Notes for Week 11/1/19 - 11/8/19

Alden Green

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Let P and Q be distributions on \mathbb{R}^d , absolutely continuous with respect to Lebesgue measure with densities p and q, and let $\mu = (P+Q)/2$. For fixed points $Z = \{z_1, \ldots, z_N\} \subset \mathcal{Z}$ for some subset \mathcal{Z} of the support of μ , suppose we observe $\ell = (\ell_1, \ldots, \ell_N) \in \mathbb{R}^n$, where ℓ_1, \ldots, ℓ_N are independent Rademacher random variables with means

$$\mathbb{E}[\ell_i] = \frac{p(z_i) - q(z_i)}{p(z_i) + q(z_i)}.$$

Let $\theta_p = (p(z_1), \dots, p(z_N))$ and similarly $\theta_q = (q(z_1), \dots, q(z_N))$; let $\theta_\mu = \frac{1}{2}\theta_p + \frac{1}{2}\theta_q$. Our goal: use the data ℓ, Z to test the following hypothesis:

$$\mathbf{H}_0: \theta_p = \theta_q \text{ versus } \mathbf{H}_a: d(\theta_p, \theta_q) > \epsilon$$

for some metric d on the space \mathbb{R}^n , and some $\epsilon > 0$. For a given test $\phi : \{-1,1\}^N \times \mathcal{Z} \to \{0,1\}$, we will evaluate our test error using the sum of Type I and Type II error

$$\mathcal{R}(\phi; \theta_p, \theta_q) = \mathbb{E}_{\theta_u, \theta_u}(\phi) + \mathbb{E}_{\theta_p, \theta_q}(1 - \phi),$$

and the worst case risk

$$\mathcal{R}(\phi, \epsilon, \Theta) = \sup_{\theta_p, \theta_q \in \Theta} \mathcal{R}(\phi; \theta_p, \theta_q)$$

where Θ is a subset of \mathbb{R}^n and the supremum is over all vectors θ_p, θ_q such that $d(\theta_p, \theta_q) \geq \epsilon$.

In particular, we propose and analyze the following projection-based test. Letting $G_{N,r}$ be the r-neighborhood graph over Z with combinatorial Laplacian L, we write the spectral decomposition of L as $L = VSV^T$, where $V = (v_1, \ldots, v_N)$ is $N \times N$ orthonormal matrix, and S is a diagonal matrix with entries $s_1 \leq s_2 \leq \ldots \leq s_N$. Our test statistic T depends on a tuning parameter C > 0 in the following manner:

$$T = T(\ell, Z) = \frac{1}{N} \sum_{k: s_k < C} (\langle \ell, v_k \rangle)^2$$

and our test $\phi := \phi(\ell, Z)$ will simply be $\phi = \mathbf{1}\{T \ge \frac{\kappa}{N} + b\tau\}$ for a threshold $\tau > 0$ to be specified later.

0.1 Moments of T.

To upper bound the test error we must show that the fluctuations of T (under null or alternative) are small compared to the difference in means $\mathbb{E}_{\theta_p,\theta_q}(T) - \mathbb{E}_{\theta_\mu,\theta_\mu}(T)$. We therefore must compute the first and second moments of T, under null and alternative. To compute the moments of T, we decompose the vector ℓ into a mean term and a noise term. Letting $\Delta_{P,Q} = \frac{\theta_P - \theta_q}{2\theta_\mu}$, we have $\ell = \Delta_{P,Q} + \varepsilon$ where $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)$ consists of n independent mean-zero random variables, distributed

$$\varepsilon_i = \begin{cases} \frac{\theta_{Q,i}}{\theta_{\mu,i}}, & \text{with probability } \frac{\theta_{P,i}}{\theta_{\mu,i}} \\ -\frac{\theta_{P,i}}{\theta_{\mu,i}}, & \text{with probability } \frac{\theta_{Q,i}}{\theta_{\mu,i}} \end{cases}$$

