A MAXIMUM PRINCIPLE ARGUMENT FOR THE UNIFORM CONVERGENCE OF GRAPH LAPLACIAN REGRESSORS

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Abstract. We study asymptotic consistency guarantees for a non-parametric regression problem with Laplacian regularization. In particular, we consider \((x_1, y_1), \ldots, (x_n, y_n)\) samples from some distribution on the cross product \(M \times \mathbb{R}\), where \(M\) is a \(m\)-dimensional manifold embedded in \(\mathbb{R}^d\). A geometric graph on the cloud \(\{x_1, \ldots, x_n\}\) is constructed by connecting points that are within some specified distance \(\varepsilon_n\). A suitable semi-linear equation involving the resulting graph Laplacian is used to obtain a regressor for the observed values of \(y\). We establish probabilistic error rates for the uniform difference between the regressor constructed from the observed data and the Bayes regressor (or trend) associated to the ground-truth distribution. We give the explicit dependence of the rates in terms of the parameter \(\varepsilon_n\), the strength of regularization \(\beta_n\), and the number of data points \(n\). Our argument relies on a simple, yet powerful, maximum principle for the graph Laplacian. We also address a simple extension of the framework to a semi-supervised setting.

1. Introduction

Given a data set \(\mathcal{X} = \{x_1, \ldots, x_n\}\) and a weighted graph structure \(\Gamma = (\mathcal{X}, W)\) on \(\mathcal{X}\), graph-based methods for learning use analytical notions like graph Laplacians, graph cuts, and Sobolev semi-norms to formulate optimization problems which offer sensible solutions to machine learning tasks. In this paper our focus is on supervised regression, where in addition to the graph structure \(\Gamma = (\mathcal{X}, W)\) we have access to values/labels \(y_i \in \mathbb{R}\) associated to some or all of the data points \(x_i\), and the goal is to learn a trend function \(\mu\) from the observed data.

Let us first consider the case where all the \(x_i\) are labeled. The optimization problem that we study takes the form:

\[
\min_u \beta R_{\Gamma}(u) + \frac{1}{n} \sum_{i=1}^{n} F(u(x_i) - y_i),
\]

where \(R_{\Gamma}\) is a regularization term and \(F : \mathbb{R} \to [0, \infty)\) is a loss function penalizing deviations from the observed data. The regularization term typically uses the graph structure and in this paper we restrict our attention to the graph Dirichlet energy

\[
R_{\Gamma}(u) := \frac{1}{n} \sum_{i,j} w_{ij} |u(x_i) - u(x_j)|^2.
\]

The parameter \(\beta \geq 0\) controls the amount of regularization imposed and serves as a way to ameliorate overfitting. Indeed, we will assume that the observed labels \(y_1, \ldots, y_n\) are noisy observations of an underlying trend \(\mu\), namely

\[y_i := \mu(x_i) + \xi_i.\]

The practical use of Laplacian regularization (or similar variants) has been considered by a number of authors in the context of non-parametric regression (see, e.g. [21, 24, 26, 29]). Other regularization methods, such as \(k\)-nearest neighbor (\(k\)-NN) regularization, have also been proposed and studied. In Section 1.3 we describe our work in the context of recent theoretical

2010 Mathematics Subject Classification. 35J05, 49J55, 60D05, 62G08, 68R10.

Key words and phrases. Empirical risk minimization, graph Laplacian, discrete to continuum, non-parametric regression.
results, as well as describing a connection between the Laplacian regularization we study here and the k-NN regularization considered in other works.

Graph-based approaches are quite flexible as they do not rely on a particular structure (e.g. Euclidean) for the data set \( \mathcal{X} \), and they are only defined in terms of the graph \( \Gamma \). However, a natural and important question to study concerns properties of the optimization problem ((1.1)) in the large \( n \) limit, when the graph \( \Gamma = \Gamma_n \) has some specific structure, often dictated by a probabilistic model. In this paper, we study the large \( n \) behavior of the solution to (1.1) when \( \Gamma \) is a realization of a random geometric graph. In our setting, \( \mathcal{X} = \mathcal{M}_n \) is a collection of \( n \) samples from a distribution supported on some compact, smooth, \( m \)-dimensional manifold \( \mathcal{M} \) embedded in Euclidean space \( \mathbb{R}^d \), and the weights are, up to rescaling, of the form

\[
    w_{ij} = \eta \left( \frac{|x_i - x_j|}{\varepsilon} \right),
\]

where \( | \cdot | \) is the Euclidean norm in \( \mathbb{R}^d \), \( \eta \) is a non-negative monotonic function with compact support, and \( \varepsilon > 0 \) is a connectivity parameter. Our asymptotic analysis relies on a careful study of the optimality conditions (i.e. the Euler-Lagrange equation) satisfied by the solution to the optimization problem (1.1). The resulting system of equations can be interpreted as an elliptic graph PDE of the form

\[
    \beta \Delta_{\Gamma} u + f(u - y) = 0,
\]

where \( f = F' \), and where \( \Delta_{\Gamma} \) represents the graph Laplacian which is defined by

\[
    \Delta_{\Gamma} u(x_i) := \sum_j w_{ij}(u(x_i) - u(x_j)),
\]

for all \( u : \mathcal{M}_n \to \mathbb{R} \). When \( F \) corresponds to quadratic loss, the graph PDE (1.3) turns out to be a linear equation, but for general \( F \) this is not the case. We use a maximum principle argument at the graph level to find \( L^\infty \) bounds of the difference between the solution to the graph PDE and a function at the continuum level \( v : \mathcal{M} \to \mathbb{R} \) which solves an analogous homogenized PDE on \( \mathcal{M} \). The proposed maximum principle (see Proposition 1.2 below) allows us to handle any sufficiently smooth, strictly convex \( F \). We also provide a characterization for how \( \beta \) must scale with \( n \) in order to recover, in the large data limit, a modified trend \( \mu_f \) which depends on \( \mu \) and on the function \( f \). Indeed, unless the function \( F \) is quadratic (i.e. \( f \) is linear), in the regime \( n \to \infty \), \( \beta := \beta_n \to 0 \) the trend \( \mu \) may not be recovered, unless further assumptions on the distribution of the noise \( \xi \) are imposed. We provide uniform rates of convergence towards the modified trend. Stated in another way, we provide quantified asymptotic consistency estimates for this class of non-parametric regression algorithms.

With exactly the same arguments we can also study a semi-supervised learning problem where only points \( x_1, \ldots, x_q \) are given labels \( y_1, \ldots, y_q \), but points \( x_{q+1}, \ldots, x_n \) are unlabeled. Indeed, the available labels can be extended to produce a function \( y : \mathcal{M}_n \to \mathbb{R} \) which is defined according to:

\[
    y(x_i) := y_i, \quad i = 1, \ldots, q,
\]

and for \( q + 1 \leq i \leq n \),

\[
    y(x_i) := y_j,
\]

where \( x_j \) is the point in \( \{x_1, \ldots, x_q\} \) that is closest to \( x_i \); notice that when \( q = n \) this reduces to the fully supervised learning set-up presented earlier. The uniform estimates that we derive are explicitly written in terms of \( n, q, \beta \) and the graph connectivity \( \varepsilon \).

With the \( L^\infty \) bounds between the solution \( u \) of the graph PDE and the modified trend in hand (for both the fully-supervised and semi-supervised settings that we study), we can construct a simple out of sample extension of \( u \) which is guaranteed to be uniformly close to the modified trend when restricted to \( \mathcal{M} \). The out-of-sample extension can be used for prediction, or in other words gives a constructive regression algorithm which satisfies the bounds that we prove in this work: see Section 2.4.
We emphasize that the estimates in our results have explicit dependence on the parameters and number of data points, up to constants depending on $\mathcal{M}$ and the underlying trend $\mu$. We believe that these results can be used to accurately estimate the impact of new labelled or unlabelled data on inferential accuracy. Empirical investigation, as well as an investigation between tradeoffs in the value of labeled vs unlabeled data, will be left to future work.

Finally, we would like to finish this introduction by emphasizing that the ideas behind our proofs are strongly grounded in PDE theory. This continues a growing body of work (which we briefly review in Section 1.3), which draws on ideas from the calculus of variations, PDE theory, optimal transport, and in general mathematical analysis, in order to effectively study unsupervised and semi-supervised learning algorithms on geometric graphs. We believe that the ideas presented in this work are amenable to use in other classification and regression problems on graphs.

1.1. Set-up. We consider an $m$-dimensional smooth, compact manifold $\mathcal{M}$ embedded in $\mathbb{R}^d$ with no boundary. A significant body of work studies how to estimate $m$ given a family of points (see e.g. [18]); for the purpose of this work we will treat $m$ as a priori known. Throughout the paper we will denote by $|x - \tilde{x}|$ the Euclidean distance in $\mathbb{R}^d$ and by $d_M(x, \tilde{x})$ the geodesic distance of two points in $\mathcal{M}$. We will denote by $i_0$ the injectivity radius of the manifold $\mathcal{M}$. We recall that the injectivity radius of a manifold is defined as the maximum radius for which the exponential map $\exp_{x} : B_m(0, i_0) \subseteq T_x \mathcal{M} \to B_{\mathcal{M}}(x, i_0)$ defines a diffeomorphism for all $x \in \mathcal{M}$. In the remainder we use $B_m$ to denote balls in $\mathbb{R}^m$, $B_{\mathcal{M}}$ for balls in $\mathcal{M}$ with the geodesic distance, and finally $B$ for balls in $\mathbb{R}^d$. We use $K$ to represent a uniform bound on the absolute value of the sectional curvature of $\mathcal{M}$ and $R$ to represent its reach. Finally, we will denote by $d\text{vol}_M$ the volume form of $\mathcal{M}$ and, after rescaling as necessary, we will assume that the volume of $\mathcal{M}$ is equal to one.

We assume that the loss function $F : \mathbb{R} \to [0, \infty)$ is a twice continuously differentiable function with $F(0) = 0$. We will further assume that $F$ is a strictly convex function, so that, in particular, its derivative $f := F'$ is strictly monotone. As a consequence, for every $s > 0$ there exists $c_s > 0$ such that $f'(t) > c_s$ for all $t \in [-s, s]$.

Let $\gamma$ be a probability distribution over $\mathcal{M} \times \mathbb{R}$. By the disintegration theorem there exists a family $\{\gamma_x\}_{x \in \mathcal{M}}$ of probability measures on $\mathbb{R}$ (the conditional distributions of the second coordinate given the first one) and a distribution $\nu$ on $\mathcal{M}$ (the marginal of the first coordinate) such that

$$\gamma(A \times D) = \int_A \gamma_x(D)d\nu(x)$$

holds for every Borel subset $A$ of $\mathcal{M}$ and every Borel subset $D$ of $\mathbb{R}$. The measure $\nu$ is assumed to have a smooth density $\rho$ with respect to $\mathcal{M}$’s volume form $d\text{vol}_M$, and the conditional distribution $\gamma_x$ is assumed to have a smooth density $p_x(\cdot)$ with respect to the Lebesgue measure in $\mathbb{R}$. We further assume that the densities $p_x$ vary smoothly in $x \in \mathcal{M}$.

