A Large-Sample Approach to Controlling the False Discovery Rate

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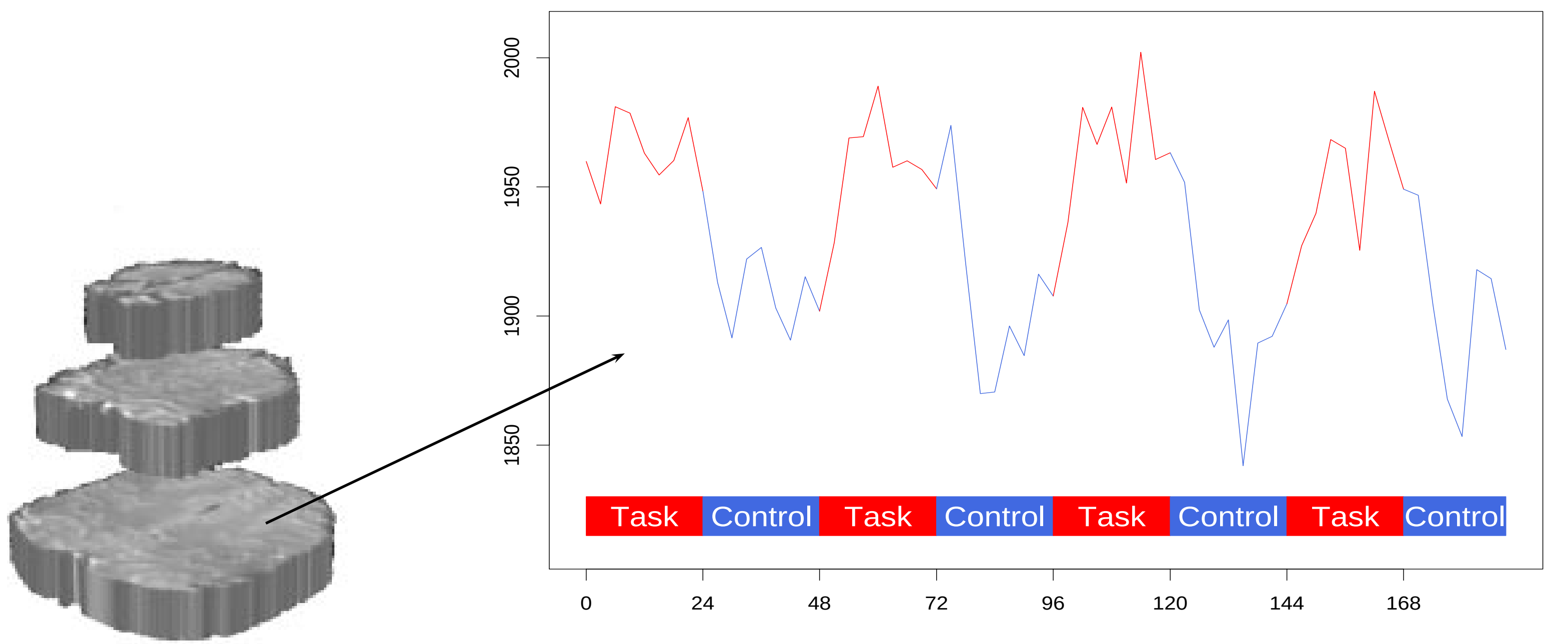
Motivating Example #1: fMRI

