# Global tests in high-dimensions

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# High-dimensional statistics

# Classical theory

- It concerns the behaviour when the *sample size* $n \to \infty$
- Suppose $Y_1, \ldots, Y_n \overset{i.i.d.}{\sim} \underset{m \times 1}{Y}$ with mean $\mu = \mathbb{E}(Y)$ and finite variance $\Sigma = \mathbb{V}\mathrm{ar}(Y)$
- *Law of large numbers*: the sample mean $\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} Y_i$ converges in probability to $\mu$
- *Central limit theorem*: the rescaled deviation $\sqrt{n}(\hat{\mu}_n - \mu)$ converges in distribution to a centered Gaussian with covariance matrix $\Sigma$
- *Consistency of maximum likelihood estimation*
- Etc.

Suppose that we are given $n = 1000$ samples from a statistical model in $m = 500$ dimensions

Will theory that requires $n \to \infty$ with the dimension $m$ remaining fixed provide useful predictions?

# High-dimensional data

- The data sets arising in many parts of modern science have a "high-dimensional flavor", with $m$ on the same order as, or possibly larger than $n$

$$m \gg n$$

- Classical "large $n$, fixed $m$" theory fails to provide useful predictions
- Classical methods can break down dramatically in high-dimensional regimes

**Reference**
Wainwright (2019)
High-Dimensional Statistics: A Non-Asymptotic Viewpoint
Cambridge University Press
Sections 1.1.1, 1.2.1, 1.3.1

# Linear discriminant analysis in high-dimensions

# Two classes

- Hypothesis testing can be used to determine whether an observed vector $x = (x_1, \ldots, x_m)^\mathsf{T} \in \mathbb{R}^m$ has been drawn from one of two possible densities $f_A \equiv \mathrm{P}(X|Y = A)$ and $f_B \equiv \mathrm{P}(X|Y = B)$, corresponding to two possible classes $A$ and $B$
- Consider testing $H_A : X_A \sim f_A$ vs $H_B : X_B \sim f_B$, where $X_A \equiv (X|Y = A)$ and $X_B \equiv (X|Y = B)$
- When these two distributions are known, then the Neyman-Pearson lemma says that the optimal decision rule is based on thresholding the log-likelihood ratio

$$\log \frac{f_B(x)}{f_A(x)}$$

- By testing $H_A$ vs $H_B$ and $H_B$ vs $H_A$ the conclusion is that the observed data $x$ is consistent with $A$ ($H_B$ rejected), with $B$ ($H_A$ rejected), with both (no rejections), or with neither (both rejected)

# Classification problem

- Let's turn to the classification problem involving the allocation of the observed unit $x$ to one of two classes $A$ and $B$
- For a Bayesian analysis suppose that the prior probabilities are $\pi_A \equiv \mathrm{P}(Y = A)$ and $\pi_B \equiv \mathrm{P}(Y = B)$ with $\pi_A + \pi_B = 1$. Then the posterior probabilities satisfy

$$\frac{\mathrm{P}(Y = B | X = x)}{\mathrm{P}(Y = A | X = x)} = \frac{\pi_B}{\pi_A} \frac{f_B(x)}{f_A(x)}$$

  giving the class with the higher posterior probability
- As a special case, suppose that the two classes are distributed as multivariate Gaussians $X_A \sim N(\mu_A, I_m)$ and $X_B \sim N(\mu_B, I_m)$, with $\pi_A = \pi_B = 1/2$

# Optimal decision

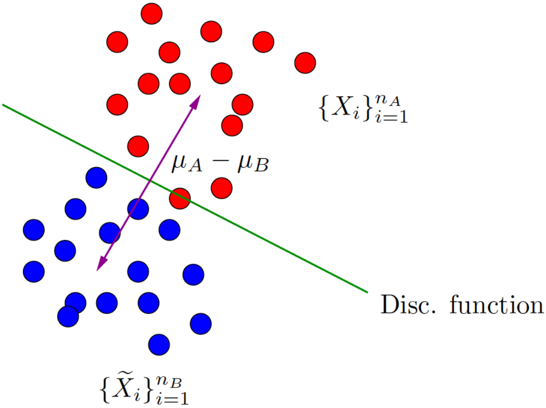
- The optimal decision rule is to threshold the log-likelihood ratio