We let $\mu : \mathcal{M} \to \mathbb{R}$ be the Bayes regressor (or trend) associated to the distribution $\gamma$. That is,

$$\mu(x) := \mathbb{E}(y|x = x) = \int ydp_x(y).$$

While all the main results in this paper can be proved in the previous general setting, for simplicity we will restrict our attention to the setting where the density $\rho$ is constant (so that the first marginal of $\gamma$ is simply the uniform measure on $\mathcal{M}$, and given that we have assumed $\mathcal{M}$ to be normalized actually $\rho \equiv 1$) and where the densities $p_x$ take the form

$$p_x(y) = p(y - \mu(x)),$$

where $p$ is a noise distribution and $\mu : \mathcal{M} \to \mathbb{R}$ is smooth trend function. For $\xi \sim p$, we assume that

$$\mathbb{E}(\xi) = 0$$

and that

$$\mathbb{P}(|\xi| \leq \sigma) = 1,$$
for some finite, positive $\sigma$. In other words, we assume the noise in the labels to be bounded. In Section 1 all our theorems and results are presented in this localized setting, but in Remark 1.8 we write precisely how they should be restated to cover the more general setting where $\rho$ is not necessarily constant and the conditional densities do not take the form $\left(1.5\right)$; no difficulties will arise when extending our theorems, other than having to deal with more cumbersome notation and longer expressions.

In the remainder we assume that $(x_1, y_1), \ldots, (x_q, y_q)$ are i.i.d. samples from $\gamma$ and that $x_{q+1}, \ldots, x_n$ are independently drawn from $\nu$.

1.1.1. Graph construction and graph PDE. Given $\mathcal{M}_n := \{x_i\}_{i=1}^n$ we construct a geometric graph as follows. We let $\eta : [0, \infty) \to [0, \infty)$ be a non-increasing function which is only non-zero on $[0, 1]$. We further assume $\eta$ to be Lipschitz continuous and normalized so that

$$\int_{\mathbb{R}^m} \eta(|z|) \, dz = 1.$$ 

We define the constant

$$\tau_\eta := \int_{\mathbb{R}^m} |z|^2 \eta(|z|) \, dz.$$ 

Between every two vertices $x_i, x_j \in \mathcal{M}_n$ we assign the weight

$$w_{i,j} = \frac{2}{\tau_\eta \varepsilon^2 + 2n} \eta \left( \frac{|x_i - x_j|}{\varepsilon} \right).$$ 

The weighted graph $(\mathcal{M}_n, w)$ is a geometric graph representing the proximity of the sample points $x_i$ in $\mathbb{R}^d$. We have rescaled the weights for convenience (in taking limits as $n \to \infty$).

1.1.2. Limiting variational problem and PDE. At the continuum level, we first define an analogue of the graph regularizer $R_\Gamma$. The Dirichlet energy of a function $v : \mathcal{M} \to \mathbb{R}$ is defined as

$$R_{\mathcal{M}}(v) := \int_{\mathcal{M}} |\nabla v|^2 \, dvol_{\mathcal{M}},$$

whenever $v$ is in the Sobolev space $H^1(\mathcal{M})$. Also, for a smooth function $v$ we define the elliptic operator $\Delta_{\mathcal{M}}$ as

$$\Delta_{\mathcal{M}} v := -\text{div}(\nabla v),$$

i.e. the negative of the Laplace-Beltrami operator on $\mathcal{M}$. It is well-known that the Euler-Lagrange equation associated to the variational problem

$$\min_v \left\{ \beta R_{\mathcal{M}}(v) + \int_{\mathcal{M}} \int_{\mathbb{R}} F(v(x) - \mu(x) - s)p(s) \, ds \, dvol_{\mathcal{M}}(x) \right\}$$

is the PDE

$$\beta \Delta_{\mathcal{M}} u + \int_{\mathbb{R}} f(u - \mu - s)p(s) \, ds = 0.$$ 

Equation (1.9) is the continuum “homogenized” analogue of the graph PDE (1.3). We notice that there are two terms that get homogenized in going from (1.3) to (1.9). On the one hand, as more feature vectors $x_i$ are available, the graph $\Gamma$ gets denser, and the graph Laplacian $\Delta_\Gamma$ starts behaving like $\Delta_{\mathcal{M}}$. On the other hand, as more labels $y_i$ are acquired, we expect an homogenization at the level of the fidelity term in (1.1). In the next section we present our main results relating the solutions to these two equations, i.e. (1.3) and (1.9).
1.2. Main results and discussion. Our first main result establishes probabilistic error bounds for
\[ \max_{i=1,\ldots,n} |u(x_i) - v(x_i)| \]
where \( u \) is the solution to the graph PDE (1.3) (with the graph \( \Gamma \) as defined in section (1.1.1)), and \( v \) is the solution to (1.9). We can view this result as a “variance” estimate.

**Theorem 1.1.** (Variance estimate) Suppose that \( x_1, \ldots, x_n \) are samples from the uniform distribution on a compact smooth manifold \( \mathcal{M} \) embedded in \( \mathbb{R}^d \). Suppose that \( u \) is the solution to the elliptic graph PDE (1.3) where \( \Delta_{\Gamma} \) is defined in (1.4) and \( v \) is the solution to the PDE (1.9). Assume that \( \mu \in C^2(\mathcal{M}) \). Then for any \( \delta, \zeta > 0 \), with probability at least
\[ 1 - 4n \exp \left( -\frac{n \delta^{m+1}}{C(1+(n\delta)^{-1})} \right) - 4n \exp(-Cn^{m} \zeta^2) - 4n \exp(-Cn^{m}) \]
\[ \max_{i=1,\ldots,n} |u_i - v_i| \leq C \left( \frac{\epsilon^2}{\beta} + \zeta + \beta \delta + \beta^{1/2} \epsilon \right), \]
where the constants \( C \) depend only on \( \mu, \eta, F, \) and \( \mathcal{M} \).

One of the main tools used to establish Theorem 1.1 is the following maximum principle at the graph level, whose proof is simple enough that we present it immediately.

**Proposition 1.2.** (Maximum principle) Let \( g : \mathbb{R} \to \mathbb{R} \) be a strictly increasing function and let \( h \in L^2(\mathcal{M}_n) \) be an arbitrary function defined on the point cloud \( \mathcal{M}_n \). Suppose that the function \( z : \mathcal{M}_n \to \mathbb{R} \) satisfies
\[ -\beta \Delta_{\Gamma} z - (g(z + h) - g(h)) \geq 0. \]
Then,
\[ z \leq 0, \]
i.e. the function \( z \) is non-positive.

**Proof.** Notice that to prove that the function \( z \) is non-positive, it is enough to show that \( z(x_i) \leq 0 \) where \( i \) is the index of the point \( x_i \) at which \( z \) is maximized. Now, we notice that at the point \( x_i \) we have
\[ \Delta_{\Gamma} z(x_i) = \sum_{j=1}^{n} w_{ij}(z(x_i) - z(x_j)) \geq 0. \]
It then follows that
\[ -(g(z(x_i) + h(x_i)) - g(h(x_i))) \geq 0, \]
or equivalently,
\[ g(z(x_i) + h(x_i)) \leq g(h(x_i)). \]
Since the function \( g \) is strictly increasing, we conclude that \( z(x_i) \leq 0 \), which concludes the proof. \( \square \)

Theorem 1.1 is proved by showing that the difference of the functions \( u \) and \( v \) (interpreting \( v \) as its restriction to \( \mathcal{M}_n \)) lies between two functions \( y^-, y^+ \) which are uniformly close to zero, i.e.,
\[ y^-(x_i) \leq u(x_i) - v(x_i) \leq y^+(x_i), \quad \forall i = 1, \ldots, n, \]
with
\[ \|y^-\|_\infty, \|y^+\|_\infty \ll 1. \]
The functions \( y^- \) and \( y^+ \) are conveniently constructed so as to ensure that the functions \( z^+ := u - v \) and \( z^- := y^- - (u - v) \) satisfy the inequality required for the maximum principle to apply with \( g \equiv f \) (which then implies (1.10)).

We also establish the following bias estimate using standard arguments from the literature of PDEs.
Theorem 1.3. (Bias estimate) Let $\mu_f$ be the solution to the equation:
\[ \int_{\mathbb{R}} f(\mu_f(x) - \mu(x) - s)p(s)ds = 0, \quad \forall x \in \mathcal{M}. \]
Then there exists a unique $v \in C^2(\mathcal{M})$ which solves the PDE (1.9). Furthermore, for $\beta$ sufficiently small, this function satisfies
\[ \sup_{x \in \mathcal{M}} |v(x) - \mu_f(x)| \leq \frac{\beta |\Delta_M \mu|_{\infty}}{c_1}, \]
where $f'(t) > c_1$ for $t \in [-|\mu_f|_{\infty}, |\mu_f|_{\infty}]$. Furthermore, assuming that $|\mu|_{C^2} < \infty$ then
\[ |v|_{C^2} \leq C, |v|_{C^3} \leq C\beta^{-1/2}, |v|_{C^4} \leq C\beta^{-1}, \]
where here $C$ is independent of $\beta$.

We can combine Theorems 1.1 and 1.3 and deduce the following:

Theorem 1.4. Under the same assumptions in Theorem 1.1 and using the same notation there as well as that in Theorem 1.3, with probability greater than $1 - 4n \exp \left( \frac{-n\delta e^{m+1}}{C(1+(n\delta e^{-1}))} \right) - 4n \exp(-Cn\varepsilon^m) - 4n \exp(-Cn\varepsilon^m)$, we have
\[ \max_{i=1,\ldots,n} |u(x_i) - \mu_f(x_i)| \leq C \left( \beta + \varepsilon^2 + \frac{\varepsilon}{\beta} + \zeta + \beta \delta + \beta^{1/2} \varepsilon \right). \]
In particular, choosing $\delta = \zeta = \beta = \varepsilon$ we have that with probability larger than $\sim 1 - n \exp(-Cn\varepsilon^{m+2})$ we have $\max |u(x_i) - \mu_f(x_i)| \leq C\varepsilon$.

Remark 1.5. We note as long as $\log(n^{1/m}) \ll \varepsilon \ll \beta^{2} \ll 1$ then the previous theorem gives asymptotic consistency. Clearly the best performance (up to constants) is obtained if we set $\varepsilon, \beta$ as stated at the end of the theorem.

