aspects of quantizations under Assumptions 1–3.

Given this mesh, for any signal \( \theta \in \mathbb{R}^n \), we can construct two vectors denoted by \( \theta_I \in \mathbb{R}^n \) and \( \theta^I \in \mathbb{R}^{Nd} \). The former \((\theta_I)\) is a signal vector that is constant within mesh cells. The latter \((\theta^I)\) has coordinates corresponding to the different nodes of the mesh (centers of cells). The precise definitions of \( \theta_I \) and \( \theta^I \) are given in Appendix A.3. Since \( \theta \) and \( \theta_I \) have the same dimension, it is natural to ask how these two relate each other, at least for the purpose of understanding the empirical process associated with the \( K\)-NN-FL estimator. Moreover, given that \( \theta^I \in \mathbb{R}^{Nd} \), one can try to relate the total variation of \( \theta^I \) along a \( d \)-dimensional grid with \( N^d \) nodes, with the total variation of the original signal \( \theta \) along the \( K \)-NN graph. We proceed to establish these connections next.

**Lemma 6.** Assume that \( K \) is chosen such that \( K/\log n \rightarrow \infty \). Then with high probability the following holds (See Lemma 10 in the Appendix for a more precise statement). Under Assumptions 1-3 there exists an \( N \) satisfying \( N \asymp (K/n)^{1/d} \) such that for the corresponding mesh \( I(N) \) we have that

\[
|e^T(\theta - \theta_I)| \leq 2 \|e\|_{\infty} \|\nabla_{G_K} \theta\|_1, \quad \forall \theta \in \mathbb{R}^n,
\]

for all \( e \in \mathbb{R}^n \). Moreover,

\[
\|D \theta^I\|_1 \leq \|\nabla_{G_K} \theta_I\|_1, \quad \forall \theta \in \mathbb{R}^n,
\]

where \( D \) is the incidence matrix of a \( d \)-dimensional grid graph \( G_{grid} = (V_{grid}, E_{grid}) \) with \( V_{grid} = [N^d] \).

Lemma 6 immediately provides a path to control the empirical process associated with the \( K \)-NN-FL estimator. In particular, by the basic inequality argument (see Wang et al. (2016) for instance), it is of interest to bound the quantity \( \hat{e}^T (\hat{\theta} - \theta^*) \). In our context this can be done by noticing that

\[
\frac{1}{n} \hat{e}^T (\hat{\theta} - \theta^*) = \frac{1}{n} \hat{e}^T (\hat{\theta} - \hat{\theta}_I) + \frac{1}{n} \hat{e}^T (\hat{\theta}_I - \theta^I) + \frac{1}{n} \hat{e}^T (\theta^I - \theta^*).
\]

Hence in the proof of our main theorem stated in the next subsection (see Appendix A.7), we proceed to bound each term in the right hand side of (25).
A.3 Quantization

We start by including some additional notation related to Lemma 6 from Section A.2.

Importantly, $I(N)$ (defined in Section A.2) can be thought of as a quantization in the domain $\mathcal{X}$; see Alamgir et al. (2014) for more general aspects of quantizations under Assumptions 1–3. For our purposes, it will be crucial to understand the behavior of $\{x_i\}_{i=1}^n$ and their relationship to $I(N)$. This is because we will use a grid embedding in order to analyze the behavior of the $K$-NN-FL estimator $\hat{\theta}$. With that goal in mind, we define a collection of cells, $\{C(x)\}_{x \in I(N)}$, in $\mathcal{X}$ as

$$C(x) = h^{-1} \left( \left\{ z \in [0, 1]^d : h(x) = \arg\min_{x' \in \text{lat}(N)} \{ \| z - x' \|_\infty : x' \in I(N) \} \right\} \right).$$

Recall that the goal in this paper is to estimate $\theta^* \in \mathbb{R}^n$. However, the mesh construction $I(N)$ has $N^d$ elements, which we denote by $u_1, \ldots, u_{N^d}$. Hence, it is not immediate how to evaluate the total variation of $\theta^*$ along the graph corresponding to the mesh. To achieve this, we consider a quantization of vectors in $\mathbb{R}^n$ to vectors in $\mathbb{R}^{N^d}$ obtained using the mesh $I(N)$.

To obtain the quantization in $\mathbb{R}^{N^d}$, we first define a discretization of any signal in $\mathbb{R}^n$ into $\mathbb{R}^n$ by incorporating information about the samples $\{x_i\}_{i=1}^n$ and the cells $\{C(x)\}_{x \in I(N)}$. To do this, for $x \in \mathcal{X}$ we write $P_I(x)$ as the point in $I$ such that $x \in C(P_I(x))$ (if there is more than one of such points we arbitrary pick one). Then we collapse measurements corresponding to different samples $x_i$ that fall in the same cell (in $\{C(x)\}_{x \in I(N)}$), into a single value associated to the sample closest to the center of the cell after mapping with the homeomorphism. Thus, for a given $\theta \in \mathbb{R}^n$, we define $\theta_I \in \mathbb{R}^n$ as

$$(\theta_I)_i = \theta_j \quad \text{where} \quad x_j = \arg\min_{x_i, I \in [n]} \| h(P_I(x_i)) - h(x_I) \|_\infty.$$

Next we construct the mapping from $\mathbb{R}^n$ to $\mathbb{R}^{N^d}$. For any $\theta \in \mathbb{R}^n$ we can induce a signal in $\mathbb{R}^{N^d}$ corresponding to the elements in $I$. We write

$I_j = \{ i \in [n] : P_I(x_i) = u_j \}, \quad j \in [N^d].$

If $I_j \neq \emptyset$, then there exists $i_j \in I_j$ such that $(\theta_I)_i = \theta_{i_j}$ for all $i \in I_j$. Here $\theta_I$ is the vector defined in (27). Using this notation, for a vector $\theta \in \mathbb{R}^n$, we write $\theta^I = (\theta_{i_1}, \ldots, \theta_{i_{N^d}})$. Where we use the convention that $\theta_{i_j} = 0$ if $I_j = \emptyset$.

Hence, for a given $\theta \in \mathbb{R}^n$, we have constructed two very intuitive signals $\theta_I \in \mathbb{R}^n$ and $\theta^I \in \mathbb{R}^m$. The former forces covariate samples in the same cell to take the same signal value. The latter has coordinates corresponding to the different nodes of the mesh (centers of cells).

A.4 Controlling counts of mesh $I(N)$

The following lemma is a well known concentration inequality for binomial random variables. In the form expressed below, such result can be found as Proposition 27 in Von Luxburg et al. (2014).

**Lemma 7.** Let $m$ be a Binomial($M, q$) distributed random variable. Then, for all $\delta \in (0, 1]$,

$$\mathbb{P}(m \leq (1 - \delta)Mq) \leq \exp\left( -\frac{1}{2} \delta^2 Mq \right),$$

$$\mathbb{P}(m \geq (1 + \delta)Mq) \leq \exp\left( -\frac{1}{2} \delta^2 Mq \right).$$

We know use Lemma 7 to bound the distance between any design point and its $K$-nearest neighbor.
Lemma 8. (See Proposition 31 in Von Luxburg et al. (2014)) Let us denote $R_K(x)$ the distance from $x \in \mathcal{X}$ to its $K$-th nearest neighbor in the set $\{x_1, \ldots, x_n\}$. Setting
\[
R_{K,\text{max}} = \max_{1 \leq i \leq n} R_K(x_i), \\
R_{K,\text{min}} = \min_{1 \leq i \leq n} R_K(x_i),
\]
we have that
\[
\mathbb{P}\left( a \left( \frac{K}{n} \right)^{1/d} \leq R_{K,\text{min}} \leq R_{K,\text{max}} \leq \tilde{a} \left( \frac{K}{n} \right)^{1/d} \right) \geq 1 - n \exp(-K/3) - n \exp(-K/12),
\]
under Assumptions 1 - 3, where $a = 1/(2 c_{2,d} p_{\text{max}})^{1/d}$, and $\tilde{a} = 2^{1/d}/(p_{\text{min}} c_{1,d})^{1/d}$.

Proof. This proof closely follows that Proposition 31 in Von Luxburg et al. (2014).

First note that for any $x \in \mathcal{X}$, by Assumptions 1–2 we have
\[
\mathbb{P}(x_1 \in B_r(x)) = \int_{B_r(x)} p(t) \mu(dt) \leq p_{\text{max}} \mu(B_r(x)) \leq c_{2,d} r^d p_{\text{max}} := \mu_{\text{max}} < 1,
\]
for small enough $r$. We also have that $R_K(x) \leq r$ if and only if there are at least $K$ data points $\{x_i\}$ in $B_r(x)$. Let $V \sim \text{Binomial}(n, \mu_{\text{max}})$. Then,
\[
\mathbb{P}(R_K(x) \leq r) \leq \mathbb{P}(V \geq K) = \mathbb{P}(V \geq 2 \mathbb{E}(V)),
\]
where the last equality follows by choosing $a = 1/(2 c_{2,d} p_{\text{max}})^{1/d}$, and $r = a(K/n)^{1/d}$. Therefore, from 7 we obtain
\[
\mathbb{P}(R_{K,\text{min}} \leq a(K/n)^{1/d}) = \mathbb{P}(\exists i : R_K(x_i) \leq a(K/n)^{1/d}) \leq n \max_{1 \leq i \leq n} \mathbb{P}(R_K(x_i) \leq r) \leq n \exp(-K/3).
\]

On the other hand,
\[
\mathbb{P}(x_1 \in B_r(x)) = \int_{B_r(x)} p(t) \mu(dt) \geq p_{\text{min}} \mu(B_r(x)) \geq c_{1,d} r^d p_{\text{min}} := \mu_{\text{min}} > 0,
\]
and we arrive with a similar argument to
\[
\mathbb{P}(R_{K,\text{max}} > \tilde{a}(K/n)^{1/d}) \leq n \exp(-K/12),
\]
where $\tilde{a} = 2^{1/d}/(p_{\text{min}} c_{1,d})^{1/d}$.

