

Notes for Week of 1/9/20 - 1/16/20

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Let $X = \{x_1, \dots, x_n\}$ be a sample drawn i.i.d. from a distribution P on \mathbb{R}^d , with density p . For a radius $r > 0$, we define $G_{n,r} = (V, E)$ to be the r -neighborhood graph of X , an unweighted, undirected graph with vertices $V = X$, and an edge $(x_i, x_j) \in E$ if and only if $K_r(x_i, x_j) = \|x_i - x_j\| \leq r$, where $\|\cdot\|$ is the Euclidean norm. We denote by $A \in \mathbb{R}^{n \times n}$ the adjacency matrix, with entries $A_{uv} = 1$ if $(u, v) \in E$ and 0 otherwise. We also denote by D the diagonal degree matrix, with entries $D_{uu} := \sum_{v \in V} A_{uv}$. The graph Laplacian is $L = D - A$, and we write its spectral decomposition as $L = VSV^T$.

Suppose in addition to the random design points $X = \{x_1, \dots, x_n\} \sim P$, we observe responses

$$y_i = f(x_i) + \varepsilon_i, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad (1)$$

To test whether $f = f_0$, we propose the following *eigenvector projection* test statistic:

$$T_{\text{spec}} := \frac{1}{n} \sum_{k=0}^{\kappa} \left(\sum_{i=1}^n v_{k,i} y_i \right)^2 \quad (2)$$

where v_k is the k th eigenvector of L (ordered according to eigenvalues $s_1 \leq s_2 \leq \dots \leq s_n$).

The eigenvector projection test is minimax optimal over the balls in higher order Holder spaces $C_d^s(\mathcal{X}; L)$.

Theorem 1. *Let $b \geq 1$ be a fixed constant, and let d and s be positive integers such that $d < 4s$. Suppose that P is an absolutely continuous probability measure over $\mathcal{X} = [0, 1]^d$ with density function $p \in C^{s-1}(\mathcal{X}; R)$ bounded above and below by constants, i.e*

$$0 < p_{\min} < p(x) < p_{\max} < \infty, \quad \text{for all } x \in \mathcal{X}.$$

Then the following statement holds: if the test $\phi_{\text{spec}} = \mathbf{1}\{T_{\text{spec}} \geq \tau\}$ is performed with parameter choices

$$n^{-1/(2(s-1)+d)} \leq r(n) \leq n^{-4/((4s+d)(2+d))}, \quad \kappa = n^{2d/(4s+d)}, \quad \tau = \frac{\kappa}{n} + b\sqrt{\frac{2\kappa}{n^2}}$$

then there exists constants c_1, c_2 which may depend on d, R , and s but are independent of the sample size n such that for every $\epsilon \geq 0$ satisfying

$$\epsilon^2 \geq c_1 \cdot b^2 \cdot n^{-4s/(4s+d)} \quad (3)$$

the worst-case risk is upper bounded

$$\mathcal{R}_\epsilon(\phi_{\text{spec}}; C_d^s(\mathcal{X}; R)) \leq \frac{c_2}{b}. \quad (4)$$

1 Proof

Let $G = (V, E)$ be a graph over vertices $V = \{v_1, \dots, v_n\}$, and let $\beta = (\beta_1, \dots, \beta_n) \in \mathbb{R}^n$ be a signal over the vertices V . We observe responses $Y = (y_1, \dots, y_n)$ according to the model

$$y_i = \beta_i + \varepsilon_i, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$$

Letting $L = VSV^T$ be the spectral decomposition of the Laplacian L of G , our graph spectral test statistic is

$$T_{\text{spec}} = \frac{1}{n} \sum_{k=1}^{\kappa} \left(\sum_{i=1}^n v_i y_i \right)^2$$

where κ is a tuning parameter. The resulting test we will use is

$$\phi_{\text{spec}} = \mathbf{1}\{T_{\text{spec}} \geq \frac{\kappa}{n} + t(b)\}, \quad \text{where } t(b) = b\sqrt{\frac{2\kappa}{n^2}} \text{ for } b \geq 1.$$

Let $S_s(\beta; G)$ be a measure of smoothness the signal β displays over the graph G , given by

$$S_s(\beta; G) := \beta^T L^s \beta$$

In Lemma 1, we upper bound the Type I and Type II error of the test ϕ_{spec} . Our bound on the Type II error will be stated as a function of $S_2(\beta; G)$ as well as the κ th eigenvalue s_κ .