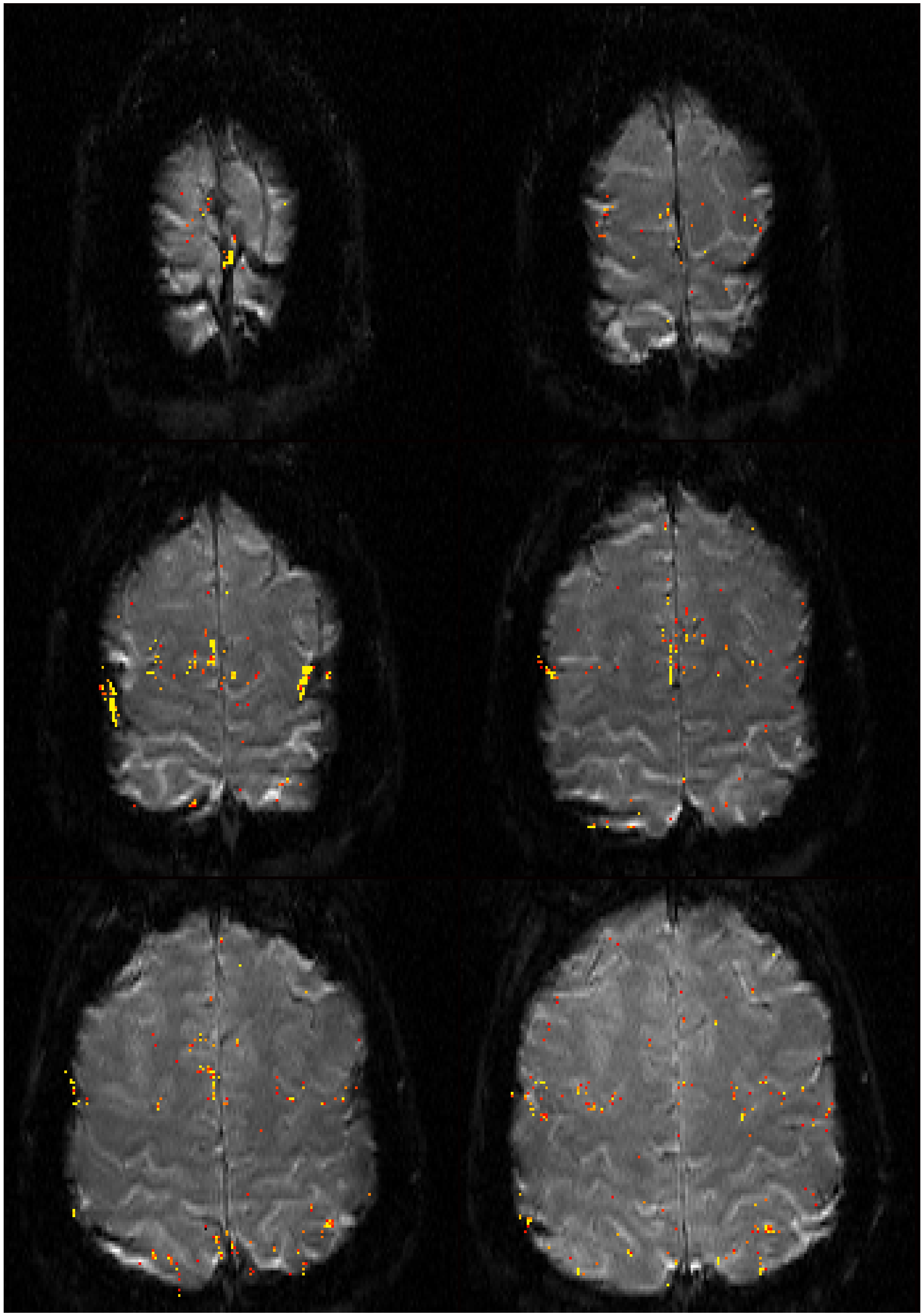
- fMRI Data: Time series of 3-d images acquired while subject performs specified tasks.



- Goal: Characterize task-related signal changes caused (indirectly) by neural activity. [See, for example, Genovese (2000), *JASA* 95, 691.]

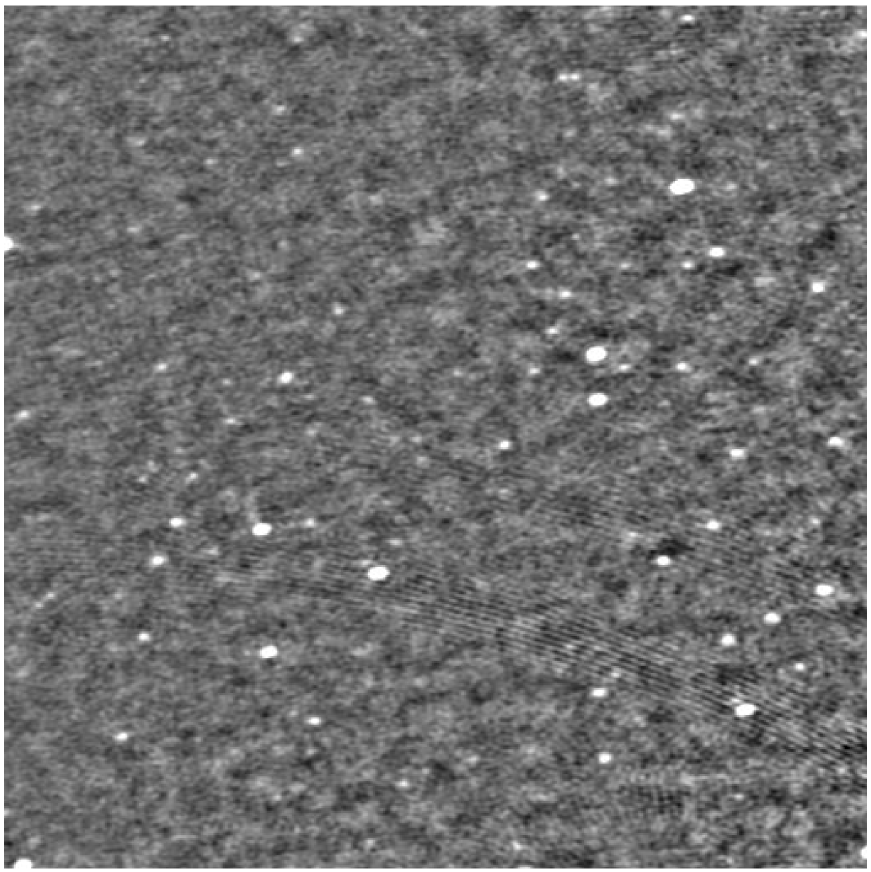
fMRI (cont'd)