The upper bound in Lemma 8 allows us to control the maximum distance between $x_i$ and $x_j$ whenever these are connected in the $K$-NN graph. Such maximum distance scales as $(K/n)^{1/d}$. The lower bound, on the other hand, prevents $x_i$ from being arbitrarily close to its $K$-th nearest neighbor. These properties are particularly important as they will be used to characterize the penalty $\|\nabla_{\theta^*} \|_1$.

As explained in Wang et al. (2016), there are different strategies for providing convergence rates in generalized lasso problems such as (2). Our approach here is similar in spirit to Padilla et al. (2018), and it is based on considering a lower bound for the penalty function induced by the $K$-NN graph. Such lower bound will arise by constructing a signal over the grid graph induced by the cells $\{C(x)\}_{x \in I(N)}$. Towards that end, we provide the following lemma characterizing the minimum and maximum number of observations $\{x_i\}$ that fall within each cell $C(x)$. With an abuse of notation we write $\|C(x)\| = |\{i \in [n] : x_i \in C(x)\}|$.

We now present a related result to Proposition 28 Von Luxburg et al. (2014).
Lemma 9. Assume that \( N \) in the construction of \( G_{\text{lat}}(N) \) is chosen as
\[
N = \left\lceil \frac{3 \sqrt{d} \left( 2 c_{2,d} p_{\max} \right)^{1/d} n^{1/d}}{L_{\min} K^{1/d}} \right\rceil.
\]
Then there exists positive constants \( \tilde{b}_1 \) and \( \tilde{b}_2 \) depending on \( L_{\min}, L_{\max}, \) \( d, \) \( p_{\min}, p_{\max}, c_{1,d}, \) and \( c_{2,d} \) such that
\[
\begin{align*}
\mathbb{P} \left( \max_{x \in I(N)} |C(x)| \geq (1 + \delta) c_{2,d} \tilde{b}_1 K \right) &\leq N^d \exp \left( -\frac{1}{3} \delta^2 \tilde{b}_2 c_{1,d} K \right), \\
\mathbb{P} \left( \min_{x \in I(N)} |C(x)| \leq (1 - \delta) c_{1,d} \tilde{b}_2 K \right) &\leq N^d \exp \left( -\frac{1}{3} \delta^2 \tilde{b}_2 c_{1,d} K \right),
\end{align*}
\]  
(29)
for all \( \delta \in (0, 1) \), with \( a = 1/(2 c_{2,d} p_{\max})^{1/d} \), and \( \tilde{a} = 2^{1/d}/(p_{\min} c_{1,d})^{1/d}. \) Moreover, the symmetric \( K \)-NN graph has maximum degree \( d_{\max} \) satisfying
\[
\mathbb{P} \left( d_{\max} \geq \frac{3}{2} p_{\max} c_{2,d} \tilde{a}^d K \right) \leq n \left[ \exp \left( \frac{-K}{12} \right) + \exp \left( -\frac{p_{\min} c_{1,d} \tilde{a}^d K}{24} \right) \right].
\]
Define the event \( \Omega \) as: “If \( x_i \in C(x'_i) \) and \( x_j \in C(x'_j) \) for \( x'_i, x'_j \in I(N) \) with \( \|h(x'_i) - h(x'_j)\|_2 \leq N^{-1} \), then \( x_i \) and \( x_j \) are connected in the \( K \)-NN graph”. Then,
\[
\mathbb{P} (\Omega) \geq 1 - n \exp(-K/3).
\]

Proof. We observe that for \( x_i \) and \( x_j \) satisfying the above property, the following holds using Assumption 3
\[
\begin{align*}
d_{\mathcal{X}}(x_i, x_j) &\leq L_{\min}^{-1} \|h(x_i) - h(x_j)\|_2 \\
&\leq L_{\min}^{-1} \sqrt{d} \|h(x_i) - h(x_j)\|_{\infty} \\
&\leq L_{\min}^{-1} \sqrt{d} \left[ \|h(x_i) - h(x'_i)\|_{\infty} + \|h(x'_i) - h(x'_j)\|_{\infty} + \|h(x'_j) - h(x_j)\|_{\infty} \right] \\
&\leq 3 L_{\min}^{-1} \sqrt{d} N^{-1} \\
&\leq a \left( \frac{K}{n} \right)^{1/d}
\end{align*}
\]
with \( a = 1/(2 c_{2,d} p_{\max})^{1/d} \), where the first inequality follows from Assumption 3. Therefore as in the proof of Lemma 8
\[
\mathbb{P} (\Omega) \geq \mathbb{P} \left( a \left( \frac{K}{n} \right)^{1/d} \leq R_{K,\min} \right) \geq 1 - n \exp(-K/3).
\]

Upper bound on counts. Assume that \( x \in h^{-1}(P_{\text{lat}}(N)) \), and \( x' \in C(x) \). Then,
\[
\begin{align*}
d_{\mathcal{X}}(x, x') &\leq \frac{1}{L_{\min}} \|h(x) - h(x')\|_2 \\
&\leq \sqrt{d} \frac{1}{L_{\min}} \|h(x) - h(x')\|_{\infty} \\
&\leq \frac{\sqrt{d}}{2 L_{\min}} N \\
&\leq \frac{\tilde{b}_1}{P_{\max}} \left( \frac{K}{n} \right)^{1/d}
\end{align*}
\]
where the first inequality follows from Assumption 3, the second from the definition of \( P_{lat}(N) \), and the third one from the choice of \( N \). Therefore,

\[
C(x) \subseteq B_{\frac{\tilde{b}_1}{p_{\max}}^{1/d}} \left( \frac{K}{n} \right)^{1/d}(x). \tag{30}
\]

On the other hand, if \( \tilde{b}_2 \) is such that

\[
\frac{(\tilde{b}_2)^{1/d}}{p_{\min}^{1/d}} \leq \frac{a}{2 L_{\max} \sqrt{3d}},
\]

then if

\[
d_N(x, x') \leq \frac{(\tilde{b}_2)^{1/d}}{p_{\min}^{1/d}} \left( \frac{K}{n} \right)^{1/d},
\]

we have that by Assumption 3, for large enough \( n \)

\[
\|h(x) - h(x')\|_{\infty} \leq \frac{1}{2^N}.
\]

And so,

\[
B_{\frac{(\tilde{b}_2)^{1/d}}{p_{\min}^{1/d}}} \left( \frac{K}{n} \right)^{1/d}(x) \subseteq C(x). \tag{31}
\]

In consequence,

\[
\mathbb{P} \left( \max_{x \in I(N)} |C(x)| \geq (1 + \delta) c_2, d \tilde{b}_1 K \right) \leq \sum_{x \in I(N)} \mathbb{P} \left( |C(x)| \geq (1 + \delta) c_2, d \tilde{b}_1 K \right) \\
\leq \sum_{x \in I(N)} \mathbb{P} \left( |C(x)| \geq (1 + \delta) n \mathbb{P}(x_1 \in C(x)) \right) \\
\leq \sum_{x \in I(N)} \exp \left( -\frac{1}{3} \delta^2 \tilde{b}_2 c_1, d K \right) \\
= N^d \exp \left( -\frac{1}{3} \delta^2 \tilde{b}_2 c_1, d K \right),
\]

where the first inequality follows from a union bound, the second from (30), and the third from (31) combined with Lemma 7.

On the other hand, with a similar argument, we have that

\[
\mathbb{P} \left( \min_{x \in I(N)} |C(x)| \leq (1 - \delta) c_1, d \tilde{b}_2 K \right) \leq \sum_{x \in I(N)} \mathbb{P} \left( |C(x)| \leq (1 - \delta) c_1, d \tilde{b}_2 K \right) \\
\leq \sum_{x \in I(N)} \mathbb{P} \left( |C(x)| \leq (1 - \delta) n \mathbb{P}(x_1 \in C(x)) \right) \\
\leq N^d \exp \left( -\frac{1}{3} \delta^2 \tilde{b}_2 c_1, d K \right).
\]

**Upper bound on degree.** We start defining the events

\[
B_i(x) = \left\{ j \in [n] \setminus \{ i \} : x_j \in B_{\tilde{a}(K/n)^{1/d}}(x) \right\}, \quad B_i = \left\{ j \in [n] \setminus \{ i \} : x_j \in B_{\tilde{a}(K/n)^{1/d}}(x_i) \right\},
\]

for \( i \in [n], x \in X \), and where \( \tilde{a} \) is given as in Lemma 8. Then,

\[
|B_i(x)| \sim \text{Binomial} \left( n - 1, \mathbb{P}(x_1 \in B_{\tilde{a}(K/n)^{1/d}}(x)) \right),
\]