Lemma 1. *Let $1 \leq \kappa \leq n$ be an integer.*

1. **Type I error:** *Under the null hypothesis $\beta = \beta_0 = 0$, the Type I error of ϕ_{spec} is upper bounded*

$$\mathbb{E}_{\beta_0}(\phi_{\text{spec}}) \leq \frac{1}{b^2}. \tag{5}$$

2. **Type II error:** *For any b and β such that*

$$\frac{1}{n} \sum_{i=1}^n \beta_i^2 \geq 2b\sqrt{\frac{2\kappa}{n^2}} + \frac{S_s(\beta; G)}{ns_\kappa} \tag{6}$$

the Type II error of ϕ_{spec} is upper bounded,

$$\mathbb{E}_\beta(1 - \phi_{\text{spec}}) \leq \frac{3}{b}. \tag{7}$$

To prove Lemma 1 we will first compute (bounds on) the expectation and variance of the test statistic T_{spec} , and then use Chebyshev's inequality to show (5) and (7).

Mean of T_{spec} : Using the notation $\langle v, w \rangle = \sum_{i=1}^n v_i w_i$, we have

$$\begin{aligned} \mathbb{E}(T_{\text{spec}}) &= \frac{1}{n} \left(\sum_{k=1}^{\kappa} \langle \beta, v_k \rangle^2 + \mathbb{E}(\langle \varepsilon, v_k \rangle^2 + 2\langle \varepsilon, v_k \rangle \langle \beta, v_k \rangle) \right) \\ &= \frac{\kappa}{n} + \frac{1}{n} \sum_{k=1}^{\kappa} \langle \beta, v_k \rangle^2. \end{aligned}$$

When $\beta = 0$, this equals κ/n . Otherwise, we have the following lower bound:

$$\begin{aligned} \sum_{k=1}^{\kappa} \langle \beta, v_k \rangle^2 &= \|\beta\|_2^2 - \sum_{k=\kappa+1}^n \langle \beta, v_k \rangle^2 \\ &\geq \|\beta\|_2^2 - \frac{1}{s_{\kappa}^s} \sum_{k=\kappa+1}^n \langle \beta, v_k \rangle^2 s_k^s \\ &\geq \|\beta\|_2^2 - \frac{S_s(\beta; G)}{s_{\kappa}^s}, \end{aligned}$$

and therefore $\mathbb{E}(T_{\text{spec}}) \geq \kappa/n + n^{-1}(\|\beta\|_2^2 - S_s(\beta; G)/s_{\kappa}^s)$.

Variance of T_{spec} : We write $T_{\text{spec}} = n^{-1}y^T V_{\kappa} V_{\kappa}^T y$ where V_{κ} is the $n \times \kappa$ matrix with eigenvectors v_1, \dots, v_{κ} as columns. Consequently,

$$\text{Var}(T_{\text{spec}}) = \frac{1}{n^2} \text{Var}(y^T V_{\kappa} V_{\kappa}^T y) \quad (8)$$

$$= \frac{1}{n^2} \text{Var}((\beta + \varepsilon)^T V_{\kappa} V_{\kappa}^T (\beta + \varepsilon)) \quad (9)$$

$$= \frac{1}{n^2} \text{Var}(2\beta^T V_{\kappa} V_{\kappa}^T \varepsilon + \varepsilon^T V_{\kappa} V_{\kappa}^T \varepsilon) \quad (10)$$

$$\leq \frac{1}{n^2} (4\beta^T V_{\kappa} V_{\kappa}^T \beta + 2\kappa) \quad (11)$$

where the last inequality follows from standard properties of the Gaussian distribution. We now move on to showing the desired inequalities (5) and (7).