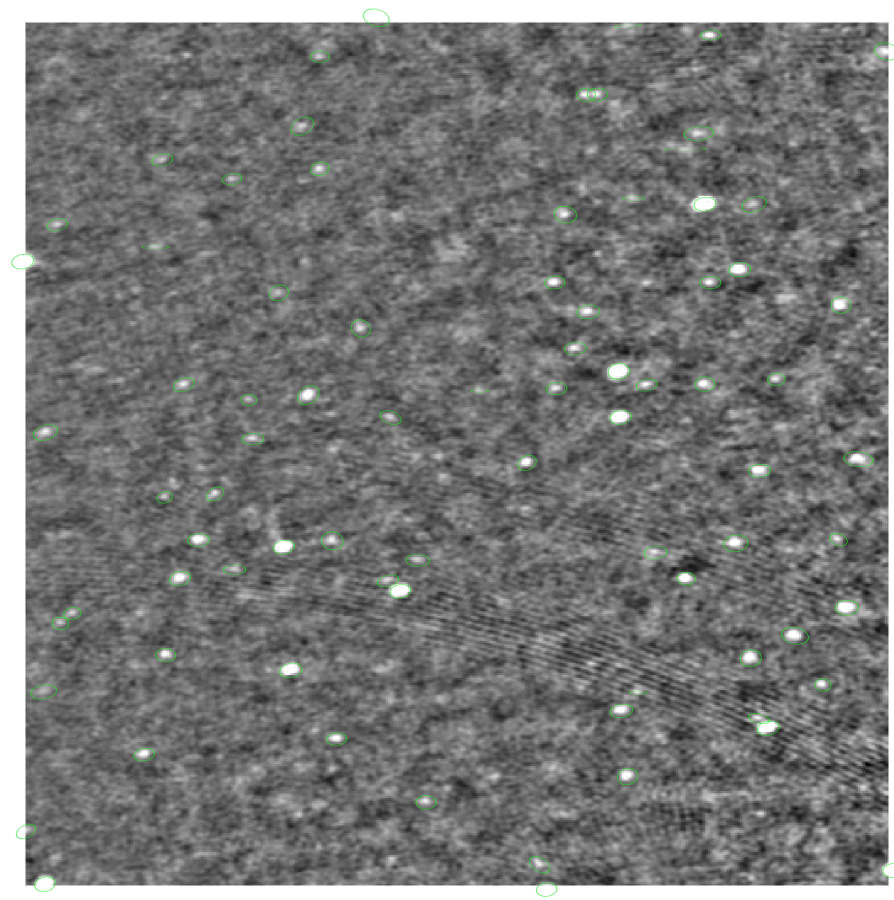
Perform hypothesis tests at many thousands of volume elements to identify loci of activation.



Motivating Example #2: Source Detection

- Interferometric radio telescope observations processed into digital image of the sky in radio frequencies.
- Signal at each pixel is a mixture of source and background signals.





Motivating Example #3: DNA Microarrays

- New technologies allow measurement of gene expression for thousands of genes simultaneously.