22
where
\[ p_{\min} c_1, d \, \tilde{a}^d \frac{K}{n} \leq \mathbb{P}(x_1 \in B_{\tilde{a}(K/n)^{1/d}}(x)) \leq p_{\max} c_2, d \, \tilde{a}^d \frac{K}{n}, \]
which implies by Lemma 7 that
\[ \mathbb{P} \left( |B_i(x)| \geq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right) \leq \mathbb{P} \left( |B_i(x)| \geq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K (n - 1) \right) \leq \exp \left( -\frac{p_{\min} c_1, d \, \tilde{a}^d}{24} K \right). \]
Hence,
\[ \mathbb{P} \left( |B_i| \geq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right) = \int_{\mathcal{X}} \mathbb{P} \left( |B_i(x)| \geq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right) p(x) \mu(dx) \leq \exp \left( -\frac{p_{\min} c_1, d \, \tilde{a}^d}{24} K \right). \]
Therefore, if \( d_i \) is the degree associated with \( x_i \) then
\[ \mathbb{P} \left( d_i \leq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right) \geq \mathbb{P} \left( \{ j \in [n] \setminus \{ i \} : d_X(x_i, x_j) \leq R_{K, \max} \} \leq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right) \geq \mathbb{P} \left( \{ j \in [n] \setminus \{ i \} : d_X(x_i, x_j) \leq \tilde{a}(K/n)^{1/d} \} \leq \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K, R_{K, \max} \leq \tilde{a}(K/n)^{1/d} \right) \geq 1 - \mathbb{P} \left( R_{K, \max} > \tilde{a}(K/n)^{1/d} \right) - \mathbb{P} \left( |B_i| > \frac{3}{2} p_{\max} c_2, d \, \tilde{a}^d K \right), \]
and the claim follows from the previous inequality and Equation (28).

As stated in the previous lemma, the number of observations \( x_i \) that fall within each cell \( C(x) \) behaves like \( K \), with high probability. We will exploit this fact in the next subsection in order to obtain an upper bound on the MSE.

### A.5 Mesh embedding for \( K \)-NN graph

**Lemma 10.** Let us assume that the event \( \Omega \) from Lemma 9 holds. Define \( N \) as in that lemma and let \( \mathcal{I} \) be the corresponding mesh. Then for all \( e \in \mathbb{R}^n \), it holds that
\[ |e^T (\theta \otimes \theta_1)| \leq 2 \| e \|_\infty \| \nabla G_{K \theta} \|_1, \quad \forall \theta \in \mathbb{R}^n. \] (32)
Moreover,
\[ \| D \theta^l \|_1 \leq \| \nabla G_{K \theta} \|_1, \quad \forall \theta \in \mathbb{R}^n, \] (33)
where \( D \) is the incidence matrix of a \( d \)-dimensional grid graph \( G_{grid} = (V_{grid}, E_{grid}) \) with \( V_{grid} = [m] \), where \( (l, l') \in E_{grid} \) if and only if
\[ \| h(P_l(x_{i_l})) - h(P_l(x_{i_{l'}})) \|_2 = \frac{1}{N}. \]
Here we use the notation from Appendix A.3.

**Proof.** We start by introducing the notation \( x_i^l = P_l(x_i) \). To prove (32) we proceed in cases.

**Case 1.** If \( (\theta_1)_1 = \theta_1 \), then clearly \( |e_1| |\theta_1 - (\theta_1)_1| = 0. \)
**Case 2.** If \( (\theta_1)_1 = \theta_i \), for \( i \neq 1 \), then
\[ \| h(x_1') - h(x_1) \|_\infty \leq \| h(x_1') - h(x_1) \|_\infty \leq \frac{1}{2N}. \]

23
Thus, $x_i' = x_i$, and so $(1, i) \in E_K$ by the assumption that the event $\Omega$ holds.

Therefore for every $i \in \{1, \ldots, n\}$, there exists $j_i \in [n]$ such that $(\theta_I)_i = \theta_{j_i}$ and either $i = j_i$ or $(i, j_i) \in E_K$. Hence,

$$|e^T(\theta - \theta_I)| \leq \sum_{i=1}^{n} |e_i| |\theta_i - \theta_{j_i}| \leq 2 \|e\|_\infty \|\nabla G_K \hat{\theta}\|_1.$$ 

To verify (33) let us observe that

$$\|D \theta^I\|_1 = \sum_{(l,l') \in E_{grid}} |\theta_{il} - \theta_{i'l'}|.$$ 

Now, if $(l, l') \in E_{grid}$, then $x_{il}$ and $x_{i'l'}$ are in neighboring cells in $I$. This implies that $(i, i')$ is an edge in the $K$-NN graph. Thus, every edge in the grid graph $G_{grid}$ corresponds to an edge in the $K$-NN graph and the mapping is injective. The claim follows.

**A.6 Bounding Empirical Process**

**Lemma 11.** With the notation from Lemma 10 we have that

$$\varepsilon^T(\hat{\theta} - \theta^*) \leq 2 \|e\|_\infty \left[ \|\nabla G_K \theta^*\|_1 + \|\nabla G_K \hat{\theta}\|_1 \right] + \varepsilon^T(\hat{\theta}_I - \theta^*_I),$$

on the event $\Omega$.

**Proof.** Let us assume that event $\Omega$ happens. Then we observe that

$$\varepsilon^T(\hat{\theta} - \theta^*) = \varepsilon^T(\hat{\theta}_I - \hat{\theta}_I) + \varepsilon^T(\hat{\theta}_I - \theta^*_I) + \varepsilon^T(\theta^*_I - \theta^*),$$

and the claim follows by Lemma 10.

**Lemma 12.** With the notation from Lemma 11, on the event $\Omega$, we have that

$$\varepsilon^T(\hat{\theta}_I - \theta^*_I) \leq \max_{u \in I} \sqrt{C(u)} \left( \|\Pi\|_2 \|\hat{\theta} - \theta^*\|_2 + \|(D^+)\|_\infty \|\nabla G_K \hat{\theta}\|_1 + \|\nabla G_K \theta^*\|_1 \right),$$

where $\varepsilon \in \mathbb{R}^{Nd}$ is a mean zero vector whose coordinates are independent and sub-Gaussian with the same constants as in (7). Here, $\Pi$ is the orthogonal projection onto the span of $1 \in \mathbb{R}^{Nd}$, and $D^+$ is the pseudoinverse of the incidence matrix $D$ from Lemma 10.

**Proof.** Here we use the notation from the proof of Lemma 10. Then,

$$\varepsilon^T(\hat{\theta}_I - \theta^*_I) = \sum_{j=1}^{Nd} \sum_{l \in I_j} \varepsilon_{lj} \left( \hat{\theta}_{ij} - \theta^*_{ij} \right) = \left[ \max_{u \in I} \{C(u)\} \right]^{1/2} \varepsilon^T(\hat{\theta}^I - \theta^*, I)$$

where

$$\varepsilon_{lj} = \left[ \max_{u \in I} \{C(u)\} \right]^{-1/2} \sum_{l \in I_j} \varepsilon_{lj}.$$
On the other hand, by Hölder’s inequality, and by the triangle inequality

\[
\epsilon^T(\hat{\theta}_I - \theta^*_I) \leq \left[ \max_{u \in I} |C(u)| \right]^{1/2} \left( \|\Pi \hat{\epsilon}\|_2 \|\hat{I} - \theta^*\|_2 + \|(D^+)^T \hat{\epsilon}\|_\infty \|D(\hat{I} - \theta^*\|_1) \right) \\
\leq \left[ \max_{u \in I} |C(u)| \right]^{1/2} \left( \|\Pi \hat{\epsilon}\|_2 \|\hat{I} - \theta^*\|_2 + \|(D^+)^T \hat{\epsilon}\|_\infty \left[ \|D\hat{I}\|_1 + \|D\theta^*\|_1 \right] \right).
\]  

(36)

Next we observe that

\[
\|\hat{I} - \theta^*\|_2 = \left[ \sum_{j=1}^{N^d} \left( \hat{\theta}_{ij} - \theta^*_{ij} \right)^2 \right]^{1/2} \leq \left[ \sum_{i=1}^{n} \left( \hat{\theta}_i - \theta^*_i \right)^2 \right]^{1/2}.
\]

(37)

Therefore, combining (36), (37) and Lemma 10 we arrive to

\[
\epsilon^T(\hat{\theta}_I - \theta^*_I) \leq \max_{u \in I} \sqrt{|C(u)|} \left( \|\Pi \hat{\epsilon}\|_2 \|\hat{I} - \theta^*\|_2 + \|(D^+)^T \hat{\epsilon}\|_\infty \left[ \|\nabla_{G\hat{K}} \hat{\theta}\|_1 + \|\nabla_{G\theta^*}\|_1 \right] \right).
\]

(38)

The following lemma is obtained with a similar argument to the proof of Theorem 2 in Hutter and Rigollet (2016).

**Lemma 13.** Let \( d > 1 \) (recall Assumptions 1-3) and let \( \delta > 0 \). With the notation from the previous lemma, given the event \( \Omega \), we have that

\[
\epsilon^T(\hat{\theta}_I - \theta^*_I) \leq \sqrt{(1 + \delta) c_{2,d} \bar{b}_1 K} \left[ 2\sigma \sqrt{2 \log \left( \frac{\delta}{5} \right)} \|\hat{\theta} - \theta^*\|_2 + \sigma C_1(d) \sqrt{\frac{2 \log n}{d} \log \left( \frac{C_2(p_{\text{max}}, L_{\text{min}}, d) n}{K\delta} \right)} \left[ \|\nabla_{G\hat{K}} \hat{\theta}\|_1 + \|\nabla_{G\theta^*}\|_1 \right] \right]
\]

(39)

with probability at least

\[
1 - 2\delta - \frac{n}{K \bar{a}_d L_{\text{max}}} \exp \left( -\frac{1}{3} \delta^2 \frac{\bar{b}_2 c_{1,d} K}{2} \right) - n \exp(-K/3),
\]

where \( C_1(d) > 0 \) is a constant depending on \( d \), and \( C_2(p_{\text{max}}, L_{\text{min}}, d) > 0 \) is another constant depending on \( p_{\text{max}}, L_{\text{min}} \), and \( d \).