0.1.1 Mean of T.

Let κ be the largest integer $k \in [N]$ such that $s_k \leq C$. (Here κ is a fixed quantity.) Then,

$$\mathbb{E}(T) = \frac{1}{N} \sum_{k=1}^{\kappa} \mathbb{E}\left[\langle v_k, \ell \rangle^2\right]$$

$$= \frac{1}{N} \sum_{k=1}^{\kappa} \mathbb{E}\left[\langle \Delta_{P,Q} + \epsilon, v_k \rangle^2\right]$$

$$= \frac{1}{N} \sum_{k=1}^{\kappa} \left\{\langle \Delta_{P,Q}, v_k \rangle^2 + \mathbb{E}\left[\langle \epsilon, v_k \rangle^2\right]\right\}$$

For a given $k \in [\kappa]$, we have

$$\mathbb{E}\left[\langle \epsilon, v_k \rangle_2^2\right] = \sum_{i=1}^N \sum_{j=1}^N \mathbb{E}\left[\varepsilon_i \varepsilon_j v_{k,i} v_{k,j}\right]$$
$$= \sum_{i=1}^N v_{k,i}^2 \mathbb{E}\left[\varepsilon_i^2\right]$$

and by a direct computation of $\mathbb{E}\left[\varepsilon_i^2\right]$ we obtain

$$\mathbb{E}(T) = \frac{1}{N} \left(\sum_{k=1}^{\kappa} \langle \Delta_{P,Q}, v_k \rangle^2 + \sum_{k=1}^{\kappa} \sum_{i=1}^{N} v_{k,i}^2 \frac{\theta_{P,i} \theta_{Q,i}}{\theta_{\mu,i}^2} \right)$$

$$= \frac{1}{N} \left(\sum_{k=1}^{\kappa} \langle \Delta_{P,Q}, v_k \rangle^2 + \kappa - \sum_{k=1}^{\kappa} \sum_{i=1}^{N} v_{k,i}^2 \Delta_{P,Q,i}^2 \right)$$

$$= \frac{1}{N} \left(\sum_{k=1}^{\kappa} \langle \Delta_{P,Q}, v_k \rangle^2 + \kappa - \sum_{i=1}^{N} \Pi_{\kappa,ii} \Delta_{P,Q,i}^2 \right)$$

$$\geq \frac{1}{N} \left(\sum_{k=1}^{\kappa} \langle \Delta_{P,Q}, v_k \rangle^2 + \kappa - \Pi_{\max} \|\Delta_{P,Q}\|^2 \right)$$

Under the null, $\Delta_{P,Q} = 0$ and therefore

$$\mathbb{E}_{\theta_{\mu},\theta_{\mu}}(T) = \frac{\kappa}{N}.\tag{1}$$

Under the alternative, we have the following lower bound on the expectation of

$$\begin{split} \sum_{k=1}^{\kappa} \langle \Delta_{P,Q}, v_k \rangle^2 &= \sum_{k=1}^{N} \langle \Delta_{P,Q}, v_k \rangle^2 - \sum_{k=\kappa+1}^{N} \langle \Delta_{P,Q}, v_k \rangle^2 \\ &= \|\Delta_{P,Q}\|_2^2 - \sum_{k=\kappa+1}^{N} \frac{1}{s_k} \langle \Delta_{P,Q}, v_k \rangle^2 s_k \\ &\geq \|\Delta_{P,Q}\|_2^2 - \frac{1}{C} \langle L\Delta_{P,Q}, \Delta_{P,Q} \rangle. \end{split}$$

leading to the lower bound

$$\mathbb{E}_{\theta_p,\theta_q}(T) \ge \frac{\kappa}{N} + \frac{(1 - \Pi_{\max})}{N} \|\Delta_{P,Q}\|^2 - \frac{1}{CN} \langle L\Delta_{P,Q}, \Delta_{P,Q} \rangle. \tag{2}$$

0.1.2 Variance of T.

Let $V_{\kappa}=(v_1\dots v_{\kappa})$ be the $n\times \kappa$ matrix containing the first κ eigenvectors of L, and let $\Pi_{\kappa}=V_{\kappa}V_{\kappa}^T$. Observing that $T=\frac{1}{N}\langle \Pi_{\kappa}(\Delta_{P,Q}+\varepsilon), \Delta_{P,Q}+\varepsilon \rangle$, we have

$$\operatorname{Var}(T) = \frac{1}{N^{2}} \operatorname{Var}(2\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle + \langle \Pi_{\kappa} \varepsilon, \varepsilon \rangle)$$

$$= \frac{1}{N^{2}} \left\{ 4 \underbrace{\operatorname{Var}(\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle)}_{=:V_{1}} + 2 \underbrace{\operatorname{Cov}(\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle, \langle \Pi_{\kappa} \varepsilon, \varepsilon \rangle)}_{=:K_{1}} + \underbrace{\operatorname{Var}(\langle \Pi_{\kappa} \varepsilon, \varepsilon \rangle)}_{=:V_{2}} \right\}, \tag{3}$$

and we now upper bound each of the three terms on the right hand side of the previous display.

