Notes for Week 4/3/20 - 4/9/20

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April 8, 2020

Suppose we observe data $(X_1, Y_1), \ldots, (X_n, Y_n)$ according to the following random design regression model. The design points $X_1, \ldots, X_n \in \mathcal{X}$ are independently sampled from a distribution P, and the responses

$$Y_i = f_0(X_i) + \varepsilon_i$$

where $f_0: \mathcal{X} \to \mathbb{R}$ is the unknown regression function and ε_i are independent N(0,1) noise samples. Our goal is to test

$$\mathbf{H}_0: f_0 = 0, \ \mathbf{H}_a: f_0 \neq 0.$$

Our test statistic $T = \|\widehat{f}\|_n^2$ will be a plug-in estimator of the L_2 -norm of f_0 . The estimator \widehat{f} of the function f_0 will be a truncated-series estimator, using eigenvectors of a graph Laplacian. We now define the graph $\overline{G}_{n,r}$ we will build over the design points $\mathbf{X} = X_1, \ldots, X_n$, which we term the histogram lattice.

Histogram Lattice. Let 0 < r < 1, and let M = 1/r. Let

$$Z = \left\{ \frac{1}{M} (2m_1 - 1, \dots, 2m_d - 1) : m \in [M]^d \right\}$$

be a set of evenly spaced grid points. (We will always assume M is an integer, merely to simplify some notational and definitional details.) A natural graph associated with Z is the lattice

$$\bar{G} = (Z, \bar{E}), (z, z') \in \bar{E} \text{ if } ||z - z'||_2 = r$$

Let $\Pi:[0,1]^d\to Z$ map points $x\in[0,1]^d$ to the nearest grid points $z\in Z,$

$$\Pi(x) := \underset{z \in Z}{\operatorname{argmin}} \ \|z - x\|_2$$

The histogram lattice $\bar{G}_{n,r} = (\mathbf{X}, \bar{E}_{n,r})$ is a product graph induced by \bar{G} and the mapping Π , with edges

$$(X_i, X_j) \in \bar{E}_{n,r} \text{ if } \Big(\Pi(X_i), \Pi(X_j)\Big) \in \bar{E}.$$

The matrix $\bar{L}_{n,r}$ is the graph Laplacian of $\bar{G}_{n,r}$ and $(\lambda_1, v_1), \ldots, (\lambda_n, v_n)$ are the eigenvector/eigenvalue pairs of $\bar{L}_{n,r}$, defined by the equation

$$\bar{L}_{n,r}v_k = \lambda_k v_k, \quad ||v_k||_n^2 = 1.$$

For a positive integer κ , the Laplacian eigenmaps estimator \hat{f}_{LE} is defined as

$$\widehat{f}_{LE} := \sum_{k=1}^{\kappa} \langle Y, v_k \rangle_n v_k.$$

and the resulting test statistic is thus

$$\widehat{T}_{LE} = \sum_{k=1}^{\kappa} (\langle Y, v_k \rangle_n)^2.$$

1 Approximation Error

We make some assumptions on the function f_0 and the distribution P.

- (A1) $f_0 \in C^s(\mathcal{X}; B)$ for some s > 0. If s > 1, then f is also compactly supported on a strict subset of \mathcal{X} .
- (A2) P admits a density p with respect to the Lebesgue measure on \mathbb{R}^d . The density $p \in C(\mathcal{X}; p_{\text{max}})$, for some k > 0.

Theorem 1. Suppose assumptions (A1) and (A2) are satisfied for some $s \ge 1$, and k = s - 1. Then, there exists a constant c such that

$$\sum_{k=1}^{\kappa} (\langle v_k, f_0 \rangle_n)^2 \ge c \cdot ||f_0||_2^2 - \kappa^{-2/d}$$

2 Proof of Theorem 1

Let $\bar{f}_0: \mathbf{X} \to \mathbb{R}$ be the histogram estimate of f_0 , defined as

$$\bar{f}_0(X) = \frac{1}{|Q(\Pi(X))|} \sum_{i=1}^n f_0(X_i) \cdot \mathbf{1} \Big\{ \pi(X_i) = \pi(X) \Big\}$$

We shall proceed according to the following steps.

1. Under the assumption (A2), for any $(\log(n)/n)^{1/d} \le r$, there exist constants c and C such that

$$c \cdot \min \left\{ nr^{d+2} \kappa^{2/d}, \deg_{\min}(\bar{G}_{n,r}) \right\} \le \lambda_{\kappa}(\bar{G}_{n,r}) \le C \cdot nr^{d+2} \kappa^{2/d}$$
(1)

and

$$c \cdot nr^d \le \deg_{\min}(\bar{G}_{n,r}) \le C \cdot nr^d$$
 (2)

with probability at least 1 - (????). Supposing (1) and (2) hold, and additionally $r < \kappa^{-1/d}$, then some straightforward algebra implies

$$cnr^{d+2}\kappa^{2/d} \le \lambda_{\kappa}(\bar{G}_{n,r}) \le \deg_{\min}(\bar{G}_{n,r}).$$