Condition 1 (Subject)

Gene	1	2	3	...
1	X_{111}	X_{121}	X_{131}	$\ldots$
2	X_{211}	X_{221}	X_{231}	$\ldots$
3	$\vdots$	$\vdots$	$\vdots$	$\ldots$
4				
5				
6				
$\vdots$				

Condition 2 (Subject)

Gene	1	2	3	...
1	X_{112}	X_{122}	X_{132}	$\ldots$
2	X_{212}	X_{222}	X_{232}	$\ldots$
3	$\vdots$	$\vdots$	$\vdots$	$\ldots$
4				
5				
6				
$\vdots$				

- Goal: Identify genes associated with differences among conditions.
- Typical analysis: hypothesis test at each gene.

Recent Work on FDR

Abromovich, et al. (2000)

Benjamini & Hochberg (1995)

Benjamini & Liu (1999)

Benjamini & Hochberg (2000)

Benjamini & Yekutieli (2001)

Efron, et al. (2001)

Finner and Roters (2001, 2002)

Genovese & Wasserman (2001,2002)

Sarkar (2002)

Storey (2001,2002)

Storey & Tibshirani (2001)

Tusher, Tibshirani, Chu (2001)

The Multiple Testing Problem

- Perform m simultaneous hypothesis tests.

  Classify results as follows:

	H_0 Retained	H_0 Rejected	Total
H_0 True	$M_{0\|0}$	$M_{1\|0}$	M_0
H_0 False	$M_{0\|1}$	$M_{1\|1}$	M_1
Total	$m - R$	R	m

  Here, $M_{i|j}$ is the number of H_i chosen when H_j true.

  Only R and m are observed.

False Discovery and Nondiscovery Proportions

- Define the False Discovery Proportion (FDP) and the False Nondiscovery Proportion (FNP) as follows:

$$\text{FDP} = \begin{cases} \dfrac{M_{1|0}}{R} & \text{if } R > 0, \\ 0, & \text{if } R = 0. \end{cases} \qquad \text{FNP} = \begin{cases} \dfrac{M_{0|1}}{m - R} & \text{if } R < m, \\ 0, & \text{if } R = m. \end{cases}$$

- Then, the False Discovery Rate (FDR) and the False Nondiscovery Rate (FNR) are given by

$$\text{FDR} = \text{E}(\text{FDP}) \qquad \text{FNR} = \text{E}(\text{FNP}).$$

Road Map

1. Preliminaries
   - Models for FDP and FNP
   - FDP and FNP as stochastic processes
2. Plug-in Procedures
   - Asymptotic behavior of BH procedure
   - Optimal Thresholds
3. Confidence Thresholds
   - Controlling probability of exceeding specified proportion of false discoveries
4. Estimating the p-value distribution

Basic Models

- Let $P^m = (P_1, \ldots, P_m)$ be the p-values for the m tests.
- Let $H^m = (H_1, \ldots, H_m)$ where $H_i = 0$ (or 1) if the i^{th} null hypothesis is true (or false).
- We assume the following model:

$$
\begin{aligned}
H_1, \ldots, H_m &\text{ iid Bernoulli}\langle a \rangle \\
\Xi_1, \ldots, \Xi_m &\text{ iid } \mathcal{L}_{\mathcal{F}} \\
P_i \mid H_i = 0, \Xi_i = \xi_i &\sim \text{Uniform}\langle 0, 1 \rangle \\
P_i \mid H_i = 1, \Xi_i = \xi_i &\sim \xi_i.
\end{aligned}
$$

where $\mathcal{L}_{\mathcal{F}}$ denotes a probability distribution on a class $\mathcal{F}$ of distributions on $[0, 1]$.

Basic Models (cont'd)

- Marginally, $P_1, \ldots, P_m$ are drawn iid from

$$G = (1 - a)U + aF,$$

where U is the Uniform$\langle 0, 1\rangle$ cdf and

$$F = \int \xi \, d\mathcal{L}_{\mathcal{F}}(\xi).$$

- Typical examples:
  - Parametric family: $\mathcal{F}_\Theta = \{F_\theta\colon\ \theta \in \Theta\}$
  - Concave, continuous distributions

$$\mathcal{F}_C = \{F\colon\ F \text{ concave, continuous cdf with } F \geq U\}.$$

- Can also work under what we call the *conditional model* where $H_1, \ldots, H_m$ are fixed, unknown.