Proof of (5): By Chebyshev's inequality,

$$\begin{aligned} \mathbb{P}_{\beta=0}(T_{\text{spec}} \geq \frac{\kappa}{n} + t(b)) &\leq \mathbb{P}_{\beta=0}(|T_{\text{spec}} - \frac{\kappa}{n}| \geq t(b)) \\ &\leq \frac{\text{Var}_{\beta=0}(T_{\text{spec}})}{t(b)^2} = \frac{1}{b^2}. \end{aligned}$$

Proof of (7): For simplicity, we introduce the notation

$$\Delta = \frac{\|\beta\|_2^2}{n} - \frac{S_s(\beta; G)}{ns_{\kappa}^s}.$$

Assumption (6) implies $\Delta \geq 2t(b)$. Then another application of Chebyshev's inequality gives us

$$\begin{aligned} \mathbb{P}_{\beta}(T_{\text{spec}} \leq \frac{\kappa}{n} + t(b)) &= \mathbb{P}_{\beta}(T_{\text{spec}} - \mathbb{E}_{\beta}(T_{\text{spec}}) \leq t(b) - \Delta) \\ &\leq \mathbb{P}_{\beta}(|T_{\text{spec}} - \mathbb{E}_{\beta}(T_{\text{spec}})| \leq \Delta - t(b)) \quad (\text{since } \Delta \geq t(b)) \\ &\leq \frac{\text{Var}_{\beta}(T_{\text{spec}})}{(\Delta - t(b))^2} \\ &\leq 4 \frac{\text{Var}_{\beta}(T_{\text{spec}})}{\Delta^2} \quad (\text{since } \Delta \geq 2t(b)) \\ &\leq 4 \frac{2\kappa/n^2 + 4\beta^T V_{\kappa} V_{\kappa}^T \beta/n^2}{\Delta^2}. \end{aligned}$$

We handle each summand in the numerator separately. For the first term, since $\Delta \geq 2t(b)$, we have

$$\frac{2\kappa}{n^2\Delta^2} \leq \frac{1}{2b^2}. \quad (12)$$

For the second term, noting that $\Delta = \beta^T V_\kappa V_\kappa^T \beta / n$, we have

$$\begin{aligned} \frac{\beta^T V_\kappa V_\kappa^T \beta / n^2}{\Delta^2} &= \frac{1}{n\Delta} \\ &\leq \frac{1}{2nt(b)} \\ &= \frac{1}{2b\sqrt{2\kappa}}, \end{aligned} \quad (13)$$

and combining (12) and (13) yields (7).

1.0.1 Step 2: Bounding neighborhood graph functionals

To make use of Lemma 1 we will need to show that when r and κ are appropriately tuned and $\|f\|_{\mathcal{L}^2(\mathcal{X})}$ is sufficiently large, the inequality (6) holds with respect to $G = G_{n,r}$ and $\beta = (f(x_1), \dots, f(x_n))$. In particular, we will show that for some constants c_1, c_2, c_3, c_4 which may depend on L, d and s but do not depend on n, f or b , the following statements:

(E1) **Graph Sobolev norm:** For $f \in C_d^s(\mathcal{X}; R)$, $p \in C_d^{s-1}(\mathcal{X}; R)$, and $1 \geq r(n) \geq n^{-1/(2(s-1)+d)}$,

$$S_s(f; G_{n,r}) \leq c_1 \cdot b \cdot n^{s+1} r^{s(d+2)} \quad (14)$$

(E2) **Eigenvalue tail bound:** For any $a > 0$ and $(\log n/n)^{1/d} n^a \leq r \leq n^{-4/((2+d)(4s+d))}$, and for $\kappa = n^{2d/(4s+d)}$,

$$s_\kappa \geq c_2 \cdot n r^{d+2} \kappa^{2/d} \quad (15)$$

(E3) **Empirical norm of f :** When $f \in C^s(\mathcal{X}; R)$ and $\|f\|_{\mathcal{L}^2} \geq c_3 \cdot b \cdot n^{-4s/(4s+d)}$,

$$\|f\|_n^2 \geq \frac{1}{b} \cdot \|f\|_{\mathcal{L}^2}^2 \quad (16)$$

each hold with probability at least $1 - c_4/b$ for sufficiently large n .

Proof of (14): We will take s to be even, as the proof when s is odd follows essentially the same steps. To simplify exposition, we introduce the iterated difference operator, defined recursively as

$$D_{jk}f(x) = (D_k f(x_j) - D_k f(x)) \frac{K_r(x_j, x)}{r^d} \quad \text{for } j \in [n], k \in [n]^q, \quad D_j f(x) = (f(x_j) - f(x)) \frac{K_r(x_j, x)}{r^d}$$

Now when s is even, letting $q = s/2$ we have the decomposition

$$f^T L^s f = \sum_{i=1}^n \sum_{k \in [n]^q} \sum_{\ell \in [n]^q} r^{ds} D_k f(x_i) D_\ell f(x_i) \quad (17)$$

For given index vectors k, ℓ and index i , let $I = |k \cup \ell \cup i|$ be the total number of unique indices. We separate our analysis into cases based on the magnitude of I , specifically whether $I < s + 1$ or $I = s + 1$, and show that

$$\mathbb{E}(D_k f(x_i) D_\ell f(x_i)) = \begin{cases} O(r^{2s}), & \text{if } I = s + 1 \\ O(r^{2r^{d(I-(2q+1))}}), & \text{otherwise} \end{cases} \quad (18)$$

uniformly over $f \in C^s(L)$. Before proving (18), we verify that (14) is directly implied by (18). In the sum on the right hand side of (17), there are $O(n^I)$ terms with exactly I distinct indices. When $I < s + 1$, the total contribution of such terms to the sum is $O(n^I r^{d(I-1)+2})$. Since $r(n) \geq n^{-1/d}$, this increases with I . Taking $I = s$ to be the largest integer less than $s + 1$, the contribution of these terms to the sum is therefore $O(n^s r^{d(s-1)+2})$ which in light of the restriction $r \geq n^{-1/(2(s-1)+d)}$ is $O(n^{s+1} r^{s(d+2)})$. On the other hand when $I = s + 1$, by (18) we immediately have that the total contribution of these terms is $O(n^{s+1} r^{2(s+d)})$. Therefore,

$$\mathbb{E}(f^T L^s f) = O(n^{s+1} r^{s(d+2)})$$

uniformly over $f \in C^s(L)$, and (14) by Markov's inequality.

Now we prove (18). Since $f \in C_d^s(R) \subseteq C_d^1(R)$, using a first-order Taylor expansion of $f(x)$ we can show that for all index vectors $k, \ell \in [n]^q$ and indices $i \in [n]$, the product of iterated difference operators $D_k f(x_i) D_\ell f(x_i)$ satisfies

$$|D_k f(x_i) D_\ell f(x_i)| \leq 4^q R^2 r^{2-2dq}$$

Moreover $D_k f(x_i) D_\ell f(x_i)$ will equal zero if there exists $x_j, j \in k \cup \ell \cup i$ such that

$$\|x_j - x_h\| > r, \text{ for all } h \neq j \in k \cup \ell \cup i$$

Therefore $D_k f(x_i) D_\ell f(x_i)$ is nonzero with probability $O(r^{d(|k \cup \ell \cup i| - 1)})$, which along with the boundedness of $D_k f(x_i) D_\ell f(x_i)$ implies the second upper bound in (18).

