

Notes for Week 5/29/19 - 5/31/19

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Consider absolutely continuous distributions \mathbb{P} and \mathbb{Q} with density functions f and g , respectively. For fixed $n \geq 0$, let $Z = (z_1, \dots, z_n)$, where for $i = 1, \dots, n$, $z_i \sim \frac{\mathbb{P} + \mathbb{Q}}{2}$ are independent. Given Z , for $i = 1, \dots, n$ let

$$\ell_i = \begin{cases} 1 & \text{with probability } \frac{f(z_i)}{f(z_i) + g(z_i)} \\ -1 & \text{with probability } \frac{g(z_i)}{f(z_i) + g(z_i)} \end{cases}$$

be conditionally independent labels, and write

$$1_X = \begin{cases} 1, & \ell_i = 1 \\ 0, & \text{otherwise} \end{cases} \quad 1_Y = \begin{cases} 1, & \ell_i = -1 \\ 0, & \text{otherwise} \end{cases}.$$

We will write $X = \{x_1, \dots, x_{N_X}\} := \{z_i : \ell_i = 1\}$ and similarly $Y = \{y_1, \dots, y_{N_Y}\} := \{z_i : \ell_i = -1\}$, where N_X and N_Y are of course random but $N_X + N_Y = n$.

Our statistical goal is hypothesis testing: that is, we wish to construct a test function ϕ which differentiates between

$$\mathbb{H}_0 : f = g \text{ and } \mathbb{H}_1 : f \neq g.$$

For a given function class \mathcal{H} , some $\epsilon > 0$, and test function ϕ a Borel measurable function of the data with range $\{0, 1\}$, we evaluate the quality of the test using *worst-case risk*

$$R_\epsilon^{(t)}(\phi; \mathcal{H}) = \sup_{f \in \mathcal{H}} \mathbb{E}_{f,f}^{(t)}(\phi) + \sup_{\substack{f, g \in \mathcal{H} \\ \delta(f, g) \geq \epsilon}} \mathbb{E}_{f, g}^{(t)}(1 - \phi)$$

where

$$\delta^2(f, g) = \int_{\mathcal{D}} (f - g)^2 dx.$$

Test statistic. For $r \geq 0$, define the r -graph $G_r = (V, E_r)$ to have vertex set $V = \{1, \dots, t\}$ and edge set E_r which contains the pair (i, j) if and only if $\|z_i - z_j\|_2 \leq r$. Let D_r denote the incidence matrix of G_r .

Define the *Laplacian Smooth* test statistic over the neighborhood graph to be

$$T_{LS} = \sup_{\theta : \|D\theta\|_2 \leq C(n, r)} \left\langle \theta, \frac{1_X}{N_X} - \frac{1_Y}{N_Y} \right\rangle$$

where we note that the test statistic is implicitly a function of r and $C(n, r)$.

1 Additional Theory

Let $\theta^* = (\theta_i^*)_{i=1}^n$, with $\theta_i^* := f(z_i) - g(z_i)$. Write $L = D^T D$ for the Laplacian matrix of the r -neighborhood graph, $\mathcal{D}f$ for the gradient of a function f , and $\mathcal{D}^2 f$ for the Hessian of a function f . We write $C^2(L)$ for the set of functions f twice continuously differentiable over \mathbb{R}^d , with bounded Hessian $\|\mathcal{D}^2 f\|_\infty \leq L$.

Lemma 1. *For all density functions $f, g \in C^2(L)$ with $\int (f - g)^2 \geq \epsilon^2$, if $r \geq c_1(\log n/n)^{1/d}$ and $\epsilon \geq c_2 n r^{d+1}$ then*

$$\sup_{\|D\theta\|_2 \leq 1} \langle \theta, \theta^* \rangle \geq \frac{c_2}{2} (\log n)^{1+2/d} n^{-2/d}$$

with probability at least $1 - \delta$.

Proof. By Lemmas 4 and 5, we have

$$\begin{aligned} \sup_{\|D\theta\|_2 \leq 1} \langle \theta, \theta^* \rangle &= \frac{1}{n} \sqrt{(\theta^*)^T L \theta^*} \\ &\geq \frac{1}{\lambda_k} (\langle \theta^*, \theta^* \rangle - \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle)^2 \end{aligned} \quad (1)$$

where the latter inequality holds for any $k = 1, \dots, n-1$. We upper bound $\langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle$ using the following relations

$$(\theta^*)^T L \theta^* \geq (P_k^\perp \theta^*)^T L^\dagger (P_k^\perp \theta^*) \geq \lambda_k \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle$$

