Nonparametric Inference and Geometric Probability

(The Curious Case of Dimension 8)

Bhaswar B. Bhattacharya

University of Pennsylvania

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Outline

The Goodness-of-Fit and the Two-Sample Problems

- Let $\mathscr{X}_m = \{X_1, X_2, \ldots, X_n\}$ be i.i.d. samples from a densiy f in $\mathbb{R}^d$. The *goodness-of-fit problem* is to test

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- *Parametric Analogues*: Suppose $\{\mathbb{P}_\theta\}_{\theta \in \Theta}$ is a parametric family of distributions in $\mathbb{R}^d$, where $\Theta \subseteq \mathbb{R}^p$ is the parameter space.
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- Throughout we will consider the asymptotic regime where $m, n \to \infty$, such that $\frac{m}{m+n} \to p \in (0, 1)$, and the dimension is fixed.

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- Most (if not all) distribution-free goodness-of-fit/two-sample tests are based on geometric graphs, like *nearest-neighbor graphs*, *minimum spanning trees*, *matchings*, etc.

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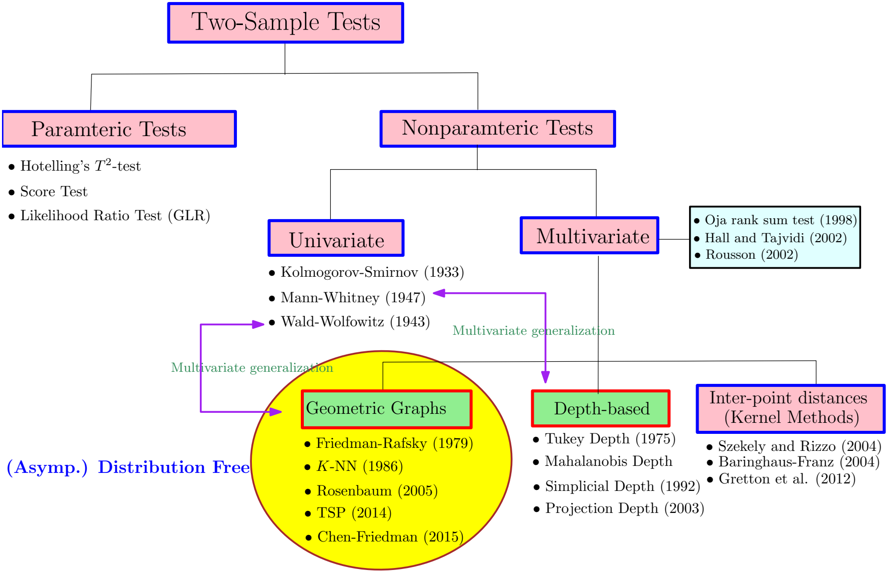
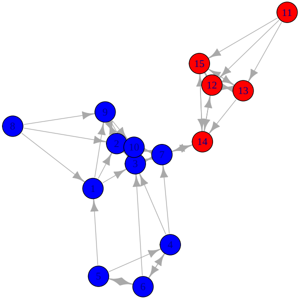
Two-Sample Tests: An Overview



Test Based on Nearest Neighbors Graphs

Bivariate normal data. Location shift. 3-NN graph.



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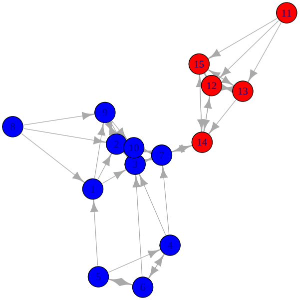

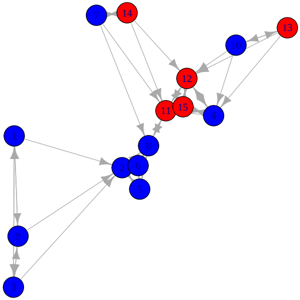

$\Delta = 2, \quad T(\mathscr{G}(\mathscr{X}_m \cup \mathscr{Y}_m)) = 1.$ $\qquad \Delta = 0.05, \quad T(\mathscr{G}(\mathscr{X}_m \cup \mathscr{Y}_m)) = 7.$