To show the first upper bound in (18), we apply the law of iterated expectation,

$$\begin{aligned} \mathbb{E}[D_k f(x_i) D_\ell f(x_i)] &= \mathbb{E}[\mathbb{E}(D_k f(x)|x_i = x) \mathbb{E}(D_\ell f(x)|x_i = x)] \\ &= \mathbb{E}[\mathbb{E}(D_k f(x)|x_i = x)^2]. \end{aligned} \quad (19)$$

By Lemma 2, we have that $\mathbb{E}(D_k f(x)) = O(r^s)$ for all values of x , implying the desired result.

Proof of (15): We prove (15) by comparing $G_{n,r}$ to the tensor product of a d -dimensional lattice and a complete graph. The latter is a highly structured graph with known eigenvalues, which as we will see are sufficiently lower bounded for our purposes.

Let $\tilde{r} = r/(3(2\sqrt{d}+1))$, $M = (1/\tilde{r})^d$, $N = n\tilde{r}^d$. Assume without loss of generality that M and N are integers. Additionally, for $t = n^{1/d}$ and $m = M^{1/d}$ let

$$\overline{X} = \left\{ \frac{1}{t}(k_1, \dots, k_d) : k \in [t]^d \right\}, \quad \overline{Z} = \left\{ \frac{1}{m}(j_1, \dots, j_d) : j \in [m]^d \right\}.$$

For a given $\bar{z}_j \in \overline{Z}$, we write $Q(z_j) = m^{-1}[j_1 - 1, j_1] \times \dots \times m^{-1}[j_d - 1, j_d]$ for the cube of side length $1/m$ with z_j at one corner.

Consider the graph $H = (\overline{X}, E_H)$, where $(\bar{x}_k, \bar{x}_\ell) \in E_H$ if

$$\text{there exists } \bar{z}_i, \bar{z}_j \in \overline{Z} \text{ such that } \bar{x}_k \in Q(\bar{z}_i), \bar{x}_\ell \in Q(\bar{z}_j), \text{ and } \|i - j\|_1 \leq 1.$$

On the one hand $H \cong \overline{G}_d^M \otimes K_N$ where \overline{G}_d^M is the d -dimensional lattice on M nodes, and K_N is the complete graph on N nodes. On the other hand, we now show that with high probability $G_{n,r} \succeq H$. If $(\bar{x}_k, \bar{x}_\ell) \in E_H$, then there exist \bar{z}_i, \bar{z}_j such that

$$\|\bar{x}_k - \bar{x}_\ell\|_2 \leq m^{-1} + \|\bar{x}_k - \bar{z}_i\|_2 + \|\bar{x}_\ell - \bar{z}_j\|_2 \leq \tilde{r}(1 + 2\sqrt{d}) = r/3.$$

Assuming (25) holds, if $(\bar{x}_k, \bar{x}_\ell) \in E_H$, then for sufficiently large n

$$\|\pi(\bar{x}_k) - \pi(\bar{x}_\ell)\|_2 \leq 2c \left(\frac{\log n}{n} \right)^{1/d} + \frac{r}{3} \leq r,$$

implying that $(\pi(\bar{x}_k), \pi(\bar{x}_\ell)) \in E$. Therefore, $G_{n,r} \succeq \bar{G}_d^M \otimes K_N$ whenever (25) holds.

The eigenvalues of lattices and complete graphs are known to satisfy, respectively

$$\lambda_k(\bar{G}_d^M) \geq \frac{k^{2/d}}{M^{2/d}} \text{ for } k = 0, \dots, M-1, \text{ and } \lambda_j(K_N) \geq N \mathbf{1}\{j > 0\} \text{ for } j = 0, \dots, N-1.$$

and by standard facts regarding the eigenvalues of tensor product graphs, we have that the spectrum $\Lambda(H)$ satisfies

$$\Lambda(H) = \left\{ N\lambda_k(\bar{G}_d^M) + M\lambda_j(K_N) : \text{for } k = 0, \dots, M-1 \text{ and } j = 0, \dots, N-1 \right\}$$