Upper bound on V_1 : Let $\Sigma := \text{Cov}(\varepsilon)$ be the covariance matrix of ε . Noting that $\Sigma \leq I$, we have

$$\operatorname{Var}(\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle) = \Delta_{P,Q}^{T} \Pi_{\kappa}^{T} \Sigma \Pi_{\kappa} \Delta_{P,Q} \le \|\Pi_{\kappa} \Delta_{P,Q}\|^{2}. \tag{4}$$

Upper bound on K_1 : Noting that $\mathbb{E}(\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle) = 0$, we have that

$$\begin{split} K_1 &= \mathbb{E}\left[\langle \Pi_{\kappa} \Delta_{P,Q}, \varepsilon \rangle \langle \Pi_{\kappa} \varepsilon, \varepsilon \rangle \right] \\ &= \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{i'=1}^{N} \mathbb{E}\left[\varepsilon_i \varepsilon_j \Pi_{\kappa,ij} \varepsilon_{i'} (\Pi_{\kappa} \Delta_{P,Q})_i \right] \\ &= \sum_{i=1}^{N} \mathbb{E}\left[\varepsilon_i^3 \right] \Pi_{\kappa,ii} (\Pi_{\kappa} \Delta_{P,Q})_i. \end{split}$$

Standard computations yield $\mathbb{E}\left[\varepsilon_i^3\right] = \frac{1}{2}(1 - \Delta_{P,Q,i}^2)(\Delta_{Q,P,i})$, and plugging in to the previous expression by Cauchy-Schwarz we have

$$K_{1} = \sum_{i=1}^{N} \mathbb{E}\left[\varepsilon_{i}^{3}\right] \Pi_{\kappa,ii} (\Pi_{\kappa} \Delta_{P,Q})_{i} = \frac{1}{2} \sum_{i=1}^{N} (1 - \Delta_{P,Q,i}^{2}) (\Delta_{Q,P,i}) \Pi_{\kappa,ii} (\Pi_{\kappa} \Delta_{P,Q})_{i}$$

$$\leq \|\Pi_{\kappa} \Delta_{P,Q}\| \cdot \left(\sum_{i=1}^{N} \Delta_{P,Q,i}^{2} \Pi_{\kappa,ii}^{2}\right)^{1/2}$$

$$\leq \Pi_{\max} \cdot \|\Pi_{\kappa} \Delta_{P,Q}\| \cdot \|\Delta_{P,Q}\|$$

$$(5)$$

Upper bound on V_2 : V_2 is a variance of a sum, which we re-express as the sum of covariances:

$$V_{2} = \operatorname{Var}(\langle \Pi_{\kappa} \varepsilon, \varepsilon \rangle)$$

$$= \sum_{i,j,i',j'=1}^{N} (\Pi_{\kappa})_{ij} (\Pi_{\kappa})_{i'j'} \operatorname{Cov}(\varepsilon_{i} \varepsilon_{j}, \varepsilon_{i'} \varepsilon_{j'}).$$

This covariance will be non-zero only when $i=i'\neq j=j',\ i=j'\neq j=i',$ or i=i'=j=j', and therefore

$$V_2 = 2\sum_{i=1}^N \sum_{j=1}^N (\Pi_\kappa)_{ij}^2 \operatorname{Var}(\varepsilon_i \varepsilon_j) + \sum_{i=1}^N (\Pi_\kappa)_{ii}^2 \operatorname{Var}(\varepsilon_i^2)$$

$$\leq 2\sum_{i=1}^N \sum_{j=1}^N (\Pi_\kappa)_{ij}^2 + \sum_{i=1}^N (\Pi_\kappa)_{ii}^2 \leq 3\operatorname{tr}(\Pi_\kappa^2) = 3\kappa.$$
(6)