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- The *2-sample test statistic based on the graph functional $\mathscr{G}$* is defined as

$$\begin{aligned}\underbrace{T(\mathscr{G}(\mathscr{X}_m \cup \mathscr{Y}_n))}_{T(\mathscr{G})} &:= \sum_{i=1}^{m}\sum_{j=1}^{n} \mathbf{1}\{(X_i, Y_j) \in E(\mathscr{G}(\mathscr{X}_m \cup \mathscr{Y}_n))\} \\ &= \#\text{ edges across the two samples.}\end{aligned}$$

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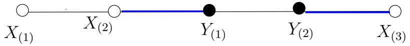

Friedman-Rafsky Test (1979)

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- Given a finite set $S \subset \mathbb{R}^d$, a *spanning tree* of S is a connected graph with vertex-set S and no cycles.
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- Other geometric graphs are often used:
  - *K-NN Test*: $\mathscr{G}$ is the K-nearest neighbor graph (Henze (1988), Schilling (1989)).
  - *Cross Match Test*: $\mathscr{G}$ is the minimum non-bipartite matching (Rosenbaum (2005)).

Properties of Tests on Geometric Graphs

- Asymptotic normality under the null of the centered statistic

$$\mathcal{R}(\mathscr{G}(\mathcal{Z}_N)) := \sqrt{N}\left(\frac{T(\mathscr{G}(\mathcal{Z}_N))}{|E(\mathscr{G}(\mathcal{Z}_N))|} - \frac{mn}{N(N-1)}\right) \xrightarrow{D} N(0, \sigma^2_{\mathscr{G}}).$$

as $N := m + n \to \infty$ such that $\frac{m}{N} \to p \in (0, 1)$.

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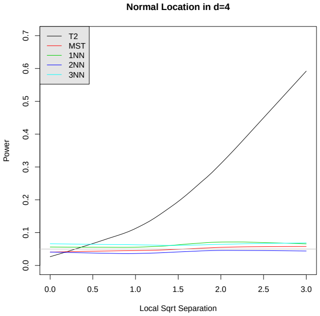
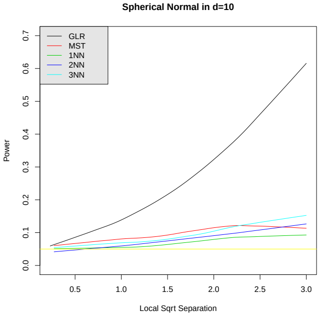
  - The performances of the different tests can be compared using these limiting power functions.

Asymptotic Efficiency of Graph-Based Tests





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(Informal) Theorem (B. (2019))

The asymptotic efficiency of the two-sample test based on an undirected graph functional $\mathscr{G}$ is

$$\mathrm{AE}(\mathscr{G}) = \frac{|C(r) \int \langle h, \nabla f(z|\theta_0)\rangle \lambda(z) \mathrm{d}z|}{\sqrt{\{\gamma_0(1-r) + (\gamma_1 - 2)(1-2r)\}}},$$

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where

- $C(r)$ *is a constant that only depends on* $r := 2p(1-p)$,
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$$\frac{N}{|E(\mathscr{G}(\mathcal{V}_N))|} \xrightarrow{P} \gamma_0, \ \ \textit{and} \ \ \frac{N\overbrace{|T_2(\mathscr{G}(\mathcal{V}_N))|}^{2-stars}}{|E(\mathscr{G}(\mathcal{V}_N))|^2} \xrightarrow{P} \gamma_1.$$

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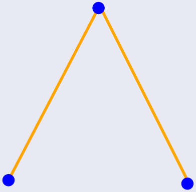
$K_{1,2}$



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The function $\lambda(\cdot)$

$$\lambda(z) = \lim_{N\to\infty} \mathbb{E}\frac{d(z, \mathscr{G}(\mathcal{V}_N^z))}{|E(\mathscr{G}(\mathcal{V}_N^z))|/N}$$
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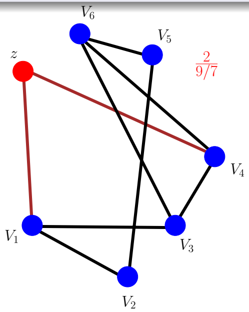

Asymptotic Efficiency of Graph-Based Tests

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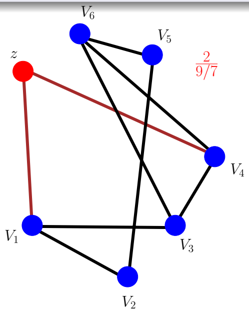