For all $j = 1, \dots, N-1$, we have that $M\lambda_j(K_N) = MN = n$. Therefore,

$$\begin{aligned} \lambda_\kappa(H) &\geq \{n \wedge N\lambda_\kappa(\bar{G}_d^M)\} \\ &\geq \{n \wedge n\tilde{r}^d \frac{\kappa^{2/d}}{M^{2/d}}\} \\ &\geq \{n \wedge (3\sqrt{d} + 3)^{-(2+d)} n r^{d+2} \kappa^{2/d}\} \\ &\geq (3\sqrt{d} + 3)^{-(2+d)} n r^{d+2} \kappa^{2/d}, \end{aligned}$$

where the last inequality can be verified by a quick calculation in light of $\kappa = n^{2d/(4s+d)}$ and $r \leq n^{-4/((2+d)(4s+d))}$. Since we've already shown that $\lambda_\kappa(G_{n,r}) \geq \lambda_\kappa(H)$ when (25) is satisfied, which happens probability $1 - o(n^{-1})$, this completes the proof of (15).

Proof of (16): Let $Z = \frac{1}{n} \sum_{i=1}^n f^2(x_i)$. We upper bound $\mathbb{E}[Z^2]$,

$$\begin{aligned} \mathbb{E}[Z^2] &\leq \mathbb{E}(f^2(x_1))^2 + \frac{1}{n} \mathbb{E}(f^4(x_1)) \\ &\leq \mathbb{E}(f^2(x_1))^2 + \frac{R^2}{n} \mathbb{E}(f^2(x_1)) \\ &\stackrel{(i)}{\leq} \mathbb{E}(f^2(x_1))^2 \left(1 + \frac{R^2}{n/\mathbb{E}(f^2(x_1))} \right) \\ &\stackrel{(ii)}{\leq} \mathbb{E}(f^2(x_1))^2 \left(1 + \frac{R^2}{c_3^2 b^2 n^{d/(4s+d)}} \right) \end{aligned}$$

where (i) follows since $f \in C_d^s(\mathcal{X}; R)$ implies $|f(x)| \leq R$, and (ii) follows by assumption. The statement then follows by the Paley-Zygmund inequality.

1.0.2 Step 3: Conclusion

We note that for all possible values of $X \in \mathcal{X}^n$, under the null hypothesis $f = f_0 = 0$ and therefore $\beta = (f(x_1), \dots, f(x_n)) = 0$ as well. Therefore by (5), we have the following bound on Type I error:

$$\mathbb{E}_{f_0}(\phi_{\text{spec}}) = \mathbb{E}(\mathbb{E}_{\beta=0}(\phi_{\text{spec}})|X) \leq \frac{1}{b^2}. \quad (20)$$

Now, we bound Type II error under the assumption $f \in C_d^s(\mathcal{X}; R)$, $p \in C_d^{s-1}(\mathcal{X}; R)$ uniformly bounded away from 0 and ∞ over \mathcal{X} , and

$$\|f\|_{\mathcal{L}^2}^2 \geq \epsilon^2 = c_3^2 \cdot b^2 \cdot n^{-4s/(4s+d)}. \quad (21)$$

Choosing $n^{-1/(2(s-1)+d)} \leq r(n) \leq n^{-4/((2+d)(4s+d))}$, we may therefore apply our conclusions in Step 2; namely, that for every possible choice of f there exists a good set $\mathcal{E}_f \subseteq \mathcal{X}^n$ with $\mathbb{P}(\mathcal{E}_f) \geq 1 - c_4/b$ such that

each of (14), (15), and (16) hold for all $X \subseteq \mathcal{E}_f$. Choosing $\kappa = n^{2d/(4s+d)}$ to balance the squared bias and variance terms on the right hand side of (6), we have that for all $X \subseteq \mathcal{E}_f$