We highlight that Theorem 1.4 gives a theoretically sound means for selecting parameter values, which is asymptotically consistent. We offer a brief computational illustration of this result. We let the domain $[0,1]^2$ play the role of $\mathcal{M}$, $n = 10,000$, and $\mu(x,y) = .5 \sin(\pi x) + .5 \sin(\pi y)$. Following the theory developed in this paper, we choose to set $\varepsilon = \beta = n^{-1/5}$. We emphasize that no tuning has been done to parameters, we select the parameter values solely using the theory developed in this work.

In Figure 1 we show the Bayes’ estimator and the computed regressor for a quadratic loss function and symmetric Bernoulli noise. In Figure 2 we show the regression errors when the loss function is quadratic and the noise is symmetric and asymmetric Bernoulli. We notice that the fit is good in both cases, particularly away from the boundaries of the domain (as expected.
since the PDE estimates will not be as good near boundaries), and that the symmetric vs.
asymmetric noise does not make a difference (due to the linear optimality conditions, which
only see the “average” noise).

In Figure 3 we show the regression errors for a quartic loss function, with the symmetric and
asymmetric Bernoulli noise. Notice that the estimator is biased in the case of asymmetric noise.
This is because the necessary conditions are no longer linear and the estimation procedure is
asymptotically biased.

Having established our probabilistic error bounds for the fully supervised setting, we turn
our attention to establishing error bounds in the semi-supervised regime.

**Theorem 1.6.** Suppose that \((x_1, y_1), \ldots, (x_q, y_q)\) are i.i.d. samples from \(\gamma\) and suppose that
\(x_{q+1}, \ldots, x_n\) are i.i.d. samples from \(\nu\). Suppose that \(q \leq cn\) for some \(c < 1\) and that the
connectivity parameter \(\varepsilon > 0\) satisfies

\[
\varepsilon \geq \max \left\{ \frac{(A \log(n))^{1/m}}{n^{1/m}}, \frac{(A \log(n))^2}{q^{1/m}} \right\}
\]

for some constant \(A > 0\) (that is large enough so that the following estimates are meaningful).
Let \( u \) be the solution to the graph PDE (1.3) where the function \( y : \mathcal{M}_n \to \mathbb{R} \) is a Voronoi extension of the labels \( y_1, \ldots, y_q \) to the whole data set \( \mathcal{M}_n \). More precisely,

\[
y(x_i) := \sum_{j=1}^{q} y_i V_j(x_i), \quad i = 1, \ldots, n,
\]

where \( V_1, \ldots, V_q \) is the Voronoi tessellation of \( \mathbb{R}^d \) induced by the points \( x_1, \ldots, x_q \). Then for any \( \delta, \zeta > 0 \), with probability at least

\[
1 - 4n \exp \left( -\frac{n \delta \varepsilon^m + 1}{C(1 + (n \delta \varepsilon)^{-1})} \right) - 4n \exp(-C n \varepsilon^m \zeta^2)
- 4n \exp(-C n \varepsilon^m) - 2n \exp \left( -\frac{C q \varepsilon^m \delta^2}{A^2 \log^2(q)} \right) - q \exp(-C q \varepsilon^m)
- C \frac{q^2 - C A}{A \log(q)} - 2q \exp \left( -\frac{C n q}{A \log(q)} \right)
\]

we have

\[
\max_{i=1, \ldots, n} |u(x_i) - \mu_f(x_i)| \leq C \left( \beta + \frac{\varepsilon^2}{\beta} + \zeta + \beta \delta + \beta^{1/2} \varepsilon \right),
\]

where the constants \( C \) only depend upon \( \mu, \eta, F, \) and \( \mathcal{M} \).

The proof of Theorem 1.6 is identical to that of the theorems in the fully supervised setting, with only slight modifications in some of the technical arguments that use concentration inequalities; specifically, only Lemma 2.4 needs to be adjusted. We notice that our estimates are only meaningful in a regime where the number of labeled data points \( q \) grows with the total number of data points \( n \) (although \( q \) is allowed to grow at a slower rate than \( n \)). We would like to emphasize that in the regime where \( q \) is constant, the standard graph Laplacian we consider does not enforce labels in the large \( n \) limit. The question of how to modify the graph Laplacian in order to address this issue has been studied in [4]. Other ways to enforce labels in the limit are based on \( p \)-Laplacian regularization (see [3, 9, 23]).

An illustration of the setting considered in Theorem 1.6 is presented in Figure 4. There we show the regression errors when the loss function is quadratic with symmetric and asymmetric noise, in the set-up where we take \( 2q = n = 10000 \), and \( \beta = \varepsilon = n^{-1/5} \). While the errors are obviously larger than the fully-supervised case, the theory provided in Theorem 1.6 still provides a robust means for estimation.
We conclude this section by making a few remarks.

**Remark 1.7.** Our results can be generalized in a straightforward way to the case where the trend function \( \mu \) is smooth everywhere except on a regular \( m-1 \) dimensional discontinuity set \( D_\mu \). In such case we can obtain similar error bounds for the difference between the solution to the graph PDE and the solution to the continuum PDE. Such error bounds are uniform away from the discontinuity set \( D_\mu \). The reason for this is that most of our estimates are local, and even those that are not, only involve averaging at the length scale \( \varepsilon \).

**Remark 1.8.** As was mentioned in Section 1.3, although we state our main results assuming the data \( x_1, \ldots, x_n \) to be uniformly distributed in \( M \) and the \( \xi_i \) to be identically distributed, it is completely straightforward to extend them to a more general setting. In particular, suppose that \((x_1, y_1), \ldots, (x_q, y_q)\) are samples from \( \gamma \) and \( x_{q+1}, \ldots, x_n \) are samples from \( \rho \), where \( \gamma \) can be decomposed as in Section 1.3 with a smooth density \( \rho \) on \( M \) that is bounded away from zero, and the function \( p_x(s) \) (representing the conditionals of labels given feature vectors) is smooth in both \( x \) and \( s \). Then, Theorems 1.1, 1.3, 1.4 and 1.6 continue to be true if we now let \( v \) be the solution to the PDE

\[
\Delta_\rho v(x) + \rho(x) \int f(v(x) - \mu(x) - s)p_x(s)ds = 0, \quad x \in M
\]

where

\[
\Delta_\rho v := -\text{div}(\rho^2 \nabla v), \quad \mu(x) := \int \text{sp}_x(s)ds, \quad \forall x \in M
\]

and if we let \( \mu_f \) be the function that satisfies

\[
\int f(\mu_f(x) - \mu(x) - s)p_x(s)ds = 0
\]

for all \( x \in M \).

**Remark 1.9.** Similar results to the ones we obtain in this paper can be deduced if we change the definition of the graph Laplacian \( \Delta_\Gamma \). Take for example the random walk graph Laplacian, which is the graph Laplacian (as defined in (1.4)) for the graph with weights \( \tilde{w}_{ij} := w_{ij} / d_i \) where \( w_{ij} \) is as in (1.7) and

\[
d_i := \sum_j w_{ij}.
\]

Proposition 2.3 would need to be changed for an analogous estimate (see [22]) and 2.4 would not require the normalization by the \( g_i \) terms.

It is important to notice that our probabilistic estimates rely only on pointwise estimates for the approximation of \( \Delta_\mathcal{M} \) with the graph Laplacian! This contrasts with some of the related literature that we will review in section 1.3.

**Remark 1.10.** In this paper we have assumed the noise of labels \( y_i \) to be bounded. While our current proofs do not allow us directly to drop this assumption, they do serve as a basis for future improved results. In a similar way, it is likely that the assumptions we have made on the loss function \( F \) can be relaxed further.

**Remark 1.11.** One direction of research which is worth further exploration is to study how these ideas can be used to address similar questions to the ones explored in this paper in the context of graph models \( \Gamma \) different from geometric graphs. An example of such a model is the stochastic block model where points \( x_1, \ldots, x_n \) have no geometric meaning and weights are determined randomly based on a probabilistic rule. We note that large \( n \) behavior of the spectra of graph Laplacians for graphs generated from a stochastic block model have been studied in [20].

1.3. Related work.
1.3.1. Analysis of large sample limits of variational problems on graphs.

In the past few years there has been a rapid development of a body of work borrowing ideas from the calculus of variations and PDE theory to study large sample asymptotics of optimization problems on geometric graphs closely connected to machine learning tasks. These works include the study of consistency of Cheeger and ratio graph cuts on graphs [13], consistency of graph Laplacian spectrum [27], and supervised and semi-supervised learning [4, 8, 10, 11]. In the previously listed papers, the convergence of discrete solutions to continuum counterparts is studied in the $TLP$-metric space introduced in [12] and later further studied in [25]. The $TLP$ topology can be thought as $Lp$ convergence after suitable matching of the ground truth measure generating the data set $Mn$ and its empirical measure. The consistency of the optimization problems is studied using variational methods, and in particular the notion of $\Gamma$-convergence (a.k.a. epi-convergence). This is a powerful notion used to establish asymptotic convergence of minimizers of optimization problems (especially in highly non-convex settings), but it does not offer direct ways to obtain rates of convergence.

Among the papers previously listed, the paper [10] by the authors is closely connected to this paper. There we consider an optimization problem of the form:

$$\min_u \beta \frac{1}{n} \sum_{i,j} w_{ij} |u(x_i) - u(x_j)| + \frac{1}{n} \sum_i |u(x_i) - y_i|,$$

which is the $L1$ version of the problem we study here. As is well known in the image analysis community the total variation functional (the first term in the above objective function) enforces sparsity [5] and hence the above optimization problem seems more appropriate for the purposes of classification when binary labels are available (in our notation $y_i \in \{0, 1\}$). In that paper we study the regimes of $\beta := \beta_n$ (and how the graph connectivity $\varepsilon$ must scale with $n$) so as to recover in the large $n$ limit the Bayes classifier with probability one. No rates of convergence are provided.

The paper [23] is also related to our work. There, $p$-Laplacian regularization for semi-supervised learning is studied. The optimization problem takes the form:

$$\min_u \beta \frac{1}{n} \sum_{i,j} w_{ij} |u(x_i) - u(x_j)|^p$$

subject to

$$u(x_i) = y_i, \quad i = 1, \ldots, q,$$

where $q$ is held fixed as $n \to \infty$. The authors are able to show that when $p$ is greater than the intrinsic dimension $m$, solutions to the $p$-Laplacian regularization problem converge uniformly to a continuum counterpart, as $n \to \infty$, which depends on the labels $y_1, \ldots, y_q$ (in other words the labels are not forgotten in the limit). The uniform convergence is proved bootstrapping the $TLP$ convergence obtained through variational methods by controlling the “oscillations” of the discrete minimizers at a certain convenient length-scale.