Putting the pieces together. Plugging (4), (5), and (6) back into (3), we obtain

$$Var(T) \le \frac{1}{N^2} \left\{ 4\|\Pi_{\kappa} \Delta_{P,Q}\|^2 + \Pi_{\max} \cdot \|\Pi_{\kappa} \Delta_{P,Q}\| \cdot \|\Delta_{P,Q}\| + 3\kappa \right\}. \tag{7}$$

0.2 Type I and Type II error.

We translate our bounds on the mean and variance of T to bounds on the Type I and Type II error of our test ϕ using Chebyshev's inequality. Recall that our test statistic is of the form $\phi = \mathbf{1}\{T \ge \frac{\kappa}{N} + b\tau\}$, and let $\tau = \frac{\sqrt{3\kappa}}{N}$.

Type I error. We apply Chebyshev's inequality, and obtain

$$\begin{split} \mathbb{P}_{\theta_{\mu},\theta_{\mu}}\left(T \geq \frac{\kappa}{N} + b\tau\right) &= \mathbb{P}_{\theta_{\mu},\theta_{\mu}}\left(T - \frac{\kappa}{N} \geq b\tau - \mathbb{E}(T)\right) \\ &= \mathbb{P}_{\theta_{\mu},\theta_{\mu}}\left((T - \frac{\kappa}{N})^{2} \geq b^{2}\tau^{2}\right) \\ &\leq \frac{\operatorname{Var}_{\theta_{\mu},\theta_{\mu}}(T)}{b^{2}\tau^{2}} = \frac{1}{b^{2}}. \end{split}$$

Type II error. To obtain meaningful bounds on Type I error, we must assume some separation between θ_P and θ_Q . In particular, letting $d(\theta_P, \theta_Q) := \|\Delta_{P,Q}\|^2$ we assume

$$\frac{1}{N}d(\theta_P, \theta_Q) \ge \frac{1}{(1 - \Pi_{\text{max}})} \left(\frac{1}{CN} \|D\Delta_{P,Q}\|^2 + 2b\tau \right). \tag{8}$$

Note that this implies

$$\mathbb{E}_{\theta_{P},\theta_{Q}}(T) - \left(\frac{\kappa}{N} + b\tau\right) \ge \frac{(1 - \Pi_{\max})}{N} \|\Delta_{P,Q}\|^{2} - \frac{1}{CN} \|D\Delta_{P,Q}\|^{2} - b\tau \ge b\tau \vee \frac{(1 - \Pi_{\max})}{2N} \|\Delta_{P,Q}\|^{2}.$$

Now, we apply Chebyshev's inequality:

$$\begin{split} \mathbb{P}\left(T \leq \frac{\kappa}{N} + b\tau\right) &= \mathbb{P}\left(T - \mathbb{E}[T] \leq \frac{\kappa}{N} + b\tau - \mathbb{E}[T]\right) \\ &= \mathbb{P}\left((T - \mathbb{E}[T])^2 \leq (\mathbb{E}[T] - \frac{\kappa}{N} - b\tau)^2\right) \\ &\leq \frac{\operatorname{Var}(T)}{(\mathbb{E}[T] - \frac{\kappa}{N} - b\tau)^2} \\ &\leq \frac{1}{N^2} \frac{4\|\Pi_{\kappa} \Delta_{P,Q}\|^2 + \Pi_{\max} \cdot \|\Pi_{\kappa} \Delta_{P,Q}\| \cdot \|\Delta_{P,Q}\| + 3\kappa}{b^2 \tau^2 \vee \frac{(1 - \Pi_{\max})^2}{4N^2} \|\Delta_{P,Q}\|^4} \\ &\leq \frac{16}{(1 - \Pi_{\max})^2 \|\Delta_{P,Q}\|^2} \vee \frac{4\Pi_{\max}}{(1 - \Pi_{\max})^2 \|\Delta_{P,Q}\|^2} \vee \frac{1}{b^2} \\ &\leq \frac{3}{L^2} \end{split}$$

where the last line follows by (8) whenever $N \geq \sqrt{48}$.

1 Upper bounds on Π_{max} .

Clearly, the critical radius established by inequality (8) is only meaningful if $1 - \Pi_{\rm max} > 0$. In fact, we will want to show that $\Pi_{\rm max} < \frac{1}{2}$ so the factor of $(1 - \Pi_{\rm max})^{-1}$ does not affect the rate at which the critical radius shrinks. We review what $\Pi_{\rm max}$ looks like on some common graphs.