$$\begin{aligned}
2b\sqrt{\frac{2\kappa}{n^2}} + \frac{S_s(\beta; G_{n,r})}{ns_\kappa} &\leq 2bn^{-4s/(4s+d)} + c \cdot b \cdot \frac{n^s r^{s(d+2)}}{s_\kappa^s} && \text{(by (14))} \\
&\leq 2bn^{-4s/(4s+d)} + c \cdot b \cdot \frac{1}{n^{4s/(4s+d)}} && \text{(by (15))} \\
&\leq \frac{1}{b} \|f\|_{\mathcal{L}^2} \\
&\leq \frac{1}{n} \sum_{i=1} \beta_i^2. && \text{(by (16))}
\end{aligned}$$

where the last two inequalities follow for a suitably large choice of c_3 in (21). We conclude that for all $X \subseteq \mathcal{E}_f$, the inequality (6) is satisfied with respect to $\beta = (f(x_1), \dots, f(x_n))$ and $G = G_{n,r}$. As a result the worst-case Type II error is bounded

$$\sup_{\substack{f \in C_d^s(\mathcal{X}; \mathcal{R}), \\ \|f\|_{\mathcal{L}^2} \geq \epsilon}} \mathbb{E}_f(1 - \phi_{\text{spec}}) \leq \sup_{\substack{f \in C_d^s(\mathcal{X}; \mathcal{R}), \\ \|f\|_{\mathcal{L}^2} \geq \epsilon}} \mathbb{E}[\mathbb{E}_\beta(1 - \phi_{\text{spec}} | X \in \mathcal{E}_f)] + \frac{c_4}{b} \leq \frac{3 + c_4}{b},$$

completing the proof of Theorem 1.

2 Supporting Results

Lemma 2. *Let s be a positive integer, and $R \geq 0$. Suppose $f \in C^s(R)$, $p \in C^{s-1}(R)$, $k \in [n]^q$ for some $q \geq 1$, and that K_r is a 2nd-order kernel. Then if $2q \leq s - 1$,*

$$\mathbb{E}(D_k f(x)) = \sum_{\ell=2q}^{s-1} O(r^\ell) \cdot f_\ell(x) + O(r^s), \tag{22}$$

for some $f_\ell \in C^{s-\ell}(L)$. If $2q \geq s$, $\mathbb{E}(D_k f(x)) = O(r^s)$. All $O(\cdot)$ terms may depend L and s , but do not depend on f or x .

Proof. We will prove Lemma 2 in the case where $d = 1$. When $d \geq 2$, using multivariate Taylor expansions we find the same result, but with more notational overhead.

We will prove by induction on q in the case where $d = 1$. The When $q = 1$ and $k \in [n]$, by taking Taylor expansions of f and p , we obtain

$$\begin{aligned}
\mathbb{E}(D_k f(x)) &= \sum_{\ell=1}^{s-1} f^{(\ell)}(x) \int (z-x)^\ell K_r(z, x) p(z) dz + O(r^s) \\
&= \sum_{\ell=1}^{s-1} \sum_{a=0}^{s-1} f^{(\ell)}(x) p^{(a)}(x) \underbrace{\int (z-x)^{\ell+a} K_r(z, x) dz}_{:= I_{\ell+a}} + O(r^s)
\end{aligned} \tag{23}$$

Since K is a 2nd-order kernel, $I_1 = 0$ and $I_t = O(r^t)$ for $t \geq 2$. Additionally, when $\ell + a \leq s - 1$, we have that $f^{(\ell)} p^{(a)} \in C^{\min\{s-\ell, s-1-a\}} \subseteq C^{s-(\ell+a)}$, and $|f^{(\ell)} p^{(a)}| \leq L^2$ for any ℓ and a . We can therefore simplify (23) by combining all terms where $\ell + a = t$, obtaining

$$\mathbb{E}(D_k f(x)) = \sum_{t=1}^{s-1} f_t(x) I_t + O(r^s) = \sum_{t=2}^{s-1} f_t(x) I_t + O(r^s), \tag{24}$$

which establishes (22) in the base case.