Multiple Testing Procedures

- A multiple testing procedure T is a map $[0,1]^m \longrightarrow [0,1]$, where the null hypotheses are rejected in all those tests for which $P_i \leq T(P^m)$. Often call T a *threshold*.
- Examples:

Uncorrected testing	$T_{\mathrm{U}}(P^m) = \alpha$
Bonferroni	$T_{\mathrm{B}}(P^m) = \alpha/m$
Fixed threshold at t	$T_t(P^m) = t$
First r	$T_{(r)}(P^m) = P_{(r)}$
Benjamini-Hochberg	$T_{\mathrm{BH}}(P^m) = \sup\{t\colon \widehat{G}(t) = t/\alpha\}$
Oracle	$T_{\mathrm{O}}(P^m) = \sup\{t\colon G(t) = (1-a)t/\alpha\}$
Plug In	$T_{\mathrm{PI}}(P^m) = \sup\{t\colon \widehat{G}(t) = (1-\widehat{a})t/\alpha\}$
Regression Classifier	$T_{\mathrm{Reg}}(P^m) = \sup\{t\colon \widehat{\mathsf{P}}\{H_1{=}1 \mid P_1{=}t\} > 1/2\}$

FDP and FNP as Stochastic Processes

- Inherent difficulty: FDP, FNP, and a general threshold all depend on the same data.
- Define the FDP and FNP processes, respectively, by

$$\mathsf{FDP}(t) \equiv \mathsf{FDP}(t; P^m, H^m) = \frac{\sum_i 1\Big\{P_i \le t\Big\}(1 - H_i)}{\sum_i 1\Big\{P_i \le t\Big\} + 1\Big\{\text{all } P_i > t\Big\}}$$

$$\mathsf{FNP}(t) \equiv \mathsf{FNP}(t; P^m, H^m) = \frac{\sum_i 1\Big\{P_i > t\Big\} H_i}{\sum_i 1\Big\{P_i > t\Big\} + 1\Big\{\text{all } P_i \le t\Big\}}.$$

- For procedure T, the FDP and FNP are obtained by evaluating these processes at $T(P^m)$.

FDP and FNP as Stochastic Processes (cont'd)

- Both these processes converge to Gaussian processes outside a neighborhood of 0 and 1 respectively.
- For example, define

$$Z_m(t) = \sqrt{m}\left(\mathsf{FDP}(t) - Q(t)\right), \quad \delta \le t \le 1,$$

  where $0 < \delta < 1$ and $Q(t) = (1-a)U/G$.

- Let Z be a mean 0 Gaussian process on $[\delta, 1]$ with covariance kernel

$$K(s,t) = a(1-a)\,\frac{(1-a)stF(s \wedge t) \;+\; aF(s)F(t)(s \wedge t)}{G^2(s)\,G^2(t)}.$$

- Then, $Z_m \rightsquigarrow Z$.

Plug-in Procedures

- Let $\widehat{G}_m$ be the empirical cdf of P^m under the mixture model. Ignoring ties, $\widehat{G}_m(P_{(i)}) = i/m$, so BH equivalent to

$$T_{\mathrm{BH}}(P^m) = \max\left\{t\colon\ \widehat{G}_m(t) = \frac{t}{\alpha}\right\}.$$

  as Storey (2002) first noted.