The paper [3] is very closely related to [23] and to this paper. In particular, it obtains analogue results to [23], but using a PDE approach rather than a calculus of variations one. A maximum principle at the graph level analogous to the one that we use in this paper is a crucial tool that is latter used in conjunction with general and flexible results on consistency of viscosity solutions to elliptic PDEs (which in general do not produce rates of convergence).

In our work we take a PDE approach as in [3], and specifically use a maximum principle, to obtain rates for the uniform convergence of graph Laplacian regressors towards continuum counterparts. Whether similar results to the ones we present here can be obtained for regressors obtained using other regularization terms different from the graph Dirichlet energy is a question that we believe is worth exploring in the future.

1.3.2. Connections to k-NN regressors and other local averaging procedures.

We now draw a connection between the graph Laplacian regressor and the classical k-NN regressor. To do this, we will focus on solutions of Equation (1.3) when $F(t) = \frac{1}{2} t^2$. As we will see, graph Laplacian
Regularization with square error loss can be interpreted as a local averaging procedure, where the “locality” is defined in terms of the intrinsic geometry of the graph.

We will briefly recall the definition of the $k$-NN regressor: For a $k \in \mathbb{N}$, with $k < n$, we define $N_k(x_i)$ to be the set of $k$ nearest neighbors of $x_i$ in the data set $M_n$. The $k$-NN regressor is then defined as the average

$$u_k(x_i) := \frac{1}{|N_k(x_i)|} \sum_{x_j \in N_k(x_i)} y_j.$$ 

A further averaging over the value of $k$ produces a regressor of the form:

$$\bar{u}(x_i) := \sum_{k=1}^{n} g(k) u_k(x_i),$$

where $g$ is some probability distribution over $k$.

The use of local averages in non-parametric regression goes as far back as the work [28], $k$-NN regression being a special case of this general idea. The book [16] presents a very complete picture of many non-parametric regression techniques and dedicates a whole chapter (Chapter 6) to $k$-NN regression. Asymptotic properties of $k$-NN regressors have been a topic of investigation for several decades see [16] and the paper [7] where $L^1$ convergence towards a trend function is proved in a very general setting. More recent results like [17] prove uniform convergence towards a trend in a quite general setting where in particular the intrinsic dimension of the underlying ground-truth may vary. The paper [6] is closely related to [17], but studies the classification problem instead.

We now show now that when $F$ is quadratic, the graph Laplacian regressor obtained by solving (1.3) can be interpreted as a local averaging procedure, where now the averaging is done using the heat kernel on the graph; for simplicity we take $F(t) := \frac{1}{2}t^2$. Indeed, in this case the solution to the graph PDE (1.3) can be explicitly written as:

$$u = (\beta \Delta_{\Gamma} + I)^{-1} y.$$ 

The fact that $\Delta_{\Gamma}$ is self-adjoint and positive semi-definite allows us to use the spectral theorem and write:

$$u = (\beta \Delta_{\Gamma} + I)^{-1} y = \int_0^\infty e^{-t(\beta \Delta_{\Gamma} + I)} y dt.$$ 

Since $\Delta_{\Gamma}$ and $I$ commute we get:

$$u = \int_0^\infty e^{-t} \left( e^{-t\beta \Delta_{\Gamma}} y \right) dt = \int_0^\infty \frac{e^{-t/\beta}}{\beta} \left( e^{-t\Delta_{\Gamma}} y \right) dt$$

where in the final step we have made a change of variables. From this formula we can conclude a couple of things. First, we notice that the function $e^{-t\Delta_{\Gamma}} y$ is simply the solution to the heat equation (on the graph) with initial condition $y$ evaluated at time $t$ and can be written as

$$e^{-t\Delta_{\Gamma}} y(x_i) = \frac{1}{n} \sum_{j=1}^{n} K_t(x_j, x_i) y_j,$$

where $K_t(x_j, x_i)$ is the heat kernel on the graph (which is not symmetric in general!) at time $t$. One can then show that the function $K_t(\cdot, x_i)$ is non-negative and moreover that $\frac{1}{n} \sum_{j=1}^{n} K_t(x_j, x_i) = 1$, and hence it follows that the function $e^{-t\Delta_{\Gamma}} y$ is obtained by computing a local average (at length-scale $t$) of $y$ around each point $x_i$. On the other hand, since the function $\frac{1}{\beta} e^{-t/\beta}$ is a probability density on $(0, \infty)$, it follows that the graph Laplacian regressor $u$ is nothing but an average of averages of $y$ over all length-scales $t$. The weight given to each length-scale is naturally determined by the parameter $\beta$, and in particular if $\beta$ is small, more relevance is given to more local length-scales, whereas if $\beta$ is large, more relevance is given to global length scales.
1.4. Outline. The rest of the paper is organized as follows. In Section 2.1 we study the bias estimates from Theorem 1.3 and establish the regularity of solutions to (1.9). We also present a simple heat kernel approach to obtain bias estimates in the linear case \( f(t) = t \). In Section 2.2 we present our bias estimate Theorem 1.3. In Section 2.2 we use our maximum principle in conjunction with two technical lemmas (where our probabilistic estimates are presented) to prove Theorem 1.1. In Section 2.3 we present the proof of Theorem 1.6.

2. Proof of Main results

2.1. Bias estimates. Here we provide a brief proof of Theorem 1.3. The techniques used herein are quite standard in the PDE literature; we provide some of the details for convenience.

Proof of Theorem 1.3. First, we define

\[
Z(w, x) := \int_{\mathbb{R}} f(w - \mu(x) - s)p(s)\,ds.
\]

We note that the function \( Z \) is smooth in both \( w \) and \( x \), and is strictly increasing in \( w \). The existence and uniqueness of the solution to the PDE within the class of \( L^2 \) functions is guaranteed by the Browder-Minty theorem (see e.g. [19] Section 10.3). Furthermore, by noting that the problem (1.8) is coercive and convex, and that the minimizer must solve the Euler-Lagrange equation, we may deduce that the \((L^2)\) solution of (1.9) is the minimizer of (1.8). Using an energy comparison argument, one may conclude that

\[
\|v\|_\infty \leq \|\mu_f\|_\infty.
\]

Then, using a bootstrapping argument, one may apply standard regularity theory [14] to establish that \( v \) is smooth.

Next, in order to prove the estimate (1.11), we note that for any point where \( v \geq \mu_f \) we have

\[
\beta \Delta_M (v - \mu_f) = Z(u, x) - \beta \Delta_M \mu_f \leq -c_1 (v - \mu_f) - \beta \Delta_M \mu_f,
\]

where we have used (2.1) and the definition of \( c_1 \). Now on the set \( E = \{x : v - \mu_f > \frac{\beta |\Delta_M \mu_f|}{c_1}\} \) we have that

\[
\beta \Delta_M (v - \mu_f) \leq 0.
\]

This implies (by the classical maximum principle) that \( v - \mu_f \) attains its maximum on the boundary of \( E \), which then implies that \( E \) is empty. This provides the desired upper bound. The lower bound is analogous.

To then establish the bounds (1.12) we note that the bound (1.11) gives that \( |\Delta v| \leq C \), with \( C \) independent of \( \beta \). Schauder regularity theory (see e.g. Theorem 6.6 in [14]) then gives the desired \( C^2 \) bound. Taking the Laplacian of the PDE and again using Schauder theory gives the desired \( C^4 \) estimates. Finally, interpolation inequalities (see e.g. Lemma 6.32 in [14]) give the intermediate bounds, which concludes the proof.

We remind the reader here that convergence is towards \( \mu_f \), not \( \mu \). One can only guarantee convergence towards \( \mu \) if one makes more specific assumptions upon the label error distribution \( p \) or on the empirical risk function \( F \).

2.1.1. A heat kernel approach for the linear case. In this subsection we describe a different version of the previous bias estimates in the case where one considers \( f(t) = t \) (i.e. \( F = \frac{1}{2} t^2 \)). Here we are able to obtain bias estimates using the spectral theorem and the heat kernel, which permits a more qualitative description of the procedure. The theory described here is given as a further insight, and not as a separate result (as the general result in the previous section does apply here).

In this linear case, we may rewrite the Euler-Lagrange equation in the form

\[
v = (\beta \Delta_M + I)^{-1} \mu,
\]

which in turn can be written as:

\[
v(x) = \int_0^\infty (e^{-t(\beta \Delta_M + I)}) \mu(x)\,dt = \int_0^\infty e^{-t} (e^{-t\beta \Delta_M} \mu)(x)\,dt.
\]
Here we are using the spectral theorem for $\Delta_M$. It follows that

$$v(x) - \mu(x) = \int_0^\infty e^{-t} \left( \int_M K_t\beta(y, x)(\mu(y) - \mu(x))dy \right) dt,$$

where $K_t\beta$ is the heat kernel on $M$. In particular,

$$|v(x) - \mu(x)| \leq \int_0^\infty e^{-t} \left( \int_M K_t\beta(y, x)|\mu(y) - \mu(x)|dy \right) dt \leq \text{Lip}(\mu) \int_0^\infty e^{-t} \int_M K_t\beta(y, x)d_M(y, x)dydt \leq C\text{Lip}(\mu)\beta,$$

where the last inequality follows using properties of the heat kernel in $M$. More precisely using Gaussian upper bounds for the heat kernel on a smooth compact manifold (see, for example, Chapter 15 in [15]). The bottom line is that

$$\|v - \mu\|_{\infty} \leq C\text{Lip}(\mu)\beta.$$

We notice that these formula (2.2) actually indicates that in this case $\|v\|_{C^k} \leq C\|\mu\|_{C^k}$, where $C$ is independent of $\beta$. We expect that similar estimates could be proved in the non-linear case, but the crude bounds on higher norms in Theorem 1.3 were sufficient for our purposes.

2.2. Variance estimates. In order to show the “variance estimates” (Theorem 1.1) we make some computations based on standard concentration inequalities (see, e.g., [1]).

**Proposition 2.1** (Hoeffding and Bernstein inequalities). Suppose $U_1, \ldots, U_n$ are independent real valued random variables, with mean zero, and for which $|U_i| \leq M$ for all $i = 1, \ldots, n$.

Suppose that

$$\frac{1}{n} \sum_{i=1}^n \text{Var}(U_i) \leq \sigma^2,$$

for some $\sigma^2$. Then,

- **(Hoeffding)** For every $\delta > 0$

  $$\mathbb{P}\left( \left| \frac{1}{n} \sum_{i=1}^n U_i \right| > \delta \right) \leq 2 \exp\left( \frac{-2n\delta^2}{M^2} \right).$$

- **(Bernstein)** For every $\delta > 0$

  $$\mathbb{P}\left( \left| \frac{1}{n} \sum_{i=1}^n U_i \right| > \delta \right) \leq 2 \exp\left( \frac{-n\delta^2}{2\sigma^2 + 2M\delta/3} \right).$$

**Remark 2.2.** In most applications these inequalities are used to prove that the empirical average $\frac{1}{n} \sum_{i=1}^n U_i$ is small with high probability, so that in particular one is typically interested in choosing $\delta \ll 1$. When the estimate on the average of variances is not significantly better than $M^2$, Bernstein’s inequality does not produce any improvement over Hoeffding’s.