Now, we assume (22) holds for all $k \in [n]^q$, and prove the desired estimate on $\mathbb{E}(D_{kj}f(x))$ for each $j \in [n]$. By the law of iterated expectation and (24),

$$\begin{aligned}\mathbb{E}(D_{kj}f(x)) &= \mathbb{E}(D_k(\mathbb{E}(D_jf))(x)) \\ &= \mathbb{E}\left(D_k\left(\sum_{t=2}^{s-1} I_t f_t + O(r^s)\right)(x)\right) \\ &= \sum_{t=2}^{s-1} I_t \cdot \mathbb{E}(D_k f_t(x)) + O(r^s)\end{aligned}$$

where the second equality follows from the linearity and boundedness of $f \mapsto \mathbb{E}(D_k f)$. We now apply the inductive hypothesis to $\mathbb{E}(D_k f_t(x))$. If $2(q+1) \geq s$, note that since $f_t \in C^{s-t}(L)$ for $t \geq 2$, we have by hypothesis $\mathbb{E}(D_k f_t(x)) = O(r^{s-t})$. As a result

$$\sum_{t=2}^{s-1} I_t \cdot \mathbb{E}(D_k f_t(x)) = \sum_{t=2}^{s-1} I_t \cdot O(r^{s-t}) = O(r^s)$$

Otherwise $2(q+1) \leq s-1$. For each $t = 2, \dots, s-1$, if additionally $2q \leq s-t-1$, then by hypothesis $\mathbb{E}(D_k f_t(x)) = \sum_{\ell=2q}^{s-t-1} O(r^\ell) \cdot g_\ell(x) + O(r^{s-t})$ for some $g_\ell \in C^{s-t-\ell}(L)$, and otherwise $\mathbb{E}(D_k f_t(x)) = O(r^{s-t})$. Therefore,

$$\begin{aligned}\sum_{t=2}^{s-1} I_t \cdot \mathbb{E}(D_k f_t(x)) &= \sum_{t=2}^{s-1-2q} I_t \cdot \left\{ \sum_{\ell=2q}^{s-t-1} O(r^\ell) \cdot g_\ell(x) + O(r^{s-t}) \right\} + \sum_{t=s-1-2q}^{s-1} I_t \cdot O(r^{s-t}) \\ &= \sum_{t=2}^{s-1-2q} I_t \cdot \left\{ \sum_{\ell=2q}^{s-t-1} O(r^\ell) \cdot g_\ell(x) \right\} + O(r^s) \\ &= \sum_{\ell=2q}^{s-3} \sum_{t=2}^{s-\ell-1} I_t \cdot O(r^\ell) \cdot g_\ell(x) + O(r^s).\end{aligned}$$

Noting that $g_\ell \in C^{s-(t+\ell)}(L)$ for some $\ell+t = 2(q+1), \dots, s-1$, and $I_t \cdot O(r^\ell) = O(r^{t+\ell})$, we can rewrite the final equation as a sum over $\ell+t = 2(q+1), \dots, s-1$, which proves (22). \square

Theorem 2 (Theorem 1 of “On the rate of Convergence of Empirical Measures in ∞ -Transportation Distance”). *Let $X = \{x_1, \dots, x_n\} \sim P$, where P is a distribution on $\mathcal{X} = [0, 1]^d$ with density p satisfying*

$$0 < p_{\min} < p(x) < p_{\max} < \infty, \quad \text{for all } x \in \mathcal{X}.$$

With probability at least $1 - o(n^{-1})$, there exists a bijection between grid points and data points $\pi : \bar{X} \rightarrow X$ such that

$$\max_{k \in [t]^d} |\bar{x}_k - \pi(\bar{x}_k)| \leq c \left(\frac{\log n}{n} \right)^{1/d} \quad (25)$$