1.1 Chain.

Suppose $G := G_{1N}$ is a length-N chain, i.e. a 1d grid graph on vertices V = 1 : N. The eigenvectors of G are given by the discrete Fourier transform;

$$v_{1,i} = \frac{1}{\sqrt{N}}, \ v_{k,i} = \sqrt{\frac{2}{N}} \cos\left(\frac{(i-.5)(k-1)\pi}{N}\right) \text{ for } i = 1, \dots, N, \ k = 2, \dots, N.$$

Clearly $\Pi_{\max} \leq \frac{2\kappa}{N}$, so that whenever $\kappa < \frac{N}{4}$ we have $\Pi_{\max} < \frac{1}{2}$ as desired.

1.2 Grid.

Now suppose $G := G_{dN}$ is a d-dimensional grid graph on N nodes, i.e. $G = G_{1M} \otimes \cdots \otimes G_{1M}$ for $M = \frac{N}{d}$ (assume M is an integer for simplicity). The product structure of G yields an expression for its eigenvectors from the eigenvectors of G_{1M} . In particular, for a given $i = (i_1, \ldots, i_d) \in [M]^d$ and $k = (k_1, \ldots, k_d) \in [M]^d$, we have

$$v_{k,i} = \prod_{j=1}^{d} \sqrt{\frac{2}{M}} \cos\left(\frac{(i_j - .5)(k_j - 1)\pi}{M}\right)$$

and therefore $v_{k,i}^2 \leq \frac{2}{M^d} = \frac{2}{N}$ for all $i, k \in [M]^d$. So we arrive at the same bound $\Pi_{\max} \leq \frac{2\kappa}{N}$ and again $\kappa < \frac{N}{4}$ implies $\Pi_{\max} < \frac{1}{2}$ as desired.

1.3 Spectral similarity.

Suppose we have graphs G and H with Laplacians L_G and L_H , such that G and H are ϵ spectrally-similar, meaning

$$(1 - \epsilon)x^T L_H x \le x^T L_G x \le (1 + \epsilon)x^T L_H x, \text{ for all } x \in \mathbb{R}^N.$$

Write $L_G = V\Lambda V^T$ and $L_H = USU^T$ for the spectral decompositions of G and H, respectively, and assume that we have

$$\max_{(i,l)\in[N]^2} u_{l,i}^2 \le \frac{2}{N},$$

which we have already shown holds for $H = G_{dN}$. For each k, and for any $L(k), R(k) \in [N]$, write

$$v_k = \sum_{l=R(k)}^{L(k)} \alpha_{k,l} u_l + \operatorname{proj}_{U_{L(k)}^{\perp}}(v_k);$$

as a result, we have that

$$v_{k,i}^{2} \leq 2 \sum_{h=R(k)}^{L(k)} \sum_{l=R(k)}^{L(k)} \alpha_{k,h} \alpha_{k,l} u_{h,i} u_{l,i} + 2(\operatorname{proj}_{U_{R(k):L(k)}^{\perp}}(v_{k}))_{i}^{2}$$

$$\leq \frac{4}{N} \|\alpha\|_{1}^{2} + 2 \|\operatorname{proj}_{U_{L(k)}^{\perp}}(v_{k})\|^{2}$$

$$\leq \frac{4}{N} (L(k) - R(k)) + 2 \|\operatorname{proj}_{U_{R(k):L(k)}^{\perp}}(v_{k})\|^{2}$$

where the last inequality follows since $\|\alpha\|_2 \le 1$, and the inequality $\|\alpha\|_1 \le \sqrt{L-R} \|\alpha\|_2$, since α is a length L-R-vector.

TODO: Upper bound $\|\operatorname{proj}_{U_{L(k)}^{\perp}}(v_k)\|^2$ using (9), and choose L(k), R(k) to make the sum in the previous display as small as possible.

2 Notation.

We write $\Pi_{\max} = \max_{i=1,...,n} \Pi_{\kappa,ii}$ where we recall $\Pi_{\kappa} = V_{\kappa} V_{\kappa}^T$ and therefore $\Pi_{\kappa,ii} = \sum_{k=1}^{\kappa} v_{k,i}^2$. We write D for the incidence matrix of L.