Our first estimates concern the pointwise convergence of $\Delta_F$ towards $\Delta_M$. Such estimates have been obtained in the literature before (see, for example, [2, 3]), but here we present them again for the convenience of the reader.

**Proposition 2.3.** (Pointwise consistency of graph Laplacian) Let $h \in C^3(M)$. Then, for every $\delta > 0$, with probability at least $1 - 2n\exp\left( -\frac{C(\|h\|_{C^3(M)}, \eta, M)^{1+(n\delta/2)+1}}{n^\delta}\right)$, we have

$$\max_{1 \leq i \leq n} |\Delta_F h(x_i) - \Delta_M h(x_i)| \leq \delta + C(m, \eta, \|h\|_{C^3})\varepsilon,$$

where the last constant depends at most linearly on $\|h\|_{C^3}$. 

Proof. Associated to the function $h$ we define a function

$$
\Delta_{\varepsilon} h(x) := \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{\mathcal{M}} \eta \left( \frac{|x - \tilde{x}|}{\varepsilon} \right) (h(x) - h(\tilde{x})) \, d\text{vol}_M(\tilde{x}), \quad x \in \mathcal{M}.
$$

This function can be interpreted as a non-local Laplacian of $h$.

Fix $i \in \{1, \ldots, n\}$ and denote by $U_1, \ldots, U_n$ the variables

$$
U_j := \frac{2}{\tau \eta \varepsilon^{m+2}} \eta \left( \frac{|x_i - x_j|}{\varepsilon} \right) (h(x_i) - h(x_j)).
$$

Notice that given $x_i$, we have

$$
E_{\tilde{x}_i}(U_j) = \Delta_{\varepsilon} h(x_i), \quad j \neq i,
$$

where $E_{\tilde{x}_i}$ stands for conditional expectation given $x_i$. Also,

$$
Var_{x_i}(U_j) \leq \frac{4}{\tau \eta \varepsilon^{m+2}} \|\eta\|_\infty \|\nabla h\|_\infty
$$

It is simple to see that for all $0 < \varepsilon < 1$ and all $x \in \mathcal{M}$ we have

$$
0 < C^{-1}_M \leq \frac{1}{\varepsilon^m} \int_{\mathcal{M}} \eta \left( \frac{|x - \tilde{x}|}{\varepsilon} \right) \, d\text{vol}_M(\tilde{x}),
$$

where $C_M$ is a positive constant. In particular it follows that

$$
\frac{1}{n} \sum_{j=1}^n Var_{x_i}(U_j) \leq \frac{1}{n \varepsilon^{m+2}} C_M \|\eta\|_\infty \|\nabla h\|_\infty^2
$$

We notice that neither $M$ nor $\sigma^2$ depend on $x_1, \ldots, x_n$, and that the $U_j - E_{x_i}(U_j)$ are independent random variables. We may now use Bernstein’s inequality (Proposition 2.1), along with the definition of $\Delta_{\Gamma} h(x_i)$ and Equations (2.4) and (2.5), to obtain

$$
P_{x_i}(\max_{i=1, \ldots, n} |\Delta_{\Gamma} h(x_i) - \Delta_{\varepsilon} h(x_i)| > \delta) \leq 2 \exp \left( -\frac{n \delta \varepsilon^{m+1}}{C(\|h\|_{C^1}, \eta, \mathcal{M})(1 + (n \delta \varepsilon)^{-1})} \right),
$$

and by the law of iterated probability get

$$
P(\max_{i=1, \ldots, n} |\Delta_{\Gamma} h(x_i) - \Delta_{\varepsilon} h(x_i)| > \delta) \leq 2 \exp \left( -\frac{n \delta \varepsilon^{m+1}}{C(\|h\|_{C^1}, \eta, \mathcal{M})(1 + (n \delta \varepsilon)^{-1})} \right).
$$

A simple union bound implies that

$$
P\left( \max_{i=1, \ldots, n} |\Delta_{\Gamma} h(x_i) - \Delta_{\varepsilon} h(x_i)| > \delta \right) \leq 2n \exp \left( -\frac{n \delta \varepsilon^{m+1}}{C(\|h\|_{C^1}, \eta, \mathcal{M})(1 + (n \delta \varepsilon)^{-1})} \right).
$$

Now we claim that for all $h \in C^3(\mathcal{M})$ and all $x \in \mathcal{M}$

$$
|\Delta_{\varepsilon} h(x) - \Delta_{h}(x)| \leq C_n \text{Lip}(\eta) \|h\|_{C^3} \varepsilon.
$$

We first replace $\Delta_{\varepsilon} h$ with a version of it that uses the geodesic distance on $\mathcal{M}$ rather than the Euclidean distance. More precisely, we set

$$
\tilde{\Delta}_{\varepsilon} h(x) := \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{\mathcal{M}} \eta \left( \frac{d_M(x, \tilde{x})}{\varepsilon} \right) (h(x) - h(\tilde{x})) \, d\text{Vol}(\tilde{x}),
$$

where $d_M(x, \tilde{x})$ is the geodesic distance between two points $x, \tilde{x}$ in $\mathcal{M}$. Now, as long as $|x - \tilde{x}| \leq c$ for some small enough $c$ (that only depends on $\mathcal{M}$) we have that

$$
|d_M(x, \tilde{x}) - |x - \tilde{x}| | \leq C(\mathcal{M}) |x - \tilde{x}|^3.
$$
From this and the Lipschitz continuity of \( \eta \) we can conclude that if \( |x - \tilde{x}| \leq 2\varepsilon \) then,
\[
\left| \eta\left( \frac{d_M(x, \tilde{x})}{\varepsilon} \right) - \eta\left( \frac{|x - \tilde{x}|}{\varepsilon} \right) \right| \leq C(M)\text{Lip}(\eta)\varepsilon^2.
\]
On the other hand, if \( 2\varepsilon < |x - \tilde{x}| \), we must also have \( d_M(x, \tilde{x}) > \varepsilon \). Therefore, in all cases we have
\[
\left| \eta\left( \frac{d_M(x, \tilde{x})}{\varepsilon} \right) - \eta\left( \frac{|x - \tilde{x}|}{\varepsilon} \right) \right| \leq C(M)\text{Lip}(\eta)\varepsilon^2 1_{B_M(2\varepsilon)}(\tilde{x}),
\]
from where it follows that for all \( x \in \mathcal{M} \),
\[
|\Delta x h(x) - \tilde{\Delta} x h(x)| \leq \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \left| \eta\left( \frac{|x - \tilde{x}|}{\varepsilon} \right) - \eta\left( \frac{d_M(x, \tilde{x})}{\varepsilon} \right) \right| |h(x) - h(\tilde{x})| d\nu_M(\tilde{x})
\]
\[
\leq C(M) \frac{\text{Lip}(\eta)}{\tau \eta} \|\nabla h\|_\infty \varepsilon.
\]

Let us now compare \( \tilde{\Delta} x h(x) \) with \( \Delta_M h(x) \). For that purpose we use the exponential map at the point \( x \),
\[
\exp_x : B_m(0, \varepsilon) \to B_M(0, \varepsilon)
\]
which takes tangent vectors \( v \) at \( x \) with norm less than \( \varepsilon \) into points \( \exp_x(v) \) in \( \mathcal{M} \) that are within geodesic distance \( \varepsilon \) of \( x \). Let \( H \) be the composition \( H := h \circ \exp_x(v) \), i.e. the function \( h \) written in normal coordinates around \( x \). The regularity of \( h \) and \( \mathcal{M} \) implies that \( H \) is also regular, and using a Taylor expansion around the origin we get
\[
H(v) = H(0) + \langle \nabla H(0), v \rangle + \frac{1}{2} \langle D^2 H(0) v, v \rangle + r(v),
\]
where the remainder \( r \) is a function that satisfies:
\[
|r(v)| \leq C \varepsilon^3, \quad \forall v \in B_m(0, \varepsilon).
\]
The constant \( C \) depends on \( \mathcal{M} \) and the third derivatives of \( h \) (and scales linearly in the third derivatives of \( h \)). In normal coordinates we can then write
\[
\tilde{\Delta} x h(x) = \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) \langle H(v) - H(0), J_x(v) \rangle dv
\]
\[
= \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) \langle \nabla H(0), v \rangle J_x(v) dv + \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) \langle D^2 H(0) v, v \rangle J_x(v) dv
\]
\[
+ \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) r(v) J_x(v) dv.
\]
We know that the Jacobian of the exponential map \( J_x \) satisfies
\[
J_x(v) = 1 + O(|v|^2),
\]
(see Section 2.2. in [2]) so we can actually write
\[
\tilde{\Delta} x h(x) = \frac{2}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) \langle \nabla H(0), v \rangle dv + \frac{1}{\tau \eta \varepsilon^{m+2}} \int_{B_m(0, \varepsilon)} \eta\left( \frac{|v|}{\varepsilon} \right) \langle D^2 H(0) v, v \rangle dv + O(\varepsilon),
\]
where the \( O \) term depends on a uniform bound on all derivatives of \( H \) up to order three and on the intrinsic dimension \( m \). We notice that the first term on the right hand side of the above expression drops due to the radial symmetry of the kernel, and also that the second term is equal to
\[
\text{trace}(D^2 H(0)) = \Delta H(0) = \Delta_M h(x).
\]
The bottom line is that, as anticipated in (2.7),
\[
|\Delta x h(x) - \Delta_M h(x)| \leq |\Delta x h(x) - \tilde{\Delta} x h(x)| + |\tilde{\Delta} x h(x) - \Delta_M h(x)| \leq C(\|h\|_{C^3, m, \eta}) \varepsilon.
\]
Combining (2.6) and (2.7) we deduce that with probability greater than 1 − 2n \exp \left(-\frac{n\delta \varepsilon^{m+1}}{C(\|h\|_{C1}, \eta, \mathcal{M})(1 + (n\delta \varepsilon)^{-1})}\right),
\max_{i=1,\ldots,n} |\Delta_{1} h(x_i) - \Delta_{\mathcal{M}} h(x_i)| \leq \delta + C(\|h\|_{C3}, m, \eta) \varepsilon.

\square

Our next result will allow us to show that the functions \(y^{-}\) and \(y^{+}\) mentioned in (1.10) and defined explicitly in (2.11), are uniformly small.