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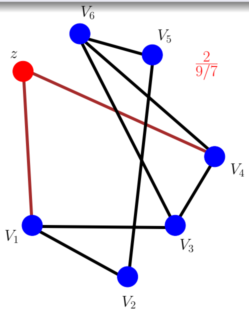

- *The function λ is like a 'centrality' measure. Small values of λ correspond to extreme points.*
- If $\mathscr{G} = MST$,

$$\frac{d(z, \mathscr{G}(\mathcal{V}_N^z))}{|E(\mathscr{G}(\mathcal{V}_N^z))|/N} \asymp d(z, \mathscr{G}(\mathcal{V}_N^z)).$$

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- What is D_d?
  - Aldous and Steele (1992) defined the MSF for *infinite* point sets which are locally finite, using the Prim's algorithm.
  - Look at the MSF on a *Poisson process of rate* 1 *with point* 0 *added to it*. *D_d is the degree of the vertex 0 in this graph.*

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Theorem

The asymptotic (Pitman) efficiency of the test based on the MST is zero.

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A translation and scale invariant graph functional $\mathscr{G}$ *stabilizes* on $\mathscr{P}_\lambda$ if there exists a random but almost surely finite variable R such that

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- Includes MST, K-NN, Delaunay graphs, etc.

Efficiency of Tests Based on Stabilizing Graphs

Theorem (B. (2019))

Let $\mathscr{G}$ be any translation and scale invariant graph functional which stabilizing $\mathscr{P}_1$, such that

$$\underbrace{\frac{\overbrace{\Delta(\mathscr{G}(\mathcal{Z}_N))}^{\text{max degree}}}{\underbrace{|E(\mathscr{G}(\mathcal{Z}_N))|/N}_{\text{average degree}}} = O_P(1)}_{\text{normality condition}}, \quad \text{and} \quad \underbrace{\sup_{N \in \mathbb{N}} \mathbb{E}\left(d(Z_1, \mathscr{G}(\mathcal{Z}_N))^s\right) < \infty}_{\text{moment condition}},$$

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Corollary

The asymptotic efficiencies of the tests based on the MST or the K-NN graphs are zero.

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  - In dimension 1, *R. Savage pointed out an issue in Lehmann's original proof.*

The Mean Difference

this manner. Since then it has been pointed out to me by R. Savage that when the limit result for

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- For dimension 1, $\frac{1}{N}\mathbb{E}T(\mathcal{N}_K(\mathcal{Z}'_N)) - \delta(f,g,p) = o(1/\sqrt{N})$, *and the Lehmann claim can be easily validated.*
- *Is this true for dimension d?* If yes, then the test will have power against $O(N^{-\frac{1}{4}})$ alternatives, and the heuristic would be correct. Otherwise, the rate of convergence competes with the Hessian term to determine the scaling for local power.

Case 1: Dimension Less or Equals 8

Theorem (B. (2020))

Suppose dimension $d \leq 8$. Then the limiting power of the directed K-NN test is given by

$$\begin{cases} \alpha & if \quad ||N^{\frac{1}{4}}\varepsilon_N|| \to 0, \\ \Phi\left(z_\alpha + c_{K,\theta_1}(h)\right) & if \quad N^{\frac{1}{4}}\varepsilon_N \to h, \\ 1 & if \quad ||N^{\frac{1}{4}}\varepsilon_N|| \to \infty. \end{cases}$$

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- *What is $c_{K,\theta_1}(h)$?*

$$c_{K,\theta_1}(h) = \begin{cases} \frac{r^2 K}{2\sigma_K}\mathbb{E}\left[\frac{h^\top \nabla_{\theta_1} f(X|\theta_1)}{f(X|\theta_1)}\right]^2 & if \quad d \leq 7, \\ \frac{r^2 K}{2\sigma_K}\mathbb{E}\left[\frac{h^\top \nabla_{\theta_1} f(X|\theta_1)}{f(X|\theta_1)}\right]^2 + \underbrace{b_{K,\theta_1}(h)}_{\text{correction term}} & if \quad d = 8. \end{cases}$$