$$\Psi(x) = \langle \mu_A - \mu_B, \left(x - \frac{\mu_A + \mu_B}{2}\right)\rangle$$

  where $\langle x, z \rangle = x^\mathsf{T} z = \sum_{j=1}^m x_j z_j$ denotes the Euclidean inner product in $\mathbb{R}^m$
- If $\Psi(x) > 0$ then classify $A$, otherwise $B$
- Error probability of the optimal rule:

$$\mathrm{Err}(\Psi) = \frac{1}{2}\mathrm{P}(\Psi(X_A) < 0) + \frac{1}{2}\mathrm{P}(\Psi(X_B) \geq 0) = \Phi\left(-\frac{\gamma}{2}\right)$$

  where $\gamma = \|\mu_A - \mu_B\|_2$, $\|\mu\|_2 = \sqrt{\mu^\mathsf{T}\mu}$, and $\Phi$ is the cdf of a standard normal variable




$$\langle \mu_A - \mu_B, \left( x - \frac{\mu_A + \mu_B}{2} \right) \rangle = 0$$

source: Wainwright

# Linear Discriminant Analysis

- Fisher's LDA: uses the plug-in principle based on $n_A$ samples from class $A$ and $n_B$ samples from class $B$

$$\hat{\Psi}(x) = \langle \hat{\mu}_A - \hat{\mu}_B, x - \frac{\hat{\mu}_A + \hat{\mu}_B}{2} \rangle$$

- Error probability of LDA (is itself a random variable)

$$\mathrm{Err}(\hat{\Psi}) = \frac{1}{2}\mathrm{P}(\hat{\Psi}(X_A) < 0) + \frac{1}{2}\mathrm{P}(\hat{\Psi}(X_B) \geq 0)$$

- Classical theory: if $(n_A, n_B) \to \infty$ and $m$ remains fixed, then $\hat{\mu}_A \overset{prob.}{\to} \mu_A$, $\hat{\mu}_B \overset{prob.}{\to} \mu_B$ and the asymptotic error probability is $\mathrm{Err}(\hat{\Psi}) \overset{prob.}{\to} \mathrm{Err}(\Psi) = \Phi(-\gamma/2)$

# High-Dimensional Theory

- What happens if $(n_A, n_B, m) \to \infty$ with
  - $m/n_A \to \delta$ with $\delta \geq 0$
  - $m/n_B \to \delta$
  - $\|\mu_A - \mu_B\|_2 \to \gamma > 0$
- Kolmogorov (1960) showed that

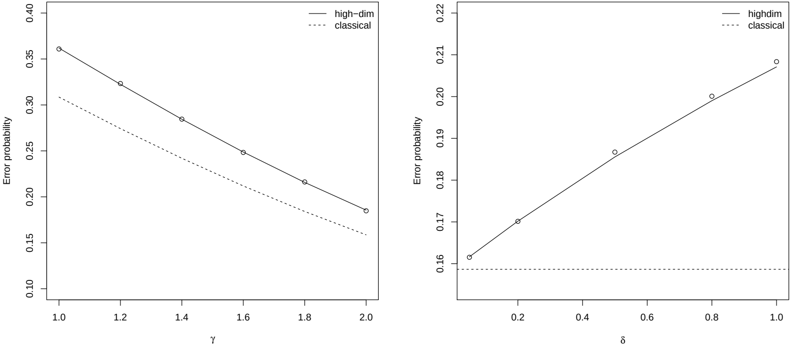
$$\mathrm{Err}(\hat{\Psi}) \overset{prob.}{\to} \Phi\Big( - \frac{\gamma^2}{2\sqrt{\gamma^2 + 2\delta}}\Big)$$

- If $m/n \to 0$, then the asymptotic error probability is $\Phi(-\gamma/2)$ as is predicted by classical theory
- If $m/n \to \delta > 0$, then the asymptotic error probability is strictly larger than $\Phi(-\gamma/2)$

The error probability of $\hat{\Phi}$, for the finite triple

$$(m, n_A, n_B) = (400, 800, 800)$$

is better described by the classical $\Phi(-\gamma/2)$, or the high-dimensional analog $\Phi(-\gamma^2/(2\sqrt{\gamma^2+2\delta}))$?




circles correspond to the empirical error probabilities, averaged over 10 trials

# What can help us in high dimensions?

- An important fact is that high-dimensional phenomena are unavoidable
- If the ratio $m/n$ stays bounded strictly above zero, then it is not possible to achieve the optimal classification rate
- Our only hope is that the data is endowed with some form of *low-dimensional structure*