Lemma 2.4. Let \(h : \mathcal{M} \to \mathbb{R}\) be a smooth function. For each \(i = 1, \ldots, n\) let \(E_i\) be defined as

\[E_i := \sum_{j=1}^{n} \frac{\eta_{ij}}{g_j} \int_{\mathbb{R}} (f(h(x_j) - s) - f(h(x_j) - \xi_j)) p(s) ds,\]

where

\[\eta_{ij} := \frac{1}{n\varepsilon^m} \eta \left(\frac{|x_i - x_j|}{\varepsilon}\right), \quad \text{and} \quad g_i := \sum_{l=1}^{n} \eta_{il}.\]

Let \(\zeta > 0\). Then with probability greater than 1 − 2n \exp \left(-c n \varepsilon^{m} \zeta^{2}\right) − 2n \exp(-c n \varepsilon^{m}),
\[|E_i| \leq \zeta, \quad \forall i = 1, \ldots, n.\]

Proof. Fix \(i = 1, \ldots, n\) and let \(U_j\) be the random variables

\[U_j := \frac{n \eta_{ij}}{g_j} f(h(x_j) - \xi_j), \quad j = 1, \ldots, n.\]

Conditioned on \(x_1, \ldots, x_n\), the variables \(U_1, \ldots, U_n\) are independent and satisfy

\[|U_j| \leq \frac{1}{\varepsilon m} \|\eta\|_{\infty} \frac{M_{h,f}}{G_{\delta}},\]

where

\[M_{h,f} := \sup_{x \in \mathcal{M}} |f(h(x) \pm \sigma)|,\]

and where

\[G_{\delta} := \min_{j=1,\ldots,n} g_j.\]

Moreover,

\[\mathbb{E}_{\delta} \left(\frac{1}{n} \sum_{j=1}^{n} U_j\right) = \frac{\eta_{ij}}{g_j} \int_{\mathbb{R}} f(h(x_j) - s) p(s) ds,\]

and

\[\frac{1}{n} \sum_{j=1}^{n} \mathbb{V}ar_{\delta}(U_j) \leq \frac{M_{h,f}^2}{n \varepsilon^{2m} G_{\delta}^2} \sum_{j=1}^{n} \eta^2 \left(\frac{|x_i - x_j|}{\varepsilon}\right) = \frac{M_{h,f}^2 \|\eta\|_{\infty}}{\varepsilon m G_{\delta}^2} g_i \leq \frac{M_{h,f}^2 \|\eta\|_{\infty}}{\varepsilon m G_{\delta}^2} G_{\delta},\]

where in the above \(\mathbb{E}_{\delta}\) and \(\mathbb{V}ar_{\delta}\) represent conditional expectation and variance given \(x_1, \ldots, x_n\), and where

\[G_{\delta} := \max_{i=1,\ldots,n} g_i.\]

Bernstein’s inequality (Proposition 2.1) then implies that:

\[\mathbb{P}_{\delta}(|E_i| \geq \zeta) = \mathbb{P}_{\delta} \left(\frac{1}{n} \sum_{j=1}^{n} U_j - \frac{1}{n} \sum_{j=1}^{N} \mathbb{E}_{\delta}(U_j) \geq \zeta\right) \leq 2 \exp \left(-\frac{-n \zeta^2}{2\|\eta\|_{\infty} M_{h,f}^2 G_{\delta}^2 G_{\delta} + \frac{2\|\eta\|_{\infty} M_{h,f} \zeta}{3\varepsilon m G_{\delta}} G_{\delta}}\right).\]

Using a simple union bound we deduce that

\[\mathbb{P}_{\delta} \left(\max_{i=1,\ldots,n} |E_i| \geq \zeta\right) \leq 2n \exp \left(-\frac{-n \varepsilon^{m} \zeta^2}{2\|\eta\|_{\infty} M_{h,f} G_{\delta}^2 G_{\delta} + \frac{2\|\eta\|_{\infty} M_{h,f} \zeta}{3\varepsilon m G_{\delta}} G_{\delta}}\right),\]
and by the law of iterated probability we obtain

\[ P \left( \max_{i=1, \ldots, n} |E_i| \geq \zeta \right) \leq 2n \mathbb{E} \left( \exp \left( \frac{n\varepsilon_m \zeta^2}{2\|y\|_{\infty} M_{1/2} L \tilde{G}_x + \frac{2\|y\|_{\infty} M_{1/2} L \zeta}{3\kappa \varepsilon}} \right) \right). \]

Now, the only terms in the above expression that depend on \( x_1, \ldots, x_n \) are \( G_{\tilde{x}} \) and \( G_{\hat{x}} \). These however can be showed to be bounded below and above by positive constants with very high probability. Indeed, we first notice that for all \( \varepsilon < 1 \) and all \( x \in M \) we have

\[ 0 < C_M^{-1} \leq K_{\varepsilon}(x) := \frac{1}{\varepsilon^m} \int_M \eta \left( \frac{|x - \tilde{x}|}{\varepsilon} \right) \text{dvol}_M(\tilde{x}) \leq C_M, \]

for some positive constant \( C_M \). On the other hand, using Hoeffding’s inequality we get that

\[ P \left( \max_{i=1, \ldots, n} |g_i - K_{\varepsilon}(x_i)| \geq \frac{1}{2C_M} \right) \leq 2n \exp \left( -cn\varepsilon^m \right), \]

from where it follows that except on a set with probability less than \( 2n \exp(-cn\varepsilon^m) \), we have

\[ \frac{1}{2C_M} \leq G_{\tilde{x}} \leq \tilde{G}_{\tilde{x}} \leq 2C_M. \]

Therefore,

\[ P \left( \max_{i=1, \ldots, n} |E_i| \geq \zeta \right) \leq 2n \exp \left( -cn\varepsilon^m \zeta^2 \right) + 2n \exp(-cn\varepsilon^m). \]

\[ \square \]

We are ready to prove Theorem 1.1.

**Proof of Theorem 1.1.** Let us first introduce some notation. For a function \( g : M_n \to M \) we denote by \( g_i \) the value of the function at \( x_i \), i.e. \( g(x_i) \). Also, we will restrict the solution of (1.9) and its Laplacian \( \Delta_M v \) to the point cloud \( M_n \), so in particular we will treat \( v \) and \( \Delta_M v \) as functions defined on \( M_n \).

First, we notice that

\[ \beta \Delta_M v + \int_M f(v - \mu - s)p(s)ds = \beta(\Delta_M v - \Delta_M v), \]

at all points in \( M_n \). Let us denote by \( a : M_n \to \mathbb{R} \) the right hand side of the above expression (i.e. \( \beta \) times the difference between \( \Delta_M v \) and \( \Delta_M v \)). By Proposition 2.3 and Theorem 1.3 we know that with probability at least \( 1 - 2n \exp \left( -\frac{m\varepsilon^2}{C(\mu, \eta, M)(1 + n\varepsilon^{-1})} \right) =: 1 - p_{n, \delta} \) we have that

\[ \max_{i=1, \ldots, n} |a_i| \leq \beta(\delta + C\beta^{-1/2}\varepsilon). \]

Now, let \( w := u - v \). Then,

\[ -\beta \Delta_G w = -\beta \Delta_G u + \beta \Delta_G v \]

\[ = f(u - y) - \int_M f(v - \mu - s)p(s)ds + a \]

\[ = f(u - \mu - \xi) - \int_M f(v - \mu - s)p(s)ds + a \]

Let us define the functions \( y^\pm \) and \( y^- \) on \( M_n \) respectively by

\[ y^+_i := \frac{\varepsilon^2}{\beta g_i} \left( \int_M f(v_i - \mu_i - s)p(s)ds - f(v_i - \mu_i - \xi_i) \right) + \rho \]

\[ y^-_i := \frac{\varepsilon^2}{\beta g_i} \left( \int_M f(v_i - \mu_i - s)p(s)ds - f(v_i - \mu_i - \xi_i) \right) - \rho \]

(2.11)
where \( g \) is as defined in Lemma 2.4 and \( \rho \) is a constant that will be chosen later on. Indeed, we will show that with the appropriate choice of \( \rho \), the following holds at all point in \( \mathcal{M}_n \):

\[
y^- \leq w \leq y^+.
\]

We focus on showing \( w \leq y^+ \), the other inequality obtained in a completely analogous way. To see that \( w \leq y^+ \), we will actually show that for an appropriate (small) value of \( \rho \), the function

\[
z := w - y^+
\]

satisfies the inequality

\[
(\beta \Delta y^+)_i = \int \left[ f(v_i - \mu_i - s)p(s)ds - f(v_i - \mu_i - \xi_i) \right]
\]

from where it follows, thanks to the maximum principle (Proposition 1.2), that \( z \leq 0 \). Let us then focus on showing (2.12). First, a direct computation shows that

\[
(\beta \Delta y^+)_i = \int f(v_i - \mu_i - s)p(s)ds - f(v_i - \mu_i - \xi_i)
\]

where in the above we are using \( \eta_j \) as defined in Lemma 2.4. It follows that

\[
(-\beta \Delta y^+)_i = f(w_i - \mu_i - \xi_i) - f(v_i - \mu_i - \xi_i) - \sum_{j=1}^n \eta_j g_j \int (f(v_j - \mu_j - s) - f(v_j - \mu_j - \xi_j))p(s)ds + a_i
\]

Since \( v - \mu \) is a bounded function (in particular thanks to their regularity as it follows from Theorem 1.3 and by the assumptions on \( \mu \), Lemma 2.4 implies that, with probability at least \( 1 - 2n \exp(-cn \varepsilon^m) - 2n \exp(-cn \varepsilon^m) =: 1 - p_{n,\varepsilon} \) we have

\[
\sum_{j=1}^n \eta_j \int (f(v_j - \mu_j - s) - f(v_j - \mu_j - \xi_j))p(s)ds \leq \varepsilon, \quad \forall i = 1, \ldots, n.
\]

Hence, by using (2.9), with probability at least \( 1 - p_{n,\varepsilon} - p_{n,\xi} \), for all \( i \) we have:

\[
(-\beta \Delta y^+)_i \geq f(w_i + v_i - \mu_i - \xi_i) - f(v_i - \mu_i - \xi_i) - \xi - \beta(\delta + C \beta^{-1/2} \varepsilon),
\]

which can be rewritten as

\[
-\beta \Delta y^+ - (f(z + v - \mu - \xi) - f(v - \mu - \xi)) \geq f(w + v - \mu - \xi) - f(z + v - \mu - \xi) - \zeta - \beta(\delta + C \beta^{-1/2} \varepsilon).
\]

Now, notice that \( \rho \) can be chosen in such a way that

\[
y^+ \geq 0.
\]