Case 1: Simulations

- For a *fixed direction $h \in \mathbb{R}^p$*, consider the hypothesis

$$H_0 : \theta_2 = \theta_1 \quad \text{versus} \quad H_1 : \theta_2 = \theta_1 + \frac{h}{N^b},$$

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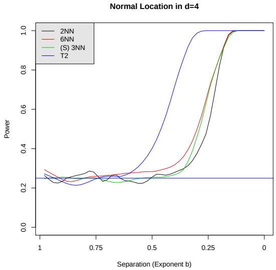

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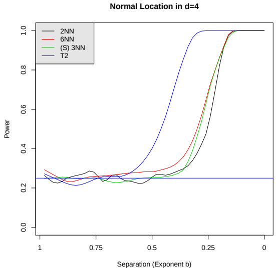

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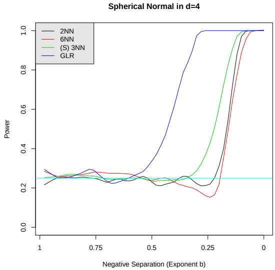

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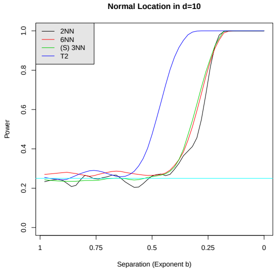

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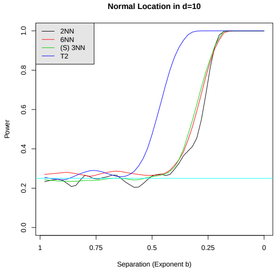

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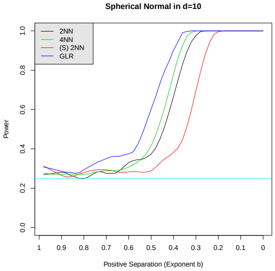

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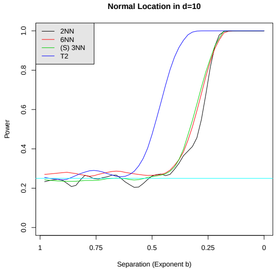

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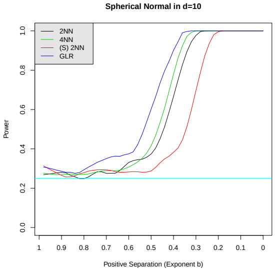

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Theorem (Continued) (B. (2020))

Suppose dimension $d \geq 9$. Then the limiting power of the K-NN test is given by

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Summarizing the Result: Critical Exponents

In general, there are two *critical exponents*,

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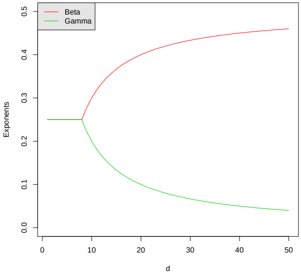

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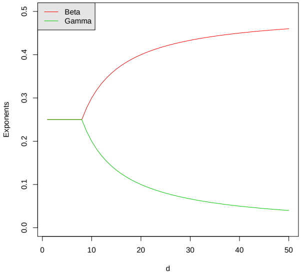

Theorem (Restated) (B. (2020))

Consider testing $H_0 : \theta_2 - \theta_1 = 0$ versus $H_1 : \theta_2 - \theta_1 = \varepsilon_N$, based on the directed K-NN graph functional. Then

- *If $||N^{\beta_d} \varepsilon_N|| \to 0$, the limiting power of the test is α.*
- *If $||N^{\gamma_d} \varepsilon_N|| \to \infty$, the limiting power of the test is 1.*

Outline

1. Preliminaries

2. Two-Sample Tests Based on Geometric Graphs
   - Definitions and Properties
   - Asymptotic Efficiency of Graph-Based Tests
   - Detection Thresholds

3. More Examples
   - Goodness-of-Fit Tests Based on Geometric Graphs
   - Independence Tests Based on Geometric Graphs

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$$\left| \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left\{ u(nD_i) - \mathbb{E}_0[u(nD_i)] \right\} \right|.$$

  Common choices of functions are $u(x) = e^{-x}$ or $u(x) = \log x$. (Pyke (1965), Hall (1986))

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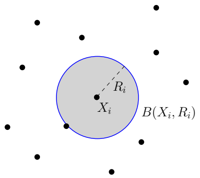

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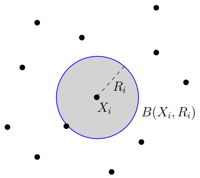

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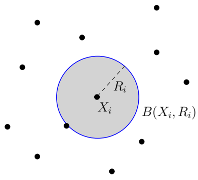

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- *The Bickel-Breiman Approximation*: Replace $\mu_{F_0}(X_i)$ by

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Properties of the Spacings Test

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- As before, can be shown that $\varepsilon_n = \frac{h}{\sqrt{n}}$ is too hard: zero Pitman efficiency.