**Proof.** Let us use the notation from Lemma 12. Then, as in the proof of Theorem 2 from Hutter and Rigollet (2016), and our choice of \( N \), we obtain that given \( \Omega \),

\[
\|(D^+)^T \hat{\epsilon}\|_\infty \leq \sigma C_1(d) \sqrt{\frac{2 \log n}{d} \log \left( \frac{C_2(p_{\text{max}}, L_{\text{min}}, d) n}{K\delta} \right)}
\]

\[
\|\Pi \hat{\epsilon}\|_2 \leq 2\sigma \sqrt{2 \log \left( \frac{\delta}{5} \right)}
\]

(39)

with probability at least \( 1 - 2\delta \), where \( C(d) \) is constant depending on \( d \), and \( C_2(p_{\text{max}}, L_{\text{min}}, d) \) is a constant depending on \( p_{\text{max}}, L_{\text{min}} \) and \( d \).

On the other hand, by Lemma 9, given the event \( \Omega \) we have

\[
\max_{x \in h^{-1}(P_{\text{hat}})} \sqrt{|C(x)|} \leq \sqrt{(1 + \delta) c_{2,d} \bar{b}_1 K}
\]

On the other hand, by Lemma 9, given the event \( \Omega \) we have

\[
\max_{x \in h^{-1}(P_{\text{hat}})} \sqrt{|C(x)|} \leq \sqrt{(1 + \delta) c_{2,d} \bar{b}_1 K}
\]
with probability at least
\[
1 - N^d \exp \left( -\frac{1}{3} \delta^2 b_2 c_{1,d} K \right) - n \exp(-K/3).
\] (40)

Therefore combining (39) and (40) the result follows.

A.7 Proof of Theorem 1

Instead of proving Theorem 1, we will prove a more general result that holds for a general choice of \( K \). This is given next. The corresponding result for \( \epsilon \)-NN-FL can be obtained with a similar argument.

**Theorem 14.** There exist constants \( C_1(d) \) and \( C_2(p_{\max}, L_{\min}, d) \), depending on \( d, p_{\max}, \) and \( L_{\min} \), such that with the notation from Lemmas 8 and 9, if \( \lambda \) is chosen as
\[
\lambda = \sigma C_1(d) \sqrt{(1 + \delta) c_{2,d} \tilde{b}_1} \frac{2 \log n}{d} \log \left( \frac{C_2(p_{\max}, L_{\min}, d)n}{K \delta} \right) K + 8\sigma \sqrt{\log n},
\]
then the \( K \)-NN-FL estimator \( \hat{\theta} \), the solution to (3), satisfies
\[
\|\hat{\theta} - \theta^*\|^2_n \leq \|\nabla_{G_K} \theta^*\|_1 \left[ \frac{4\sigma C_1(d)}{n} \sqrt{(1 + \delta) c_{2,d} \tilde{b}_1} \frac{2 \log n}{d} \log \left( \frac{C_2(p_{\max}, L_{\min}, d)n}{K \delta} \right) K \right. \\
+ \left. \frac{32 \sqrt{\log n}}{n} + \frac{16 \sigma^2 (1 + \delta) c_{2,d} \tilde{b}_1 K \log(\tilde{z})}{n} \right],
\]
with probability at least \( \eta_n \left( 1 - n \exp(-K/3) \right) \). Here,
\[
\eta_n = 1 - 2\delta - N^d \exp \left( -\frac{1}{3} \delta^2 b_2 c_{1,d} K \right) - n \exp(-K/3) - \frac{C}{n^r},
\]
where \( C \) is the constant in (7) and \( N \) is given as in Lemma 9. Consequently, taking \( K \asymp \log^{1+2r} n \) we obtain the result in Theorem 1.

**Proof.** We notice that by the basic inequality argument, see for instance Wang et al. (2016), that
\[
\frac{1}{2}\|\hat{\theta} - \theta^*\|^2_n \leq \frac{1}{n} \left[ \varepsilon^T (\hat{\theta} - \theta^*) + \lambda \left[ -\|\nabla_{G_K} \hat{\theta}\|_1 + \|\nabla_{G_K} \theta^*\|_1 \right] \right].
\] (41)

On the other hand, (7) and a union bound,
\[
\mathbb{P} \left( \max_{1 \leq i \leq n} |\varepsilon_i| > 4\sigma \sqrt{\log n} \mid \Omega \right) = \mathbb{P} \left( \max_{1 \leq i \leq n} |\varepsilon_i| > 4\sigma \sqrt{\log n} \right) \leq \frac{C}{n^r}. \] (42)

Therefore, combining (41), (42), Lemma 11, Lemma 12, and Lemma 13 we obtain that conditioning on \( \Omega \),
\[
\frac{1}{2}\|\hat{\theta} - \theta^*\|^2_n \leq \sqrt{(1 + \delta) c_{2,d} \tilde{b}_1 K} \frac{2 \sqrt{2 \log (\tilde{z})} \|\hat{\theta} - \theta^*\|_2 + \sigma C_1(d) \sqrt{\frac{2 \log n}{d} \log \left( \frac{C_2(p_{\max}, L_{\min}, d)n}{K \delta} \right) K}}{n} \\
+ \frac{8\sigma \sqrt{\log n}}{n} \left[ \|\nabla_{G_K} \hat{\theta}\|_1 + \|\nabla_{G_K} \theta^*\|_1 \right] + \frac{\lambda}{n} \left[ -\|\nabla_{G_K} \hat{\theta}\|_1 + \|\nabla_{G_K} \theta^*\|_1 \right] \\
\leq \|\nabla_{G_K} \theta^*\|_1 \left[ \frac{\sigma C_1(d)}{n} \sqrt{(1 + \delta) c_{2,d} \tilde{b}_1} \frac{2 \log n}{d} \log \left( \frac{C_2(p_{\max}, L_{\min}, d)n}{K \delta} \right) K \right. \\
+ \frac{8\sigma \sqrt{\log n}}{n} \left. + 2\sqrt{2(1 + \delta) c_{2,d} \tilde{b}_1 K \log(\tilde{z})} \right] \|\hat{\theta} - \theta^*\|_2;
\]
with probability at least $\eta_n$. Hence by the inequality $a b - 4^{-1} b^2 \leq a^2$, we obtain that conditioning on $\Omega$,  
\[
\frac{1}{2} \left\| \hat{\theta} - \theta^* \right\|^2 \leq \left\| \nabla_{G_K} \theta^* \right\|_1 \left[ \frac{\sigma c_1(d)}{n} \sqrt{(1 + \delta) c_{2,d} b_1^{1/2} \log n} \right] \leq \frac{8 \sigma \sqrt{\log n}}{n} + 4 \sigma^2 (1 + \delta) c_{2,d} b_1 K \log \left( \frac{\eta}{\delta} \right),
\]
with high probability. The claim follows. \qed

### A.8 Useful Lemma

Throughout we use the notation from Appendix A.3.

**Lemma 15.** Assume that $N$ in the construction of $G_{\text{lat}}$ is chosen as  
\[
N = \left\lfloor \frac{(c_{1,d} p_{\min})^{1/d} n^{1/d}}{2^{1/d} L_{\max} K^{1/d}} \right\rfloor,
\]
then there exist positive constants $b_1'$ and $b_2'$ depending on $L_{\min}$, $L_{\max}$, $d$, $p_{\min}$, $c_{1,d}$, and $c_{2,d}$, such that  
\[
P \left( \max_{x \in h^{-1}(P_{\text{lat}})} |C(x)| \geq (1 + \delta) c_{2,d} b_1' K \right) \leq N^d \exp \left( -\frac{1}{3} \delta^2 b_2' c_{1,d} K \right),
\]
\[
P \left( \min_{x \in h^{-1}(P_{\text{lat}})} |C(x)| \leq (1 - \delta) c_{1,d} b_2' K \right) \leq N^d \exp \left( -\frac{1}{3} \delta^2 b_2' c_{1,d} K \right),
\]
for all $\delta \in (0,1]$. Moreover, let $\tilde{\Omega}$ denote the event: “For all $i, j \in [n]$, if $x_i$ and $x_j$ are connected in the $K$-NN graph, then $\| h(x_i') - h(x_j') \|_2 < 2 N^{-1}$ where $x_i \in C(x_i')$ and $x_j \in C(x_j')$ with $x_i', x_j' \in I(N)$”. Then  
\[
P \left( \tilde{\Omega} \right) \geq 1 - n \exp(-K/3).
\]

**Proof.** Let $i, j \in [n]$ such that $x_i$ and $x_j$ are connected in the $K$-NN graph where $x_i \in C(x_i')$ and $x_j \in C(x_j')$ with $x_i', x_j' \in I(N)$. Then,  
\[
\| h(x_i') - h(x_j') \|_2 \leq \| h(x_i') - h(x_i) \|_2 + \| h(x_i) - h(x_j) \|_2 + \| h(x_j) - h(x_j') \|_2 \\
\leq \frac{1}{N} + \| h(x_i) - h(x_j) \|_2 \\
\leq \frac{1}{N} + L_{\max} d_{\chi}(x_i, x_j) \\
\leq \frac{1}{N} + L_{\max} R_{K,\max}
\]
Therefore,  
\[
P \left( \tilde{\Omega} \right) \geq P \left( R_{K,\max} \leq \bar{a}(K/n)^{1/d} \right) \geq 1 - n \exp(-K/12),
\]
where $\bar{a}$ is given as in Lemma 8.