Indeed, since we have assumed that the noise \( \xi \) is bounded, we can conclude that \( y^+ \geq -C_2^2 + \rho \) for some constant \( C_2 \), from where it follows that if \( \rho \) is chosen to be larger than \( C_2^2 \beta^{-1/2} \) we can conclude that \( y^+ \geq 0 \). In particular, for such choice of \( \rho \) we have \( w = z + y^+ \geq z \) and thus by the fundamental theorem of Calculus:

\[
f(w + v - \mu - \xi) - f(z + v - \mu - \xi) = \int_{s_1}^{s_2} f'(s)ds \geq c(s_2 - s_1) = cy^+,
\]

for some constant \( c > 0 \) (using the assumed strict monotonicity of \( f \)) and where

\[
s_2 := w + v - \mu - \xi, \quad s_1 := z + v - \mu - \xi.
\]
Plugging this back into (2.15) we deduce that (with probability at least 1 − \( p_{n,\delta} - p_{n,\zeta} \))
\[ -\beta \Delta_{f} z - (f(z + v - \mu - \xi) - f(v - \mu - \xi)) \geq \epsilon y^{+} - \zeta - \beta \delta - C\beta^{1/2} \epsilon \geq c \rho C_{2} \frac{\epsilon^{2}}{\beta} - \zeta - \beta \delta - C\beta^{1/2} \epsilon. \]
Hence if we let \( \rho \) be defined according to
\[ \rho := \frac{C_{2} \epsilon^{2}}{\beta} + \frac{\zeta + \beta \delta + C\beta^{1/2} \epsilon}{c}, \]
we conclude that, with probability at least 1 − \( p_{n,\delta} - p_{n,\zeta} \)
\[ -\Delta_{f} z - (f(z + v - \mu - \xi) - f(v - \mu - \xi)) \geq 0, \]
as we wanted to show. Repeating this argument for \( y^{-} \), and using a union bound completes the proof.

\[ \square \]

2.3. Semi-supervised learning. In this section we prove Theorem 1.6

Proof of Theorem 1.6. The proof of Theorem 1.6 is almost exactly as that of Theorem 1.4 with only a minor modification needed in the variance estimate (Theorem 1.1). To begin, for every fixed \( i \), we define
\[ \xi_{j} := \xi_{i}, \]
where \( i \) is the index of the point in \( x_{1}, \ldots, x_{q} \) that is closest to \( x_{j} \) among the points \( x_{1}, \ldots, x_{q} \). With this new interpretation of \( \xi_{1}, \ldots, \xi_{n} \), the functions \( y^{+} \) and \( y^{-} \) are defined exactly as in 2.11. Following the proof of Theorem 1.1, we notice that all computations therein continue to hold in this new setting and that the only point that needs to be adjusted is the probabilistic estimate for the absolute values of the terms
\[ E_{i} := \frac{1}{nc^{m}} \sum_{j=1}^{n} \eta_{ij} \int_{\mathbb{R}} (f(h_{j} - s) - f(h_{j} - \xi_{j}))p(s)ds, \quad i = 1, \ldots, n. \]
To control these terms, we notice that for any fixed \( i \), \( E_{i} \) can be written as
\[ E_{i} = \frac{1}{nc^{m}} \sum_{l=1}^{q} \sum_{x_{l} \in V_{l} \cap M_{n}} \eta_{ij} \int_{\mathbb{R}} (f(h_{j} - s) - f(h_{j} - \xi_{j}))p(s)ds \]
\[ = \frac{1}{nc^{m}} \sum_{l=1}^{q} \sum_{x_{l} \in V_{l} \cap M_{n}} \eta_{ij} \int_{\mathbb{R}} (f(h_{j} - s) - f(h_{j} - \xi_{i}))p(s)ds \]
\[ = \frac{1}{q} \sum_{l=1}^{q} \frac{1}{nc^{m}} \sum_{x_{l} \in V_{l} \cap M_{n}} \eta_{ij} \int_{\mathbb{R}} (f(h_{j} - s) - f(h_{j} - \xi_{i}))p(s)ds \]
where the sets \( V_{1}, \ldots, V_{q} \) are
\[ V_{l} := \{ x \in \mathbb{R}^{d} : |x_{l} - x| \leq |x_{j} - x|, \quad \forall j = 1, \ldots, q \}. \]
In other words the \( E_{i} \) are still defined as the average of independent random variables (conditioned on the \( x^{‘} \)s), but this time only \( q \) terms are involved. More precisely, we notice that for a fixed \( i \),
\[ E_{i} = \frac{1}{q} \sum_{l=1}^{q} U_{l}, \]
where \( U_{1}, \ldots, U_{q} \) are the random variables
\[ U_{l} := \frac{q}{nc^{m}} \sum_{x_{l} \in V_{l} \cap M_{n}} \eta_{ij} \int_{\mathbb{R}} (f(h_{j} - s) - f(h_{j} - \xi_{i}))p(s)ds, \quad l = 1, \ldots, q. \]
Conditioned on \(x_1, \ldots, x_n\), the variables \(U_1, \ldots, U_q\) are independent and satisfy:

\[
|U_l| \leq \frac{q}{n\varepsilon^m} M_{h,f} \sum_{x_j \in V_l} \frac{\eta_{lj}}{g_j} \leq \frac{q}{n\varepsilon^m} M_{h,f} \|\eta\|_\infty \#(V_l \cap \mathcal{M}_n \cap B(x_i, \varepsilon)) \leq \frac{q}{n\varepsilon^m} M_{h,f} \|\eta\|_\infty \frac{K_{\mathcal{G}}}{G_{\mathcal{G}}} =: M_{\mathcal{G}},
\]

where

\[
K_{\mathcal{G}} := \max_{i=1, \ldots, n} \max_{l=1, \ldots, q} \#(V_l \cap \mathcal{M}_n \cap B(x_i, \varepsilon)), \quad G_{\mathcal{G}} := \min_{j=1, \ldots, n} g_j.
\]

In addition,

\[
\mathbb{E}_{\mathcal{G}}(U_l) = 0, \quad \forall l = 1, \ldots, q
\]

and

\[
\frac{1}{q} \sum_{l=1}^{q} \text{Var}_{\mathcal{G}}(U_l) \leq \frac{qM_{h,f}^2}{n^2 \varepsilon^2 m G_{\mathcal{G}}^2} \left( \sum_{l=1}^{q} \sum_{x_j \in V_l} \frac{\eta_{lj}}{g_j} \right)^2 \leq \frac{qM_{h,f}^2 \|\eta\|_\infty^2}{n^2 \varepsilon^2 m G_{\mathcal{G}}^2} (\#(\{l : V_l \cap \mathcal{M}_n \cap B(x_i, \varepsilon) \neq \emptyset\}) \cdot (\max_{l=1, \ldots, q} \#(V_l \cap \mathcal{M}_n \cap B(x_i, \varepsilon)))^2 \leq \frac{qM_{h,f}^2 \|\eta\|_\infty^2}{n^2 \varepsilon^2 m G_{\mathcal{G}}^2} N_{\mathcal{G}} \cdot (K_{\mathcal{G}})^2 =: \hat{\sigma}_{\mathcal{G}}^2,
\]

where

\[
N_{\mathcal{G}} := \max_{i=1, \ldots, n} \#\{l : V_l \cap \mathcal{M}_n \cap B(x_i, \varepsilon) \neq \emptyset\}.
\]

As in the proof of Lemma 2.4, we use concentration inequalities to deduce that conditioned on \(x_1, \ldots, x_n\) we have

\[
\mathbb{P}_{\mathcal{G}}\left(\max_{i=1, \ldots, n} |E_i| \geq \delta\right) \leq 2n \exp\left(-\frac{q\delta^2}{2\hat{\sigma}_{\mathcal{G}}^2 + \frac{2}{3} M_{\mathcal{G}} \delta}\right),
\]

and by the law of total probability we deduce that

\[
\mathbb{P}\left(\max_{i=1, \ldots, n} |E_i| \geq \delta\right) \leq 2n \mathbb{E}\left(\exp\left(-\frac{q\delta^2}{2\hat{\sigma}_{\mathcal{G}}^2 + \frac{2}{3} M_{\mathcal{G}} \delta}\right)\right).
\]

It remains to find probabilistic upper bounds for \(\hat{\sigma}_{\mathcal{G}}^2\) and \(M_{\mathcal{G}}\). In turn, these will depend on upper bounds for \(N_{\mathcal{G}}\) and \(K_{\mathcal{G}}\) as well as a lower bound for \(G_{\mathcal{G}}\) (which was already obtained in (2.8)). In the Appendix we show that for every \(r > 0\) with \(r \leq \varepsilon\) we have

\[
\mathbb{P}(N_{\mathcal{G}} \leq Cqr^m, K_{\mathcal{G}} \leq Cnr^m) \geq 1 - \left( q \exp(-cq^m) \frac{8q + 2}{\gamma^m} \exp(-cq^m) + 2q \exp(-cnr^m) \right).
\]

These estimates are based on the standard concentration inequalities that we have been using in the other probabilistic estimates. Now, with (2.18) at hand, we may combine with (2.8) to conclude that

\[
\mathbb{P}(N_{\mathcal{G}} \leq Cqr^m, K_{\mathcal{G}} \leq Cnr^m, G_{\mathcal{G}} \geq C) \geq 1 - \left( q \exp(-cq^m) \frac{8q + 2}{\gamma^m} \exp(-cq^m) + 2q \exp(-cnr^m) + 2n \exp(-cn^m) \right).
\]
Therefore,

$$\mathbb{P}\left( \max_{i=1,...,n} |E_i| \geq \delta \right) \leq 2n \mathbb{E}\left( \exp\left( \frac{-q\delta^2}{2\hat{\delta}^2 + \frac{2}{3}M\delta} \right) \right)$$

$$\leq 2n \exp\left( -\frac{cq\varepsilon^m\delta^2}{q^2r^{2m}(r/\varepsilon)^m + qr^m\delta} \right)$$

(2.19)

$$+ \mathbb{P}\left( N_\delta \geq Cqr^m \bigcup K_\delta \geq Cnr^m \bigcup G_\delta \leq C \right)$$

$$\leq 2n \exp\left( -\frac{cq\varepsilon^m\delta^2}{q^2r^{2m} + qr^m\delta} \right)$$

$$+ \mathbb{P}\left( N_\delta \geq Cqr^m \bigcup K_\delta \geq Cnr^m \bigcup G_\delta \leq C \right).$$

Picking $r = \left( \frac{A\log(q)}{q} \right)^{1/m}$ for large enough $A$, we can guarantee that the second term on the right hand side of the above expression converges to zero (and moreover is summable). Also,

$$\mathbb{P}\left( \max_{i=1,...,n} |E_i| \geq \delta \right) \leq 2n \exp\left( -\frac{cq\varepsilon^m\delta^2}{A^2\log^2(q)} \right) + q \exp(-cq\varepsilon^m)$$

$$+ C \frac{q^2-cA}{A\log(q)} + 2q \exp\left( -\frac{cmq}{A\log(q)} \right) + 2n \exp(-cn\varepsilon^m).$$

\[\square\]

2.4. **Out of sample extension convergence.** With the $L^\infty$ bounds between $u$ and $\mu_f$ in hand (for both the fully-supervised and semi-supervised settings that we have considered), we can now construct a simple out of sample extension $u : \mathbb{R}^d \to \mathbb{R}$ of $u$ that is guaranteed to be uniformly close to the modified trend $\mu_f$ when restricted to $\mathcal{M}$. The out-of-sample extension can be used for prediction.