- What is the underlying cause of the inaccuracy of the prediction for the LDA in high-dimensions?
- The squared Euclidean error

$$\|\hat{\mu} - \mu\|_2^2 = \sum_{j=1}^{m} (\hat{\mu}_j - \mu_j)^2$$

concentrates sharply around $m/n$, i.e. for $t \in (0, 1)$

$$\mathrm{P}\left(\left|\|\hat{\mu} - \mu\|_2^2 - \frac{m}{n}\right| \geq \frac{m}{n} t\right) = \mathrm{P}\left(\left|\frac{1}{m} \sum_{j=1}^{m} Z_j^2 - 1\right| \geq t\right) \leq 2e^{-\frac{mt^2}{8}}$$

where $Z_j = \sqrt{n}(\hat{\mu}_j - \mu_j) \sim N(0, 1)$; for the upper bound see Wainwright (2019), Example 2.11

# Sparsity

- Suppose that the $m$-vector $\mu$ is *sparse*, with only $s$ of its $m$ entries being nonzero, for some sparsity parameter $s \ll m$
- If sparsity holds, we can obtain a better estimator by thresholding the sample means

$$\tilde{\mu}_j = \hat{\mu}_j \mathbb{1}\{|\hat{\mu}_j| > \lambda\}$$

where

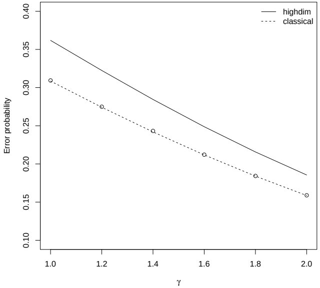
$$\lambda = \sqrt{\frac{2 \log m}{n}}$$

# Thresholded mean

Suppose to replace $\hat{\mu}$ by the thresholded mean $\tilde{\mu}$, then

$$\tilde{\Psi}(x) = \langle \tilde{\mu}_A - \tilde{\mu}_B, x - \frac{\tilde{\mu}_A + \tilde{\mu}_B}{2} \rangle$$

approaches the optimal $\mathrm{Err}(\Psi)$ if $\log \binom{m}{s}/n \to 0$. For $s = 5$:




circles correspond to the empirical error probabilities, averaged over 10 trials

# Inference for the mean vector

- Random sample of $n$ observations from $y \sim N_m(\mu, \Sigma)$

$$\left( \begin{array}{c} y_1 \\ \vdots \\ y_m \end{array} \right) \sim N_m \left( \left( \begin{array}{c} \mu_1 \\ \vdots \\ \mu_m \end{array} \right), \left[ \begin{array}{cccc} \sigma_1^2 & \sigma_{12} & \cdot & \sigma_{1m} \\ \sigma_{21} & \sigma_2^2 & \cdot & \sigma_{2m} \\ \cdot & \cdot & \cdot & \cdot \\ \sigma_{m1} & \cdot & \cdot & \sigma_m^2 \end{array} \right] \right)$$

- The parameter of interest is $\mathbb{E}(y) = \mu$, where $\mu_j = 0$ means "no effect" and $\mu_j \neq 0$ means "effect" in the $j$th component
- The nuisance parameter is the variance/covariance matrix $\mathbb{V}\text{ar}(y) = \Sigma$

# Three questions

1. *Detecting effects*: There is at least one $\mu_j$ different from 0?
2. *Counting effects*: How many $\mu_j$ are different from 0?
3. *Identifying effects*: Which $\mu_j$ are different from 0?

# Global null hypothesis

Testing the global null hypothesis aims at detecting any effect

$$H_0 : \mu = 0, \text{ i.e. } \bigcap_{j=1}^{m} \{\mu_j = 0\}$$

$$H_1 : \mu \neq 0, \text{ i.e. } \bigcup_{j=1}^{m} \{\mu_j \neq 0\}$$

One-sided alternative

$$H_0 : \bigcap_{j=1}^{m} \{\mu_j = 0\}$$

$$H_1 : \bigcup_{j=1}^{m} \{\mu_j > 0\}$$

# MaxT and SumT

- For simplicity, assume $\Sigma = I_m$ and $n = 1$ and consider the one-sided alternative
- $T_j = y_j \sim N(\mu_j, 1)$ for $j = 1, \ldots, m$
- $(T_1, \ldots, T_m)' \overset{H_0}{\sim} N_m(0, I_m)$
- MaxT
$$T_{\max} = \max(T_1, \ldots, T_m)$$
- SumT
$$T_{\text{sum}} = \sum_{j=1}^{m} T_j$$