**Upper bound on counts.** Assume that $x \in h^{-1}(P_{\text{lat}}(N))$, and $x' \in C(x)$. Then,  
\[
d_{\chi}(x, x') \leq \frac{1}{l_{\text{max}}} \| h(x) - h(x') \|_2 \\
\leq \frac{1}{2 l_{\min} N} \| h(x) - h(x') \|_2 \\
\leq \frac{1}{2 l_{\min}} \| h(x) - h(x') \|_2 \\
= \left( b_1' \right)^{1/d} \left( \frac{K}{n} \right)^{1/d},
\]
where the first inequality follows from Assumption 3, the second from the definition of \( P_{lat}(N) \), and the third one from the choice of \( N \). Therefore,

\[
C(x) \subset B_{(b_1')^{1/d}(K/b_1')}^{1/d}(x).
\] (44)

On the other hand, we can find \( b_2' \) with a similar argument the proof of Lemma 9, and the proof follows the same steps from such lemma.

\[\square\]

### A.9 Proof of Theorem 2

**Proof.** Throughout, we extend the domain of the function \( g_0 \) to be \( \mathbb{R}^d \) by simply making it take the value zero in \( \mathbb{R}^d - [0, 1]^d \). We will proceed to construct smooth approximations to \( g_0 \) that will allow us to obtain the desired result. To that end, for any \( \epsilon > 0 \) we construct the regularizer (or mollifier) \( g_\epsilon : \mathbb{R}^d \to \mathbb{R} \) defined as

\[
g_\epsilon(z) = \psi_\epsilon \ast g_0(z) = \int \psi_\epsilon(z') g_0(z - z') dz',
\]

where \( \psi_\epsilon(z') = \epsilon^{-d} \psi(z' / \epsilon) \). Then given Assumption 4, by the proof of Theorem 5.3.5 from Zhu et al. (2003), it follows that there exists a constant \( C_2 \) such that

\[
\limsup_{\epsilon \to +0} \int_{(0,1)^d} \|\nabla g_\epsilon(z)\|_1 \, dz < C_2
\]

which implies that there exists \( \epsilon_1 > 0 \) such that

\[
\sup_{0 < \epsilon < \epsilon_1} \int_{(0,1)^d} \|\nabla g_\epsilon(z)\|_1 \, dz < C_2.
\] (45)

Next, for \( N \) as in Lemma 15, we set \( \epsilon = N^{-1} \) and consider the event

\[
\Lambda_\epsilon = \left\{ h(x_1) \in B_{4 \epsilon}(S) \cup \left[ (0,1)^d \setminus \Omega_{4 \epsilon} \right] \right\},
\] (46)

and note that

\[
\mathbb{P}(\Lambda_\epsilon) = \int_{h^{-1}(B_{4 \epsilon}(S) \cup (0,1)^d \setminus \Omega_{4 \epsilon})} \mu(dz) \\
\leq p_{\text{max}} \mu \left( h^{-1}(B_{4 \epsilon}(S) \cup (0,1)^d \setminus \Omega_{4 \epsilon}) \right) \\
\leq p_{\text{max}} C_S 4 \epsilon,
\] (47)

where the last inequality follows from Assumption 5. Defining

\[
J = \left\{ i \in [n] : h(x_i) \in \Omega_{4 \epsilon} \setminus B_{4 \epsilon}(S) \right\},
\] (48)

by the triangle inequality we have

\[
\left| \sum_{(i,j) \in E, i,j \in J} |\theta_i^* - \theta_j^*| - \sum_{(i,j) \in E, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| \right| \\
= \left| \sum_{(i,j) \in E, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| - \sum_{(i,j) \in E, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| \right|
\] (49)
\begin{align*}
&\leq \sum_{(i,j) \in E_k, i,j \in J} \left[ g_0(h(x_i)) - g_\epsilon(h(x_i)) + |g_0(h(x_j)) - g_\epsilon(h(x_j))| \right] \\
&\leq K \tau_d \sum_{i \in J} |g_0(h(x_i)) - g_\epsilon(h(x_i))| \\
&\leq K \tau_d \sum_{i \in J} \int \psi_\epsilon(h(x_i) - z) |g_0(h(x_i)) - g_0(z)| \, dz \\
&\leq K \tau_d C_1 \epsilon^{-d} \sum_{i \in J} \int_{|h(x_i) - z| \leq \epsilon} |g_0(h(x_i)) - g_0(z)| \, dz,
\end{align*}

where \( \tau_d \) is a positive constant and the second inequality happens with high probability as shown in Lemma 9.

We then bound the last term in (50) using Assumption 5. Thus,

\begin{align*}
\epsilon^{-d} \sum_{i \in J} \int_{|h(x_i) - z| \leq \epsilon} |g_0(h(x_i)) - g_0(z)| \, dz &= \epsilon^{-d} \sum_{A \in \mathcal{P}_k} \sum_{i \in J, h(x_i) \in A} \int_{|h(x_i) - z| \leq \epsilon} |g_0(h(x_i)) - g_0(z)| \, dz \\
&\leq \left[ \max_{z \in P_{min}(N)} |C(h^{-1}(z))| \right] S_1(g_0, \mathcal{P}_{N-1, S}) N^d \epsilon \\
&\leq \left[ (1 + \delta) c_{2,d} b_1' K \right] S_1(g_0, \mathcal{P}_{N-1, S}) N^d \epsilon,
\end{align*}

with probability at least

\[
1 - \frac{n}{K \bar{a}^d L_{max}^d} \exp \left( -\frac{1}{3} \delta^2 b_2' c_{1,d} K \right),
\]

which follows from Lemma 15.

If \( h(x_i) \notin \Omega_\epsilon \setminus B_\epsilon(S) \), then

\[
|g_0(h(x_i)) - g_0(h(x_j))| \leq 2 \|g\|_{L_\infty(0,1)^d}.
\]

We now proceed to put the different pieces together. Setting \( \bar{n} = |[n] \setminus J| \), we observe that

\[\bar{n} \sim \text{Binomial} \left( n, \mathbb{P}(A_\epsilon) \right).\]

If

\[n' \sim \text{Binomial} \left( n, p_{\max} C_S \epsilon 4 \right),\]

then

\[
\mathbb{P} \left( \bar{n} \geq \frac{3}{2} n p_{\max} C_S \epsilon 4 \right) \leq \mathbb{P} \left( n' \geq \frac{3}{2} n p_{\max} C_S \epsilon 4 \right) \\
\leq \exp \left( -\frac{1}{12} n (p_{\max} C_S \epsilon 4) \right) \\
= \exp \left( -\frac{p_{\max} 4 C_S}{12} n \left( \frac{2^{1/d} L_{max} K^{1/d} \epsilon^{1/d}}{c_{1,d} p_{\max}^{1/d} n^{1/d}} \right) \right) \\
= \exp \left( -\tilde{C} n^{1-1/d} K^{1/d} \right),
\]

where the first inequality follows from (47), the second from Lemma 7, and \( \tilde{C} \) is a positive constant that depends \( p_{\min}, p_{\max}, L_{\min}, L_{\max}, d \), and \( C_S \). Consequently, combining the above inequality with (49), (51)
and (52) we arrive at

$$\sum_{(i,j) \in E_K} |\theta^*_i - \theta^*_j| = \sum_{(i,j) \in E_K, i,j \in J} |\theta^*_i - \theta^*_j| + \sum_{(i,j) \in E_K, i \notin J \text{ or } j \notin J} |\theta^*_i - \theta^*_j|$$

$$\leq \sum_{(i,j) \in E_K, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| +$$

$$K \tau_d C_1 [(1 + \delta) c_{2,d} b'_1 K] S_1(g_0, \mathcal{P}_{N-1}) N^d \epsilon$$

$$+ 2 \|g_0\|_{L_\infty(0,1)^d} K \tau_d \tilde{n}$$

$$< \sum_{(i,j) \in E_K, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| + C_6 n^{1-1/d} K^{1+1/d}$$

$$+ 2 \|g_0\|_{L_\infty(0,1)^d} K \tau_d \tilde{n},$$

for some positive constant $C_6 > 0$, which happens with high probability (see above). Hence, from (53)

$$\sum_{(i,j) \in E_K} |\theta^*_i - \theta^*_j| \leq \sum_{(i,j) \in E_K, i,j \in J} |g_\epsilon(h(x_i)) - g_\epsilon(h(x_j))| + C_6 n^{1-1/d} K^{1+1/d}$$

(54)

where $C_7 > 0$ is a constant, and the last inequality holds with probability approaching one provided that $K/ \log n \to \infty$.