2. **Deterministic bounds:** Specifically as a consequence of the upper bound $\lambda_k(\bar{G}_{n,r}) \geq \deg_{\min}(\bar{G}_{n,r})$, we have that

$$\sum_{k=1}^{\kappa} (\langle v_k, f_0 \rangle_n)^2 = \sum_{k=1}^{\kappa} (\langle v_k, \bar{f}_0 \rangle_n)^2$$
(3)

For any $f \in \mathbb{R}^n$, we have

$$||f||_n^2 - \frac{f^T \bar{L}_{n,r}^s f}{n \lambda_\kappa(\bar{G}_{n,r})} \tag{4}$$

Neither the equality nor the inequality follow from probabilistic reasoning (except through the reasoning used to establish $\lambda_k(\bar{G}_{n,r}) \ge \deg_{\min}(\bar{G}_{n,r})$). The equality follows from the product graph structure of $\bar{G}_{n,r}$. The inequality is a standard inequality used in the analysis of truncated-series estimators, and would hold for any graph G on the vertices \mathbf{X} .

3. Under the assumptions (A1) and (A2), the graph Sobolev seminorm is upper bounded

$$\bar{f}_0^T \bar{L}_{n,r}^s \bar{f}_0 \le n^{s+1} r^{s(d+2)} B^2$$

with probability at least $1 - C_1 r^{-d} \exp\{-c_2 n r^d\}$.

4. The empirical norm of the histogram estimate \bar{f}_0 is lower bounded

$$\|\bar{f}_0\|_n^2 \ge c \|f_0\|_{L_2}^2$$

with probability at least 1 - ???.

2.1 Step 1: Bounds on graph eigenvalues

2.2 Step 2: Deterministic bounds

2.2.1 Proof of (3).

The graph $\bar{G}_{n,r}$ is a certain type of product graph, which we term the (Alden product graph). We shall show that all product graphs of this type satisfy an equality similar to (3).

(Alden product graph). Let $G = ([\mathcal{M}], E)$ be a graph on $\mathcal{M} \geq 1$ vertices, and let $n_1, \ldots, n_{\mathcal{M}}$ each be positive integers; let $N = \sum_{i=1}^{\mathcal{M}} n_i$. The (Alden product) graph $G^{\square}(G; n_1, \ldots, n_{\mathcal{M}})$ is defined as

$$G^{\square}(G; n_1, \dots, n_{\mathcal{M}}) = \left(\bigcup_{m=1}^{\mathcal{M}} \bigcup_{i=1}^{n_m} (m, i), \quad E^{\square}\right), \quad \text{where } \left((\ell, i), (m, j)\right) \in E^{\square} \text{ if } (\ell, m) \in E.$$

We will simply write G^{\square} when it is clear from context what G and $n_1, \ldots, n_{\mathcal{M}}$ are. Lemma 1 characterizes some of the eigenvectors of G^{\square} .

Lemma 1. For any $m \in \mathcal{M}$, and any $i \neq j \in [n_m]$, the vector

$$g[(m',k)] = \mathbf{1}\{(m',k) = (m,i)\} - \mathbf{1}\{(m',k) = (m,j)\}$$
 (5)

is an eigenvector of G^{\square} , with eigenvalue $\deg((m,i); G^{\square})$.

Proof of Lemma 1. content...

We can see from Lemma 1 that any eigenvector g of G^{\square} which does not satisfy (5) must instead be piecewise constant, i.e. g[(m,i)] = g[(m,j)] for all $m \in [\mathcal{M}]$ and $i,j \in [n_m]$. For any such eigenvector, and for any $f: \bigcup_{m=1}^{\mathcal{M}} \bigcup_{i=1}^{n_m} (m,i) \to \mathbb{R}$, we have that

$$\sum_{m=1}^{\mathcal{M}} \sum_{i=1}^{n_m} f\big[(m,i)\big] g\big[(m,i)\big] = \sum_{m=1}^{\mathcal{M}} \sum_{i=1}^{n_m} \bar{f}\big[(m,i)\big] g\big[(m,i)\big]$$

for $\bar{f}[(m,i)] = (n_m)^{-1} \sum_{i=1}^{n_m} f[(m,i)]$. Corollary 1 follows immediately from this reasoning.

Corollary 1. Let k be an integer such that $\lambda_k(G^{\boxdot}) < \deg((m,i); G^{\boxdot})$. Then the eigenvectors $v_1(G^{\boxdot}), \ldots, v_k(G^{\boxdot})$ are all piecewise constant. As a result, for any function f,

$$\sum_{k=1}^{\kappa} \left(\sum_{m=1}^{\mathcal{M}} \sum_{i=1}^{n_m} f\left[(m,i)\right] v_k\left[(m,i)\right] \right)^2 = \sum_{k=1}^{\kappa} \left(\sum_{m=1}^{\mathcal{M}} \sum_{i=1}^{n_m} \bar{f}\left[(m,i)\right] v_k\left[(m,i)\right] \right)^2$$

We obtain the equality (3) by applying Corollary 1 to the graph $G_{n,r}$.

2.3 Step 3: Upper bound on the graph Sobolev semi-norm

2.4 Step 4: Lower bound on the empirical norm of the histogram estimate