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- *Connections?*

Thank

You

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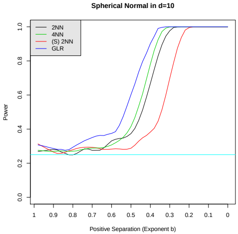

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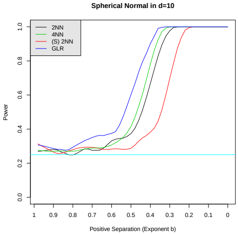

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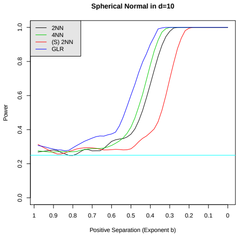

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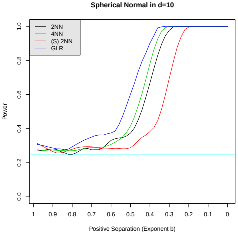

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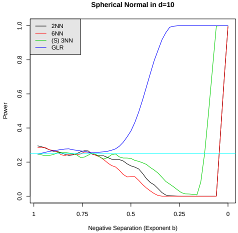

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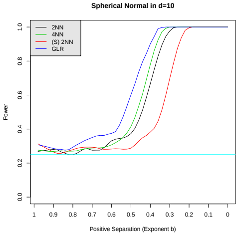

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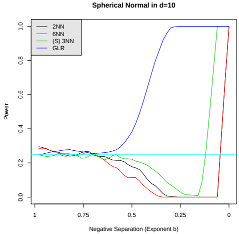

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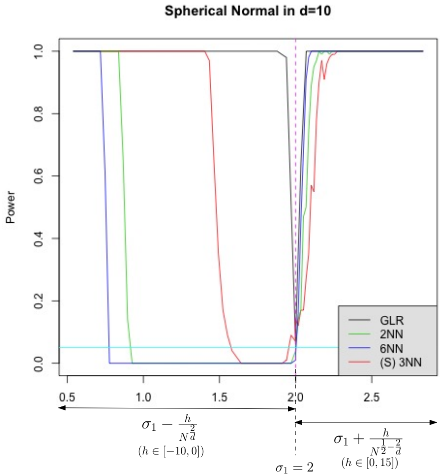
Zooming in at Thresholds: Spherical Normal

- We can zoom in at the two thresholds $O(N^{-\frac{1}{2}+\frac{2}{d}})$ and $O(N^{-\frac{2}{d}})$, and observe the phase transitions of the power function.



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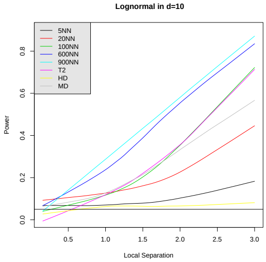
  - Consider K-NN graphs with $K = K_N \to \infty$.
  - In this case, $O(N^{-\frac{1}{2}})$ detection thresholds (Pitman efficiency) can be attained, when K grows with N sufficiently fast.
  - *How fast is fast enough?* Trade-off with computation time.



$$\mathbb{P}_\theta \sim \exp(N(\theta, \mathrm{I}))$$
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Theorem (Zhou and Rao (1993), B. (2019+))

Suppose dimension $d \leq 8$. Then the limiting power of the multivariate spacings test, for a fixed function $u : [0, \infty) \to \mathbb{R}$, is given by

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$$\begin{cases} \alpha & if \quad ||n^{\frac{1}{4}} \varepsilon_n|| \to 0, \\ \Phi\left(-z_{\frac{\alpha}{2}} + c_{\theta_0}(u,h)\right) + \Phi\left(-z_{\frac{\alpha}{2}} - c_{\theta_0}(u,h)\right) & if \quad ||n^{\frac{1}{4}} \varepsilon_n|| \to h, \\ 1 & if \quad ||n^{\frac{1}{4}} \varepsilon_n|| \to \infty. \end{cases}$$