For an arbitrary $x \in \mathbb{R}^d$ we define the 1-NN extension of $u$ to be

$$u(x) := \sum_{i=1}^n u_i \mathbf{1}_{V_i}(x),$$

where the $\{V_i\}_{i \in \mathbb{N}}$ is the Voronoi tessellation in $\mathbb{R}^d$ induced by $\mathcal{M}_n$, that is,

$$V_i := \{x \in \mathbb{R}^d : |x - x_i| \leq |x - x_j|, \quad \forall j = 1, \ldots, n\}.$$

We use the above definition for vectors $x$ that only belong to one of the Voronoi cells. If $x$ belongs to the interface of more than one Voronoi cell, we define $u$ as the average of the $u_i$ associated to those cells $x$ belongs to.

To see that such extension is uniformly close to $\mu_f$, take, for simplicity, a vector $x \in \mathcal{M}$ which belongs only to the cell $V_i$. Then, the triangle inequality implies that we can pick $r > 0$ such that with very high probability,

$$|u(x) - \mu_f(x)| \leq |u_i - \mu_f(x_i)| + |\mu_f(x_i) - \mu_f(x)|$$

$$\leq \sup_{j=1,\ldots,n} |u_j - \mu_f(x_j)| + Lip(\mu_f) |x - x_i|$$

$$\leq \sup_{j=1,\ldots,n} |u_j - \mu_f(x_j)| + Lip(\mu_f) diam_\mathcal{M}(V_i)$$

$$\leq \sup_{j=1,\ldots,n} |u_j - \mu_f(x_j)| + CLip(\mu)r,$$

where in the last inequality we have used the estimates in the Appendix (specifically (A.2)). The term $\sup_{j=1,\ldots,n} |u_j - \mu_f(x_j)|$ is controlled in Theorem 1.6 or Theorem 1.4 (depending on whether we are in the semi-supervised or in the fully supervised settings).
3. Conclusions

In this paper we have used ideas from PDE theory, and specifically a maximum principle argument, to establish a convergence rate of graph Laplacian regressors on random geometric graphs. We believe that the ideas presented in this work are amenable to be used in other classification/regression problems on graphs in the geometric graph setup as well as for other probabilistic models relevant to machine learning like the stochastic block model.

Our error estimates are explicitly written in terms of the number of data points $n$, the number of labeled data $q$, the parameter $\beta$ controlling the strength of regularization, and the connectivity parameter $\epsilon$. The variance estimate essentially splits into two terms, one due to the error of approximation of geometry of the feature vectors $x_i$ (the graph Laplacian approximation of the true Laplacian) and another term that is linked directly to the observed labels $y_i$. The interplay between geometry and observed labels and how they can be used to reinforce the overall learning is an important and interesting topic to be explored in the future.

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Appendix A. Proof of 2.18

In what follows it will be convenient to let $M_q$ be the set of the first $q$ data points

$$M_q := \{x_1, \ldots, x_q\}.$$

Fix $r > 0$ small enough, and in particular smaller than $\varepsilon$.

Our first claim is that

(A.1) \[ P(\text{diam}_{M}(V_l) \leq cr, \quad \forall l = 1, \ldots, q) \geq 1 - 2 \frac{1}{\rho m} \exp(-cqr^m), \]

where $\text{diam}_{M}(V_l)$ is the diameter of the set $V_l$ (as defined in (2.17)). By a standard localization argument, in order to prove this inequality it actually suffices to prove it for the case where the points $M_q = \{x_1, \ldots, x_q\}$ are i.i.d. samples from the uniform distribution on $[0, 1]^m$. We consider a tiling of $[0, 1)^m$ into boxes of the form

$$Q = [a_1 r, b_1 r) \times \cdots \times [a_m r, b_m r),$$

where for every $j = 1, \ldots, m$, $a_j \in \{0, \ldots, \lfloor \frac{1}{r} \rfloor - 1\}$ and $b_j = a_j + 1$ if $a_j < \lfloor \frac{1}{r} \rfloor - 1$, and $b_j = \frac{1}{r}$ if $a_j = \lfloor \frac{1}{r} \rfloor - 1$.

Following Bernstein’s inequality we deduce that for every such $Q$

$$P\left(\left|\frac{\#M_q \cap Q}{q} - \text{vol}(Q)\right| > \text{vol}(Q)\right) \leq 2 \exp\left(\frac{-q\text{vol}(Q)^2}{2q\text{vol}(Q) + 2\text{vol}(Q)/3}\right) \leq 2 \exp(-cq r^m).$$

We notice that the event:

$$\left|\frac{\#M_q \cap Q}{q} - \text{vol}(Q)\right| > \text{vol}(Q)$$

is contained in the event

$$\#M_q \cap Q \geq 1,$$

and so we conclude that

$$P\left(\#M_q \cap Q \geq 1\right) \leq 1 - 2 \exp(-cq r^m).$$

Taking a union bound over all boxes $Q$ in the tiling we deduce that

$$P\left(\#M_q \cap Q \geq 1, \quad \forall Q\right) \geq 1 - \frac{2}{\rho m} \exp(-cq r^m).$$

On the other hand, notice that in the event $\#M_q \cap Q \geq 1$ for all $Q$, we also have

$$\text{diam}(V_l) \leq Cr, \quad \forall l = 1, \ldots, q.$$
for some large enough $C$ of order one. This is because a point $x \in V_l$ cannot be at distance higher than $Cr$ for otherwise one would be able to find a point in $M_q$ closer to $x$ than $x_l$ (violating the definition of the Voronoi cells). From this fact, we conclude that

\[(A.2) \quad P(diam(V_l) \leq Cr, \quad \forall l = 1, \ldots, q) \geq 1 - \frac{2}{r^m} \exp(-cqr^m),\]

which was our claim (A.1).

Having established (A.1), we notice that in the event

\[diam_M(V_l) \leq Cr\]

we have

\[vol_M(V_l) \leq C_diam(V_l)^m \leq Cr^m, \quad \forall l = 1, \ldots, q.\]

Now, notice that $\#V_l \cap M_n - 1 = \#V_l \cap (M_n \setminus M_q)$, and that the points $M_n \setminus M_q$ are independent from $M_q$. Bernstein’s inequality implies that

\[
P_{M_q} \left( \left| \frac{\#V_l \cap M_n - 1}{n - q} - vol_M(V_l) \right| \geq Cr^m \right) \leq 2 \exp \left( -\frac{(n - q)Cr^{2m}}{2\text{vol}_M(Q) + Cr^m} \right), \quad \forall l = 1, \ldots, q,
\]

where we use $P_{M_q}$ to represent conditional probability given $M_q$. By the law of total probability, (A.1), and a union bound we see that

\[
P \left( \left| \frac{\#V_l \cap M_n - 1}{n - q} - vol_M(V_l) \right| \geq Cr^m, \quad \forall l \right) \leq 2 \sum_l \mathbb{E} \left( \exp \left( -\frac{(n - q)Cr^{2m}}{2\text{vol}_M(Q) + Cr^m} \right) \right) \leq 2q \exp(-c(n - q)r^m) + \frac{4q}{r^m} \exp(-cqr^m).
\]

In particular,

\[
P \left( \frac{\#V_l \cap M_n - 1}{n - q} \geq Cr^m + vol_M(V_l), \quad \forall l \right) \leq 2q \exp(-c(n - q)r^m) + \frac{4q}{r^m} \exp(-cqr^m).
\]

Using again (A.1) we see that

\[
P \left( \frac{\#V_l \cap M_n - 1}{n - q} \geq 2Cr^m, \quad \forall l \right) \leq 2q \exp(-c(n - q)r^m) + \frac{4q + 2}{r^m} \exp(-cqr^m).
\]

Finally, we can use the definition of $K_{x_l}$ and notice that

\[K_{x_l} \leq \max_{l=1, \ldots, q} \#V_l \cap M_n,
\]

and so

\[
P(K_{x_l} \leq Cnr^m) \geq P(K_{x_l} \leq (n - q)Cr^m + 1) \geq 1 - \left( 2q \exp(-c(n - q)r^m) + \frac{4q + 2}{r^m} \exp(-cqr^m) \right) \geq 1 - \left( 2q \exp(-cnr^m) + \frac{4q + 2}{r^m} \exp(-cqr^m) \right),
\]

where we have used the assumption that $q \leq cn$ for some $c < 1$ and $nr^m \geq 1$.

We now focus on establishing a probabilistic estimate for $N_{x_l}$. We start by noticing that in the event $diam(V_l) \leq Cr$ for all $l$, we have

\[N_{x_l} \leq \max_{s=1, \ldots, q} \max_{l=1, \ldots, q} \#(M_q \cap B(x_s, \varepsilon + 2Cr)).\]

This last inequality follows from the fact that if $V_l \cap B(x_i, \varepsilon) \neq \emptyset$ for some $i = 1, \ldots, n$ and $l = 1, \ldots, q$, then we can let $s$ be the index of the Voronoi cell that $x_i$ belongs to and notice that

\[d_M(x_l, x_s) \leq d_M(x_l, x_i) + d(x_i, x_s) \leq \varepsilon + 2diam_M(V_l).
\]

Using the same concentration bounds as earlier we can show that

\[
P(\#B(x_l, r) \cap M_q \leq Cq(\varepsilon + r)^m) \geq 1 - \left( q \exp(-cq(\varepsilon + r)^m) + \frac{2q}{r^m} \exp(-cqr^m) \right).
\]
From this we conclude (also using the fact that we had taken $r \leq \epsilon$) that

$$P(N_{\vec{x}} \leq Cqr^m) \geq P(N_{\vec{x}} \leq Cq(\epsilon + r)^m) \geq 1 - \left( q \exp(-cq(\epsilon + r)^m) + \frac{4q}{r^m} \exp(-cqr^m) \right)$$

$$\geq 1 - \left( q \exp(-cqr^m) + \frac{4q}{r^m} \exp(-cqr^m) \right).$$

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