Therefore, it remains to bound the first term in the right hand side of inequality (54). To that end, we notice that if $(i, j) \in E_K$, then from the proof of Lemma 15 we observe that

$$\|h(x_i) - h(x_j)\|_2 \leq L_{\max} R_{K,\max} \leq \epsilon,$$

where the last inequality happens with high probability. Hence, with high probability, if $z$ is in the segment connecting $h(x_i)$ and $h(x_j)$, then $z \notin B_{2\epsilon}(S) \cup ((0,1)^d \setminus \Omega_{2\epsilon})$ provided that $i, j \in J$. As a result, by the mean value theorem, for $i, j \in J$ there exists a $z_{i,j} \in \Omega_{2\epsilon} \setminus B_{2\epsilon}(S)$ such that

$$g_\epsilon(h(x_i)) - g_\epsilon(h(x_j)) = \nabla g_\epsilon(z_{i,j})^T (h(x_i) - h(x_j)),$$

and this holds uniformly with probability approaching one.
Then,

\[
\sum_{(i,j) \in E_K} \left| g_c(h(x_i)) - g_c(h(x_j)) \right| \\
= \sum_{(i,j) \in E_K} |\nabla g_c(z_{i,j})^T(h(x_i) - h(x_j))| \\
\leq \sum_{(i,j) \in E_K} \|\nabla g_c(z_{i,j})\| \left\lceil \frac{2}{N} \right\rceil \\
= 2 \sum_{A \in \mathcal{P}_c, A \cap (\Omega_2 \setminus B_{2k}(S)) \neq \emptyset} \left[ \sum_{(i,j) \in E_K} \sum_{s.t. i,j \in J, and z_{i,j} \in A} \|\nabla g_c(z_{i,j})\| \|1\text{ Vol}(B_c(z_{i,j})) \frac{C_{\theta} N^d}{N} \right] \\
\leq 2 \sum_{A \in \mathcal{P}_c, A \cap (\Omega_2 \setminus B_{2k}(S)) \neq \emptyset} \left[ \sum_{s.t. i,j \in J, and z_{i,j} \in A} \frac{1}{B_c(z_{i,j})} \right] \int \|\nabla g_c(z)\|dz \frac{C_{\theta} N^d}{N} + \\
2 \sum_{A \in \mathcal{P}_c, A \cap (\Omega_2 \setminus B_{2k}(S)) \neq \emptyset} \left[ \sum_{s.t. i,j \in J, and z_{i,j} \in A} \frac{1}{B_c(z_{i,j})} \int \|\nabla g_c(z)\|dz \right] \frac{C_{\theta} N^d}{N} \\
= T_1 + T_2.
\]

Therefore we proceed to bound $T_1$ and $T_2$. Let us assume that $(i, j) \in E_K$ with $i, j \in J$, and $z_{i,j} \in A$ with $A \in \mathcal{P}_c$. Then by Lemma 15 we have two cases. Either $h(x_i)$ and $h(x_j)$ are in the same cell (element of $\mathcal{P}_c$), or $h(x_i)$ and $h(x_j)$ are in adjacent cells. Denoting by $c(A')$ the center of a cell $A' \in \mathcal{P}_c$, then if $z' \in B_c(z_{i,j}) \cap A'$ it implies that

\[
\|c(A') - c(A)\|_{\infty} \leq \|c(A') - z'\|_{\infty} + \|z' - z_{i,j}\|_{\infty} + \|z_{i,j} - c(A)\|_{\infty} \leq 2\epsilon.
\]

And if in addition $h(x_i) \in A_i$ and $h(x_j) \in A_j$, then

\[
\|c(A_i) - c(A)\|_{\infty} \leq \|c(A_i) - h(x_i)\|_{\infty} + \|h(x_i) - z_{i,j}\|_{\infty} + \|z_{i,j} - c(A)\|_{\infty} \leq 2\epsilon,
\]

and the same is true for $c(A_j)$. Hence,

\[
\int_{B_c(z_{i,j})} \|\nabla g_c(z)\|dz \leq \sum_{A' \in \mathcal{P}_c : \|c(A) - c(A')\|_{\infty} \leq 2\epsilon} \int_{A'} \|\nabla g_c(z)\|dz.
\]

Since the previous discussion was for an arbitrary $z_{i,j}$ with $i, j \in J$, we obtain that

\[
T_1 \leq \sum_{A \in \mathcal{P}_c, A \cap (\Omega_2 \setminus B_{2k}(S)) \neq \emptyset} \left[ \sum_{s.t. i,j \in J, and z_{i,j} \in A} \frac{1}{A'} \int_{A'} \|\nabla g_c(z)\|dz \right] \frac{2C_{\theta} N^d}{N} \\
\leq \frac{2C_{\theta} N^d}{N} \sum_{A \in \mathcal{P}_c} \left[ \{A' \in \mathcal{P}_c : \|c(A) - c(A')\|_{\infty} \leq 2\epsilon\} \right] \max_{x \in h^{-1} (\Pi_{lat}(N))} |C(x)|^2 \int_{A} \|\nabla g_c(z)\|dz \\
\leq C_{\theta} N^{d-1} \max_{x \in h^{-1} (\Pi_{lat}(N))} |C(x)|^2 \sum_{A \in \mathcal{P}_c} \int_{A} \|\nabla g_c(z)\|dz.
\]

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where \( C_9 \) is positive constant depending on \( d \) which can be obtained with an entropy argument similar to (70). As a result, form (45) we obtain

\[
T_1 \leq C_2 C_9 N^{d-1} \max_{x \in h^{-1}(P_{au}(N))} |C(x)|^2. \tag{57}
\]

It remains to bound \( T_2 \) in (55). Towards that goal, we observe that

\[
\int_{B_r(z_{i,j})} \left| \nabla g_\epsilon(z_{i,j}) \right|_1 \leq \left| \nabla g_\epsilon(z) \right|_1 \int_{B_r(z_{i,j})} \left| \frac{\partial g_\epsilon}{\partial z_l}(z_{i,j}) - \frac{\partial g_\epsilon}{\partial z_l}(z) \right| dz
\]

\[
= \int_{B_r(z_{i,j})} \sum_{l=1}^d \left| \frac{1}{\epsilon^{d+1}} \int_{B_r(0)} \frac{\partial \psi}{\partial z_l}(z'/\epsilon) \left( g_0(z_{i,j} - z') - g_0(z - z') \right) dz' \right| dz
\]

\[
\leq \int_{B_r(z_{i,j})} \sum_{l=1}^d \epsilon^{d} \|z_{i,j} - z\|_2 \int_{B_r(0)} \frac{\partial \psi}{\partial z_l}(z'/\epsilon) \left( g_0(z_{i,j} - z') - g_0(z - z') \right) dz'
\]

which implies that for some \( C_{10} > 0 \)

\[
\int_{B_r(z_{i,j})} \left| \nabla g_\epsilon(z_{i,j}) \right|_1 \leq C_{10} \epsilon^d \sup_{z \in B_r(z_{i,j})} \sum_{l=1}^d \int_{B_r(0)} \frac{\partial \psi}{\partial z_l}(z'/\epsilon) \left( g_0(z_{i,j} - z') - g_0(z - z') \right) dz'
\]

and so

\[
T_2 \leq \sum_{A \in \mathcal{P}_c, A \cap (\Omega_{2\epsilon} \setminus B_{2\epsilon}(S)) \neq \emptyset} \left[ \sum_{(i,j) \in E_K} \sum_{l=1}^d \int_{B_r(z_{i,j})} \frac{\partial \psi}{\partial z_l}(z'/\epsilon) \left( g_0(z_{i,j} - z') - g_0(z - z') \right) dz' \right]
\]

\[
: 2 C_{10} C_8 \epsilon^d N^{d-1}
\]

\[
= \sum_{A \in \mathcal{P}_c, A \cap (\Omega_{2\epsilon} \setminus B_{2\epsilon}(S)) \neq \emptyset} \left[ \sum_{(i,j) \in E_K} \sum_{l=1}^d T(g_0, z_{i,j}) \epsilon^d \right] \cdot 2 C_{10} C_8 N^{d-1}, \tag{58}
\]

with \( T(g_0, z) \) as in (12). Now, if \( z_{i,j} \in A, h(x_i) \in A_i \) and \( h(x_j) \in A_j \), then just as in (56) we obtain that

\[
\max \{ |c(A_i) - c(A)|_\infty, |c(A_j) - c(A)|_\infty \} \leq 2\epsilon.
\]

Hence, since by construction we also have \( z_{i,j} \in \Omega_{2\epsilon} \setminus B_{2\epsilon}(S) \) then

\[
\sum_{(i,j) \in E_K} T(g_0, z_{i,j}) \leq \left| \{ i, j \} : \max \{ |c(A_i) - c(A)|_\infty, |c(A_j) - c(A)|_\infty \} \leq 2\epsilon \right|
\]

\[
\sup_{z_A \in A \cap (\Omega_{2\epsilon} \setminus B_{2\epsilon}(S))} T(g_0, z_A),
\]

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which combined with (58) implies that

\[ T_2 \leq \sum_{A \in \mathcal{P}_e(\mathcal{A} \cap \Omega_2 \setminus B_{2\rho}(S))} \sup_{x \in \mathcal{A} \cap \Omega_2 \setminus B_{2\rho}(S)} \left[ \sum_{i,j} T(g_{0z}, \theta_i, \theta_j) c_d \right] \cdot 2 C_{10} C_8 N^{-d-1}. \]

(59)

|\{i, j\} : \max \{\|c(A_i) - c(A)\|_{\infty}, \|c(A_j) - c(A)\|_{\infty}\} \leq 2\varepsilon|

\leq C_{11} N^{-d-1} \max_{x \in h^{-1}(\mathcal{P}_{na}(N))} |C(x)|^2,

for some positive constant \( C_{11} \), where the last inequality follows from Assumption 5 and that fact that for every \( A \) the set of pairs of cells with centers within distance \( 2\varepsilon \) is constant.