and obtain

$$\begin{aligned} \frac{1}{\lambda_k} (\langle \theta^*, \theta^* \rangle - \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle)^2 &\geq \frac{1}{\lambda_k} \left(\langle \theta^*, \theta^* \rangle - \frac{(\theta^*)^T L \theta^*}{\lambda_k} \right)^2 \\ &\geq \frac{1}{\lambda_k} \left(c_1 n \epsilon^2 - \frac{c_2 n^2 r^{d+2}}{\lambda_k} \right)^2 \end{aligned} \quad (\text{Lemmas 2 and 3})$$

where the latter inequality occurs with probability at least $1 - 2\delta$. Choose $k = n-1$. As $r \geq c_1(\log n/n)^{1/d}$, we have that $G \preceq \text{Grid}$, and as a result $4 \geq \lambda_{n-1} \geq 1$. Therefore,

$$\begin{aligned} \frac{1}{\lambda_k} \left(c_1 n \epsilon^2 - \frac{c_2 n^2 r^{d+2}}{\lambda_k} \right)^2 &\geq \frac{1}{4} (c_1 n \epsilon^2 - c_2 n^2 r^{d+2})^2 \\ &\geq \frac{1}{4} (c_2 n^2 r^{d+2})^2 \\ &\geq \frac{1}{4} \left(c_2 n^{1-2/d} \log(n)^{1+2/d} \right)^2 = \frac{c_2^2}{4} n^{2-4/d} \log(n)^{2+4/d}, \end{aligned}$$

and the proof is complete. \square

Lemma 2. *For any $f, g \in L^2(\mathbb{R}^d)$ satisfying the **regularity conditions**, such that $\int_{\mathbb{R}^d} (f - g)^2 dx \geq \epsilon^2$ there exists constant c_1 such that*

$$\langle \theta^*, \theta^* \rangle \geq c_1 n \epsilon^2$$

with probability at least $1 - \delta$.

Lemma 3. *For any $f, g \in C^2(L)$ satisfying the **regularity conditions**, there exists a constant c_2 such that*

$$(\theta^*)^T L \theta^* \leq c_2 n^2 r^{d+2}$$

with probability at least $1 - \delta$.

2 Linear Algebra

Lemma 4. For any unweighted, undirected, connected graph $G = (V, E)$ with incidence matrix D , and any vector $v \in \mathbb{R}^n$ with $\sum_{i=1}^n v_i = 0$,

$$\sup_{\theta: \|D\theta\|_2 \leq C} \langle \theta, v \rangle = C \sqrt{v^T L^\dagger v}$$

Additionally, for any vector $v \in \mathbb{R}^n$ (not necessarily $\sum_{i=1}^n v_i = 0$), under the additional constraint $\theta^T \mathbf{1} = 0$, the same statement holds. That is,

$$\sup_{\substack{\theta: \|D\theta\|_2 \leq C, \\ \theta^T \mathbf{1} = 0}} \langle \theta, v \rangle = C \sqrt{v^T L^\dagger v}$$

Proof. Note that the condition $\|D\theta\|_2 \leq C$ is equivalent to $\theta^T L \theta \leq C$. The solution then follows from the KKT conditions. \square

Let L be the Laplacian matrix of a connected graph, and L^\dagger be the pseudo-inverse L . Write the eigendecomposition of $L^\dagger = U \Lambda^\dagger U^T$, where Λ is an $n \times n$ diagonal matrix with entries $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{n-1}$ and U is an orthogonal matrix with columns $U = (u_0 \dots u_{n-1})$. For each $k = 0, \dots, n-1$, write $U_k = (u_0 \dots u_{k-1})$ for the first k columns of U , P_k as the projection operator onto the span of U_k , and P_k^\perp for the projection operator onto the subspace orthogonal to the span of U_k .

Lemma 5. For any $k = 1, \dots, n$,

$$(\theta^*)^T L^\dagger \theta^* \geq \frac{1}{\lambda_k} (\langle \theta^*, \theta^* \rangle - \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle)^2$$

Proof. Note that Λ^\dagger is a diagonal matrix, with entries $\rho_{1,1} = 0$ and $\rho_{k,k} = \frac{1}{\lambda_k}$ for $k = 1, \dots, n$. Therefore,

$$(\theta^*)^T L^\dagger \theta^* = \sum_{k=1}^n \frac{\langle \theta^*, u_k \rangle^2}{\lambda_k}.$$

Clearly, for any $k = 1, \dots, n$,

$$\sum_{k=1}^n \frac{\langle \theta^*, u_k \rangle^2}{\lambda_k} \geq \frac{\langle P_k \theta^*, P_k \theta^* \rangle^2}{\lambda_k}$$

and as $\langle P_k \theta^*, P_k \theta^* \rangle + \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle = \langle \theta^*, \theta^* \rangle$, we obtain

$$\frac{\langle P_k \theta^*, P_k \theta^* \rangle^2}{\lambda_k} = \frac{1}{\lambda_k} (\langle \theta^*, \theta^* \rangle - \langle P_k^\perp \theta^*, P_k^\perp \theta^* \rangle)^2.$$

\square