# MaxT

- The critical value $t_{1-\alpha}$ of $T_{\max}$ is

$$\mathrm{P}_0(T_{\max} \geq t_{1-\alpha}) = \alpha$$

where $t_{1-\alpha}$ is the $1-\alpha$ quantile of the distribution of the maximum of $m$ independent standard normal variables

$$\int_{t_{1-\alpha}}^{\infty} m\phi(y)\Phi(y)^{m-1}dy = \alpha$$

where $\phi$ and $\Phi$ are the density and cdf of $N(0,1)$

# Critical value approximation

– We can replace $t_{1-\alpha}$ by $z_{1-\frac{\alpha}{m}}$

$$\begin{aligned} P_0(T_{\max} \geq z_{1-\frac{\alpha}{m}}) &= P_0\Big(\bigcup_{j=1}^{m}\{T_j \geq z_{1-\frac{\alpha}{m}}\}\Big) \\ &\leq \sum_{j=1}^{m} P_0(T_j \geq z_{1-\frac{\alpha}{m}}) = m\frac{\alpha}{m} = \alpha \end{aligned}$$

– The union bound might seem crude, but with independent $T_j$s the size of the test is very near $\alpha$

$$\begin{aligned} P_0(T_{\max} \geq z_{1-\frac{\alpha}{m}}) &= 1 - \prod_{j=1}^{m} P_0(T_j < z_{1-\frac{\alpha}{m}}) \\ &= 1 - \Big(1 - \frac{\alpha}{m}\Big)^m \overset{m\to\infty}{\to} 1 - e^{-\alpha} \end{aligned}$$

For $\alpha = 0.05$, $1 - e^{-\alpha} = 0.0487$

# Magnitude of the critical value

- How large is the threshold $z_{1-\frac{\alpha}{m}}$? For large $m$

$$
\begin{aligned}
z_{1-\frac{\alpha}{m}} &\approx \sqrt{2\log m} - \frac{\log(2\log m) + \log 2\pi}{2\sqrt{2\log m}} \\
&\approx \sqrt{2\log m}
\end{aligned}
$$

with no dependence on $\alpha$

# Proof

$$\frac{\phi(t)}{t}(\frac{t^2}{t^2+1}) \leq \mathrm{P}(N(0,1) > t) \leq \frac{\phi(t)}{t}$$

where $\phi(t)$ is the probability density function of $N(0,1)$. This result implies that for large $t$, $\frac{\phi(t)}{t}$ is a good approximation to the normal tail probability. Let $z^* = z_{1-\frac{\alpha}{m}}$. We have $\frac{\alpha}{m} = \mathrm{P}(N(0,1) > z_{1-\frac{\alpha}{m}}) \approx \frac{\phi(z^*)}{z^*}$, which implies $\alpha/m \approx \frac{1}{z^*\sqrt{2\pi}} e^{-\frac{(z^*)^2}{2}}$. Taking the logarithm

$$\log m \approx \frac{1}{2}\log(2\pi) + \frac{1}{2}(z^*)^2 + \log(z^*) + \log(\alpha)$$

Note that $z^*$ is increasing in $m$, i.e. $m \to \infty$ induces $z^* \to \infty$. As $\frac{1}{2}\log(2\pi) + \log(z^*) + \log(\alpha)$ is negligible compared to $(z^*)^2$ when $m$ goes to $\infty$, it gives

$$z_{1-\frac{\alpha}{m}} \approx \sqrt{2\log m}$$

# Needle in a haystack problem

$$H_0 : \mu_j = 0 \text{ for all } j = 1, \ldots, m$$
$$H_1 : \mu_j = c_m > 0, \mu_k = 0 \text{ for } k \neq j$$

- What is the limiting power of the MaxT test?

$$\lim_{m \to \infty} \mathrm{P}_1(T_{\max} > z_{1-\frac{\alpha}{m}})$$

It depends on the limiting ratio

$$\lim_{m \to \infty} \frac{c_m}{\sqrt{2 \log m}} \lesseqgtr 1$$

where $c_m$ is the value of the single non-zero mean, which depends on $m$

Two cases:

- Assume without loss of generality that $\mu_1 = c_m$. Suppose $c_m > (1+\epsilon)\sqrt{2\log m}$. Then, for $m \to \infty$

  $$P_1(T_{\max} > z_{1-\frac{\alpha}{m}}) \geq P_1(T_1 > z_{1-\frac{\alpha}{m}}) = P(N(0,1) > z_{1-\frac{\alpha}{m}} - c) \to 1$$

- Suppose $c_m < (1-\epsilon)\sqrt{2\log m}$. Then for $m \to \infty$

  $$\begin{aligned} P_1(T_{\max} > z_{1-\frac{\alpha}{m}}) &\leq P(T_1 > z_{1-\frac{\alpha}{m}}) + P(\max_{j>1} T_j > z_{1-\frac{\alpha}{m}}) \\ &= P(N(0,1) > z_{1-\frac{\alpha}{m}} - c) + P(\max_{j>1} T_j > z_{1-\frac{\alpha}{m}}) \\ &\to 0 + (1 - e^{-\alpha}) \end{aligned}$$

  and the MaxT test has no power

# SumT

$$T_{\text{sum}} = \sum_{j=1}^{m} T_j \sim N(\sum_{j=1}^{m} \mu_j, m)$$

- $\frac{T_{\text{sum}}}{\sqrt{m}} \overset{H_0}{\sim} N(0,1)$; $\frac{T_{\text{sum}}}{\sqrt{m}} \overset{H_1}{\sim} N(\theta_m, 1)$ with

$$\theta_m = \frac{\sum_{j=1}^{m} \mu_j}{\sqrt{m}}$$

  but if $\theta_m \to 0$ when $m \to \infty$, then $T_{\text{sum}}$ has no power
- By the Neyman-Pearson lemma, $T_{\text{sum}}$ is the UMP test for

  $H_0 : \mu_j = 0$ for all $j$
  $H_1 : \mu_j = c_m > 0$ for all $j$

  where $\theta_m = \sqrt{m} c_m$, but if $c_m = \frac{1}{m}$ the UMP test has no power

# Comparison

- **Few strong effects**:
  $m^{1/4}$ of the $\mu_j$s are equal to $\sqrt{2\log m}$, the rest 0.
  E.g. when $m = 10^6$, $m^{1/4} \approx 36$ and $\sqrt{2\log m} \approx 5.3$. In this setting $T_{\text{max}}$ has full power, but $T_{\text{sum}}$ has no power because

$$\theta_m = \frac{m^{1/4}\sqrt{2\log m}}{\sqrt{m}} \to 0$$

- **Small, distributed effects**:
  $\sqrt{2m}$ of the $\mu_j$s are equal to 3, the rest 0.
  The $T_{\text{sum}}$ has (almost) full power, but $T_{\text{max}}$ has no power because when $m$ is large it's very likely that the largest $y_j$ value comes from a null $\mu_j$

# MinP

- Let $p_j = 1 - \Phi(T_j)$ be the $j$th $p$-value
- $p_1, \ldots, p_m \overset{i.i.d.}{\sim} U(0,1)$ under $H_0$
- The MinP test is based on the minimum $p$-value

$$p_{\min} = \min(p_1, \ldots, p_m) \overset{H_0}{\sim} \mathrm{Beta}(1, m)$$

- The MinP test rejects $H_0$ if $p_{\min} \leq 1 - (1-\alpha)^{\frac{1}{m}}$ and has size $\alpha$:

$$\begin{aligned} \mathrm{P}_0(p_{\min} \leq 1 - (1-\alpha)^{\frac{1}{m}}) &= 1 - \mathrm{P}_0\Big(\bigcap_{i=1}^{m} \{p_i > 1 - (1-\alpha)^{\frac{1}{m}}\}\Big) \\ &= 1 - \big[(1-\alpha)^{\frac{1}{m}}\big]^m = \alpha \end{aligned}$$