The proof concludes by combining the last equation with (54), (57), (55), (59) and Lemma 15.

**Bound when \( g_0 \) is piecewise Lipschitz.** Using the notation from before, we observe that (47) still holds and for \( J \) in (48) we have that

\[ \sum_{(i,j) \in E_K} |\theta_i - \theta_j^*| = \sum_{(i,j) \in E_K, i,j \in J} |\theta_i - \theta_j^*| + \sum_{(i,j) \in E_K, i \notin J \text{ or } j \notin J} |\theta_i^* - \theta_j^*| \leq |f_0(x_i) - f_0(x_j)| + 2\|g_0\|_{L_{\infty}(0,1)} K \tau_\delta \tilde{\mathbb{N}}. \]

(60)

So the claim follows from combining Lemma 8, (53), and the piecewise Lipschitz condition.

\[ \square \]

**A.10 Proof of Theorem 3**

**Proof.** For \( i \in [n] \) we write \( l(i) := j \in [\ell] \) if \( i \in A_j \). We also introduce the following notation:

\[ N_K(x_i) = \{ \text{set of nearest neighbors of } x_i \text{ in the } K\text{-NN graph constructed from points } \{x_{i'}\}_{i'=1,...,n} \}, \]

\[ \tilde{N}_K(x_i) = \{ \text{set of nearest neighbors of } x_i \text{ in the } K\text{-NN graph constructed from points } \{x_{i'}\}_{i' \in A_l(i)} \}, \]

\[ \tilde{R}_{K,\max}^l = \max_{i \in A_l} \max_{x \in \tilde{N}_K(x_i)} d_X(x, x_i), \]

and we denote by \( \nabla G_l^i \) the incidence matrix of the \( K\text{-NN graph corresponding to the points } \{x_i\}_{i \in A_l} \).

Next we observe that just as in the proof of Lemma 9,

\[ \mathbb{P} \left( \tilde{R}_{K,\max}^l > \tilde{a}_l(K/n_l)^{1/d} \right) \leq n_l \exp(-K/12), \]

(61)

for some positive constant \( \tilde{a}_l \). We write \( \epsilon_l = \tilde{a}_l(K/n_l)^{1/d} \), and consider the sets

\[ A_l = \{ i \in A_l : \text{ such that } N_K(x_i) = \tilde{N}_K(x_i) \}. \]

Our goal is to use these sets in order to modify the basic inequality for the \( K\text{-NN-FL to be split into different } \)

processes corresponding to the different sets \( A_l \). To that end let us pick \( l \in [\ell] \). We notice that if \( \partial A_i = \emptyset \),

then by Assumption 6 we have that \( N_K(x_i) = \tilde{N}_K(x_i) \) for all \( i \in A_l \) with high probability.

Let us instead assume that \( \partial A_l \neq \emptyset \). Let \( i \in A_l \). Then

\[ \mathbb{P} \left( x_i \in B_{\epsilon_l}(\partial A_l, d_X) \right) \geq pl_{\min} \mu_l \left( B_{\epsilon_l}(\partial A_l, d_X) \right) \geq c_l \epsilon_l^{d_l}, \]

(62)
where $p_{t,\min} = \min_{x \in \mathcal{X}_t} p_t(x)$, and $c'_t$ is a positive constant that exists because $X_t$ satisfies Assumption 2.

On the other hand, (15) implies that for $i \in A_t$ we have

$$p_t(x_i \in B_{\epsilon_t}(\partial \mathcal{X}_t)) \leq p_{t,\max} \mu_t \left( B_{\epsilon_t}(\partial \mathcal{X}_t, d_X) \cap \mathcal{X}_t \right) \leq p_{t,\max} \tilde{c}_t \epsilon_t,$$

(63)

where $p_{t,\max} = \max_{x \in \mathcal{X}_t} p_t(x)$, and $\tilde{c}_t$ is a positive constant.

Therefore, combining (16), (61), (62), and (63) with Lemma 7, we obtain that

$$\mathbb{P} \left( n_l - |\Lambda_l| \leq \frac{3}{2} p_{t,\max} \tilde{c}_t n_l \epsilon_l \right) \geq 1 - p_{\max} \exp \left( -\frac{1}{2} c'_t a'_t d_i^n K \right) - n_l \exp(-K/12).$$

(64)

Next we see how the previous inequality can be used to put an upper-bound on the penalty term of the $K$-NN-FL. Thus, for any $\theta \in \mathbb{R}^n$ we have

$$\|\nabla_{G_K} \theta\|_1 = \sum_{l=1}^\ell \sum_{i=1}^{n_l} \sum_{j \in \mathcal{N}_K(x_i)} |\theta_i - \theta_j| = \sum_{l=1}^\ell \sum_{i=1}^{n_l} \sum_{j \notin \mathcal{N}_K(x_i)} |\theta_i - \theta_j| + R(\theta),$$

where

$$|R(\theta)| \leq 4 \tau_d \|\theta\|_\infty K \sum_{l=1}^\ell |[n_l]\setminus \Lambda_l|$$

(65)

where $\tau_d$ is a positive constant depending only on $d$ and the second inequality follows from the well known bound on the maximum degree of $K$-NN graphs see Corollary 3.23 in Miller et al. (1997). Combining with (64), we obtain that

$$R(\theta) - R(\hat{\theta}) = O_{\mathbb{P}} \left( \sqrt{\log n} \lambda K^{1+1/d_i} \sum_{l=1}^\ell n_l^{1-1/d_i} \right).$$

(66)

Not that if $\partial X_t = \emptyset$, then (66) will still hold as $R(\theta) = 0$ for all $\theta \in \mathbb{R}^n$ with high probability.

To conclude the proof we notice by the basic inequality that

$$\|\theta^* - \hat{\theta}\|_n^2 \leq \frac{1}{n} \varepsilon_T^T (\hat{\theta} - \theta^*) + \frac{\lambda}{n} \left[ \|\nabla_{G_K} \theta^*\|_1 - \|\nabla_{G_K} \hat{\theta}\|_1 \right]$$

$$= \sum_{l=1}^\ell \varepsilon_{A_l}^T (\hat{\theta}_{A_l} - \theta^*_{A_l}) + \sum_{l=1}^\ell \frac{\lambda}{n} \left[ \|\nabla_{G'_K} \theta^*_{A_l}\|_1 - \|\nabla_{G'_K} \hat{\theta}_{A_l}\|_1 \right] + \frac{\lambda}{n} \left[ R(\theta^*) - R(\hat{\theta}) \right],$$

(67)

here for a vector $x$ we denote $x_{A_l}$ by removing the coordinates with index not in $A$. The proof follows from (66) and because bounding each term

$$\frac{1}{n} \varepsilon_{A_l}^T (\hat{\theta}_{A_l} - \theta^*_{A_l}) + \frac{\lambda}{n} \left[ \|\nabla_{G'_K} \theta^*_{A_l}\|_1 - \|\nabla_{G'_K} \hat{\theta}_{A_l}\|_1 \right],$$

can be done as in the proof of Theorem 14.

\[\square\]
A.11 Proof of Example 1

Proof. We begin noticing that if $i, j \in A_2$ with $i \neq j$, then for the choice of $\epsilon > 0$ in this example, we have that
\[
\Pr(d_X(x_i, x_j) \leq \epsilon) \leq p_{2, \text{max}} \int_{\mathcal{X}} \Pr(d_X(x, x_j) \leq \epsilon) \mu_2(dx) \leq \tilde{C}_1 \frac{(\text{poly}(\log n))^3}{n^{3/4}}.
\]
Let $m > n^{3/4-a}$, and $j_1 < j_2 < \ldots < j_m$ elements of $A_2$. Then the event
\[
\Lambda = \bigcap_{s=1}^{m} \{d_X(x_{j_s}, x_i) > \epsilon, \; \forall l \in A_2 \setminus \{j_s\}\},
\]
satisfies
\[
\Pr(\Lambda) \geq 1 - c_2 n^{3/2-3/4-a} (\text{poly}(\log n))^3,
\]
for some positive constant $c_2$. Therefore,
\[
\mathbb{E} \left[ \sum_{i=1}^{n} (\theta^*_{i} - \hat{\theta}_{e,i})^2 \right] \geq \mathbb{E} \left[ \sum_{i=1}^{n} (\theta^*_{i} - \hat{\theta}_{e,i})^2 | \Lambda \right] \Pr(\Lambda) \geq m \sigma^2 (1 - c_2 n^{3/2-3/4-a} (\text{poly}(\log n))^3) \geq C_1 n^{3/4-a}
\]
for some positive constant $C_1$ if $n$ is large enough.