- *What is $c_{\theta_0}(u,h)$?*

$$c_{\theta_0}(u,h) = \begin{cases} \frac{1}{\sigma(u)} \mathbb{E}\left[\frac{h^\top \nabla_{\theta_1} f(X|\theta_1)}{f(X|\theta_1)}\right]^2 \int_0^\infty e^{-t}(\frac{t^2}{2} - t)u'(t)\mathrm{d}t & if \quad d \leq 7, \\ \frac{1}{\sigma(u)} \mathbb{E}\left[\frac{h^\top \nabla_{\theta_1} f(X|\theta_1)}{f(X|\theta_1)}\right]^2 \int_0^\infty e^{-t}(\frac{t^2}{2} - t)u'(t)\mathrm{d}t + \underbrace{b_{\theta_0}(u,h)}_{\textit{correction term}} & if \quad d = 8. \end{cases}$$

  - Can be optimized over u to obtain the "optimal" test among the class of tests $T_n(u)$:

Case 1: Dimension Less or Equals 8

Theorem (Zhou and Rao (1993), B. (2019+))

Suppose dimension $d \leq 8$. Then the limiting power of the multivariate spacings test, for a fixed function $u : [0, \infty) \to \mathbb{R}$, is given by

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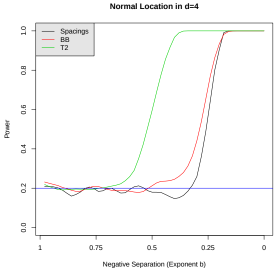
- Can be optimized over u to obtain the "optimal" test among the class of tests $T_n(u)$: *Global test for uniformity, irrespective of the alternative.*

Case 1: Simulations

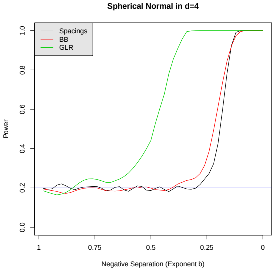
- For a fixed direction $h \in \mathbb{R}^p$, consider the hypothesis

$$H_0 : \theta = \theta_0 \quad \text{versus} \quad H_1 : \theta = \theta_0 + \frac{h}{N^b},$$

as b varies from $(0, 1)$.



$\mathbb{P}_\theta \sim N(\theta, \mathrm{I})$
$H_0 : \theta = 0 \quad \text{vs} \quad H_1 : \theta = -\frac{\mathbf{1}}{N^b}$



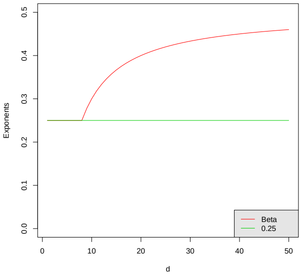
$\mathbb{P}_\sigma \sim N(0, \sigma^2 \mathrm{I})$
$H_0 : \sigma = 4 \quad \text{vs} \quad H_1 : \sigma = 4 - \frac{3}{N^b}.$

Case 2: Dimension Greater Than 8

Again, there are two *critical exponents*,

$$\beta_d = \begin{cases} \frac{1}{4} & \text{if} \quad d \leq 8 \\ \frac{1}{2} - \frac{2}{d} & \text{if} \quad d \geq 9, \end{cases}$$

and the *constant* $\frac{1}{4}$.



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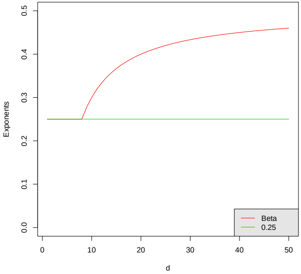

Theorem (B. (2019+))

The limiting power of the multivariate spacings test, for a fixed function $u : [0, \infty) \to \mathbb{R}$*, satisfies:*

- *If* $||N^{\beta_d} \varepsilon_N|| \to 0$*, the limiting power of the test is* α*.*
- *If* $||N^{\frac{1}{4}} \varepsilon_N|| \to \infty$*, the limiting power of the test is* 1*.*