# Simes test

- $p_1, \ldots, p_m \overset{i.i.d.}{\sim} U(0,1)$ under $H_0$
- Sort the $p$-values

$$p_{(1)} \leq p_{(2)} \leq \cdots \leq p_{(m)}$$

- The null distribution of $j$th ordered $p$-value is

$$p_{(j)} \overset{H_0}{\sim} \mathrm{Beta}(j, m-j+1)$$

- The Simes test $p$-value

$$p_{\mathrm{s}} = \min_{j=1,\ldots,m} \left\{ p_{(j)} \frac{m}{j} \right\} \overset{H_0}{\sim} U(0,1)$$

- It rejects $H_0$ if

$$\exists\, j : p_{(j)} \leq \frac{\alpha j}{m}$$

# Fisher combination

- $p_1, \ldots, p_m \overset{i.i.d.}{\sim} U(0,1)$ under $H_0$
- Fisher's method of combining $p$-values

$$T_{\mathrm{f}} = \sum_{j=1}^{m} 2 \log\left(\frac{1}{p_j}\right) \overset{H_0}{\sim} \chi^2_{2m}$$

# Higher criticism

- Empirical cdf $\hat{F}_m(t) = \dfrac{\sum_{j=1}^m \mathbb{1}\{p_j \leq t\}}{m}$ for $t \in [0,1]$.
- Since $p_1, \ldots, p_m \overset{i.i.d.}{\sim} U(0,1)$ under $H_0$, then

$$m\hat{F}_m(t) \overset{H_0}{\sim} \text{Binomial}(m, t)$$

- The higher criticism test is

$$T_{\text{hc}} = \sup_{t \in [0,1]} \frac{\hat{F}_m(t) - t}{\sqrt{t(1-t)/m}}$$

or equivalently

$$T_{\text{hc}} = \max_{j=1,\ldots,m} \sqrt{m} \frac{(i/m) - p_{(i)}}{\sqrt{p_{(i)}(1 - p_{(i)})}}$$


**Reference**
Donoho, Jin (2015)
Higher Criticism for Large-Scale Inference, Especially for Rare and Weak Effects
Statistical Science, 30:1–25

- For $m \to \infty$, $b_m T_{\text{hc}} - c_m$ converges weakly to the standard Gumbel distribution, where $b_m = \sqrt{2 \log \log m}$ and $c_m = \frac{1}{2}(\log \log \log(m) - 4\pi)$
- For any fixed $\alpha$ and $m \to \infty$, its critical value is

$$t_{1-\alpha} \approx (1 + a)\sqrt{2 \log \log m}$$

  for some $a > 0$, e.g. $a = 1.08$ for $m \approx 10^6$ and $\alpha = 0.05$

# Mixture distribution

- We assume that our samples follow a mixture of $N(0,1)$ and $N(\mu,1)$ distributions

$$\begin{aligned} H_0 &: \quad y_j \overset{i.i.d}{\sim} N(0,1) \\ H_1 &: \quad y_j \overset{i.i.d}{\sim} \pi_0 N(0,1) + \pi_1 N(\mu,1) \end{aligned}$$

  where $\pi_1 = 1 - \pi_0$

- To carry out asymptotic analysis, we must specify the dependence scheme of $\pi_1 = \pi_1(m)$ and $\mu = \mu(m)$ on $m$:

$$\begin{aligned} \pi_1 &= m^{-\beta} & \frac{1}{2} < \beta < 1 \\ \mu &= \sqrt{2r\log m} & 0 < r < 1 \end{aligned}$$

- The needle in a haystack problem: $\beta = 1$ and $r = 1$; small distributed effects: $\beta = 1/2$

# Threshold curve

Consider the following threshold curve for $r$

$$\rho_{\text{hc}}(\beta) = \begin{cases} \beta - \frac{1}{2} & \text{if } \frac{1}{2} < \beta \leq \frac{3}{4} \\ (1 - \sqrt{1-\beta})^2 & \text{if } \frac{3}{4} \leq \beta \leq 1 \end{cases}$$

- If $r > \rho_{\text{hc}}(\beta)$ the Neyman-Pearson optimal test achieves

  $$\mathrm{P}_0(\text{Type I Error}) + \mathrm{P}_1(\text{Type II Error}) \to 0$$

  The Higher Criticism is asymptotically equivalent to the optimal test without knowledge of $\pi_1$ and/or $\mu$
- If $r < \rho_{\text{hc}}(\beta)$ then for *any* test

  $$\liminf_{m \to \infty} \mathrm{P}_0(\text{Type I Error}) + \mathrm{P}_1(\text{Type II Error}) \geq 1$$

# Detectable region