A.12 Proof of Theorem 4

Proof. Throughout we use the notation from Appendix A.3. We start by noticing that
\[
\mathbb{E}_{x \sim \mu} \left| f_0(x) - \hat{f}(x) \right|^2 = \int \left( f_0(x) - \hat{f}(x) \right)^2 p(x) \mu(dx)
\]
\[
= \int \left[ f_0(x) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i)
\right.
\]
\[
+ \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} \hat{f}(x_i) \right]^2 p(x) \mu(dx)
\]
\[
\leq 2 \int \left( f_0(x) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) \right)^2 p(x) \mu(dx) +
\]
\[
2 \int \left( \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\]
Therefore we proceed to bound the second term in the last inequality. We observe that
\[
\int \left( \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\]
\[
= \sum_{x ' \in I(N)} \int_{C(x')} \left( \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx).
\]
(67)
Let $x' \in \mathcal{X}$, then there exists $u(x') \in I(N)$ such that $x \in C(u(x'))$ and
\[
\|h(x') - h(u(x'))\|_2 \leq \frac{1}{2N}.
\]

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Moreover, by Lemma 9, with high probability, there exists \( i(x') \in [n] \) such that \( x_{i(x')} \in C(u(x')) \). Hence,

\[
d_X(x', x_{i(x')}) \leq \frac{1}{L_{\min}} \| h(x') - h(x_{i(x')}) \|_2 \leq \frac{1}{L_{\min} N}.
\]

The above implies that there exists \( x_{i_1}, \ldots, x_{i_K}, i_1, \ldots, i_K \in [n] \) such that

\[
d_X(x', x_{i_l}) \leq \frac{1}{L_{\min} N} + R_{K, \max}, \quad l = 1, \ldots, K.
\]

Thus, with high probability, we have that for any \( x' \in \mathcal{X} \),

\[
\mathcal{N}(x') \subset \left\{ i : d_X(x', x_i) \leq \frac{1}{L_{\min} N} + R_{K, \max} \right\}
\subset \left\{ i : \| h(x') - h(x_i) \|_2 \leq \frac{L_{\max}}{L_{\min} N} + L_{\max} R_{K, \max} \right\}
\subset \left\{ i : \| h(u(x')) - h(x_i) \|_2 \leq \left( \frac{1}{2} + \frac{L_{\max}}{L_{\min}} \right) \frac{1}{N} + L_{\max} R_{K, \max} \right\}
=: \mathcal{N}(u(x'))
\]

As a result, denoting by \( u_1, \ldots, u_{N^d} \) the elements of \( I(N) \), we have that for \( j \in [N^d] \),

\[
\int_{C(u_j)} \left( \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} f_0(x_i) - \frac{1}{|\mathcal{N}(x)|} \sum_{i \in \mathcal{N}(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\leq \int_{C(u_j)} \sum_{i \in \mathcal{N}(x)} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\leq \frac{1}{K} \int_{C(u_j)} \sum_{i \in \mathcal{N}(u_j)} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 p(x) \mu(dx)
= \frac{1}{K} \left[ \sum_{i \in \mathcal{N}(u_j)} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 \right] \int_{C(u_j)} p(x) \mu(dx).
\]
The above combined with (67) leads to

\[
\int \left( \frac{1}{|N(x)|} \sum_{i \in N(x)} f_0(x_i) - \frac{1}{|N(x)|} \sum_{i \in N(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\]

\[
\leq \sum_{j=1}^{N^d} \left[ \frac{1}{K} \left( \sum_{i \in N(u_j)} (f_0(x_i) - \hat{f}(x_i))^2 \right) \right] \int_{C(u_j)} p(x) \mu(dx)
\]

\[
\leq \left[ \sum_{j=1}^{N^d} \frac{1}{K} \sum_{i \in N(u_j)} (f_0(x_i) - \hat{f}(x_i))^2 \right] \max_{1 \leq j \leq N^d} \int_{C(u_j)} p(x) \mu(dx)
\]

\[
\leq \left[ \sum_{i=1}^{n} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 \right] \left[ \max_{i \in [n]} \left\{ j : \| h(x_i) - h(u_j) \|_2 \leq \left( \frac{1}{2} + \frac{L_{\max}}{L_{\min}} \right) \frac{1}{N} + L_{\max} R_{K,\max} \right\} \right].
\]

\[
\frac{1}{K} \max_{1 \leq j \leq N^d} \int_{C(u_j)} p(x) \mu(dx).
\]

(69)

On the other hand, by Lemma 9, there exists a constant \( \tilde{c} \) such that \( R_{K,\max} \leq \tilde{c}/N \) (with high probability). This implies that with high probability for a positive constant \( \tilde{C} \) we have that

\[
\max_{i \in [n]} \left\{ j \in [N^d] : \| h(x_i) - h(u_j) \|_2 \leq \left( \frac{1}{2} + \frac{L_{\max}}{L_{\min}} \right) \frac{1}{N} + L_{\max} R_{K,\max} \right\}
\]

\[
\leq \max_{i \in [n]} \left\{ j \in [N^d] : \| h(x_i) - h(u_j) \|_2 \leq \frac{\tilde{c}}{N^3} \right\}
\]

\[
\leq \max_{i \in [n]} N_{1,\text{pack}}^{C} \left( B_{\tilde{C}} \left( \frac{h(x_i)}{N} \right) \right)
\]

\[
\leq N_{1,\text{tor}}^{C} \left( B_{\tilde{C}} \left( 0 \right) / N \right)
\]

\[
< C',
\]

(71)

for some positive constant \( C' \). And so, there exists a constant \( C_1 \) such that

\[
\int \left( \frac{1}{|N(x)|} \sum_{i \in N(x)} f_0(x_i) - \frac{1}{|N(x)|} \sum_{i \in N(x)} \hat{f}(x_i) \right)^2 p(x) \mu(dx)
\]

\[
\leq \left[ \sum_{i=1}^{n} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 \right] \frac{C_1}{K} \max_{1 \leq j \leq N^d} \int_{C(u_j)} p(x) \mu(dx)
\]

\[
\leq \left[ \sum_{i=1}^{n} \left( f_0(x_i) - \hat{f}(x_i) \right)^2 \right] \frac{C_1 p_{\max}}{K} \mu \left( B_{\tilde{C}} \left( \frac{K}{p_{\max}} \right)^{1/d}(x) \right)
\]

where the last equation follows as in (30). The claim then follows. \( \square \)
A.13 Proof of Theorem 5

Proof. Throughout we use the notation from Lemma 9 and Appendix A.3. We denote by \( u_1, \ldots, u_{N^d} \) the elements of \( h^{-1}(P_{\text{lat}}(N)) \), and so

\[
\text{AErr} = \int \left( f_0(x) - \frac{1}{K} \sum_{i \in N(x)} f_0(x_i) \right)^2 p(x) \, \mu(dx)
\]

\[
= \sum_{j \in [N^d]} \int_{C(u_j)} \left( f_0(x) - \frac{1}{K} \sum_{i \in N(x)} f_0(x_i) \right)^2 p(x) \, \mu(dx)
\]

\[
\leq \sum_{j \in [N^d]} \int \sum_{i \in N(x)} \frac{1}{K} \left( f_0(x) - f_0(x_i) \right)^2 p(x) \, \mu(dx)
\]

\[
= \sum_{j \in [N^d]} \int_{C(u_j)} \sum_{i \in N(x)} \frac{1}{K} \left( f_0(x) - f_0(x_i) \right)^2 p(x) \, \mu(dx)
\]

\[
\leq 4 \left| \{ j \in [N^d] : C(u_j) \cap S \neq \emptyset \} \right| \| f_0 \|_\infty^2 \max_{1 \leq j \leq N^d} \int_{C(u_j)} p(x) \, \mu(dx)
\]

\[
+ \sum_{j \in [N^d]} \int_{C(u_j)} \sum_{i \in N(x)} \frac{1}{K} \left( g_0(h(x)) - g_0(h(x_i)) \right)^2 p(x) \, \mu(dx)
\]

\[
\leq \left[ c_{2,d} 4 \tilde{b} \| f_0 \|_\infty^2 \right] \frac{K}{n} \left| \{ j \in [N^d] : C(u_j) \cap S \neq \emptyset \} \right|
\]

\[
+ \sum_{j \in [N^d]} \int_{C(u_j)} \sum_{i \in N(x)} \frac{1}{K} \| h(x) - h(x_i) \|^2 p(x) \, \mu(dx)
\]

\[
\leq \left[ c_{2,d} 4 \tilde{b} \| f_0 \|_\infty^2 \right] \frac{K}{n} \left| \{ j \in [N^d] : C(u_j) \cap S \neq \emptyset \} \right|
\]

\[
+ L_0 \left[ \sum_{j \in [N^d]} \int_{C(u_j)} p(x) \, \mu(dx) \right] \left[ \frac{L_{\text{max}}}{L_{\text{min}}} \frac{1}{N} + L_{\text{max}} R_{K,\text{max}} \right]^2
\]

\[
\leq \left[ c_{2,d} 4 \tilde{b} \| f_0 \|_\infty^2 \right] \frac{K}{n} \left| \{ j \in [N^d] : C(u_j) \cap S \neq \emptyset \} \right|
\]

\[
+ L_0 \left[ \frac{L_{\text{max}}}{L_{\text{min}}} \frac{1}{N} + L_{\text{max}} R_{K,\text{max}} \right]^2,
\]

where the first inequality holds by convexity, the second equality by properties of integration, the second inequality also by elementary properties of integrals, the third inequality by (30), the fourth inequality
by Assumptions 2–3, the fifth inequality by same argument from (68), and the sixth inequality from by properties of integration. The result follows from the inequality above combined with Lemma 8 and the proof of Proposition 23 from Hutter and Rigollet (2016) which uses Lemma 8.3 from Arias-Castro et al. (2012).

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