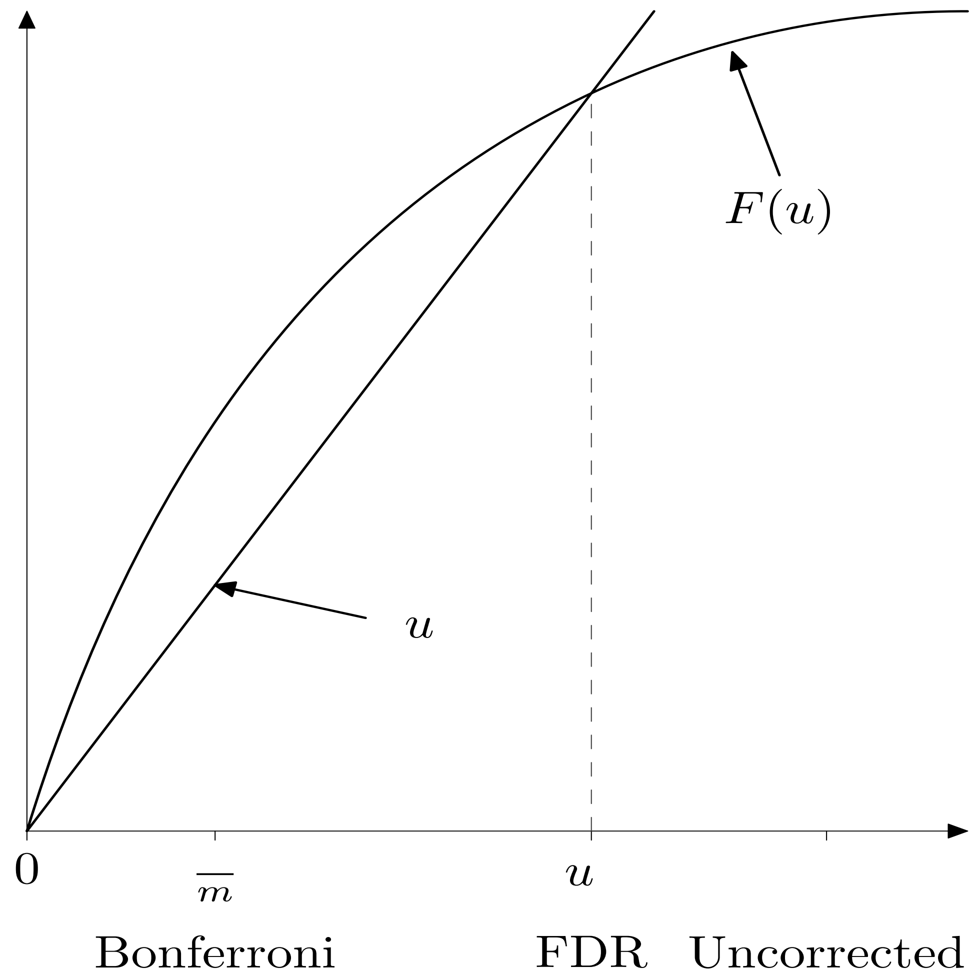
- One can think of this as a plug-in procedure for estimating

$$\begin{aligned} u^*(a, G) &= \max\left\{t\colon\ G(t) = \frac{t}{\alpha}\right\} \\ &= \max\left\{t\colon\ F(t) = \beta t\right\}, \end{aligned}$$

  where $\beta = (1 - \alpha + \alpha a)/\alpha a$.

Asymptotic Behavior of BH Procedure

This yields the following picture:



Optimal Thresholds

- Under the mixture model and in the continuous case,

$$\mathsf{E}(\mathsf{FDP}(T_{\mathrm{BH}}(P^m))) = (1-a)\alpha.$$

- The BH procedure overcontrols FDR and thus will not in general minimize FNR.
- This suggests using T_{PI}, the plug-in estimator for

$$\begin{aligned} t^*(a,G) &= \max\left\{t\colon\ G(t) = \frac{(1-a)t}{\alpha}\right\} \\ &= \max\left\{t\colon\ F(t) = (\beta - 1/\alpha)t\right\}, \end{aligned}$$

where $\beta - 1/\alpha = (1-a)(1-\alpha)/a\alpha$.
- Note that $t^* \geq u^*$.

Optimal Thresholds (cont'd)

- For each $0 \leq t \leq 1$,

$$\mathsf{E}(\mathsf{FDP}(t)) = \frac{(1-a)\,t}{G(t)} + O\left((1-t)^m\right)$$

$$\mathsf{E}(\mathsf{FNP}(t)) = a\,\frac{1-F(t)}{1-G(t)} + O\left((a+(1-a)t)^m\right).$$

- Ignoring $O()$ terms and choosing t to minimize E(FNP(t)) subject to E(FDP(t)) $\leq \alpha$, yields $t^*(a, G)$ as the optimal threshold.
- GW (2002) show that

$$\mathsf{E}(\mathsf{FDP}(t^*(\widehat{a}, \widehat{G}))) \leq \alpha + O(m^{-1/2}).$$

Confidence Thresholds

- In practice, it would be useful to have a procedure T_C that guarantees

$$\mathsf{P}_G\Big\{\mathsf{FDP}(T_C) > c\Big\} \leq \alpha$$

  for some specified c and α.

  We call this a $(1-\alpha, c)$ *confidence threshold procedure*.

- Four approaches: (i) an asymptotic Bootstrap threshold, (ii) an asymptotic closed-form threshold, (iii) an exact (small-sample) threshold requiring numerical search, and (iv) a Bayesian threshold.

- Here, I'll discuss the case where a is known.

  In general, all of this works using an estimator, but this introduces additional complexity.

Bootstrap Confidence Thresholds

- First guess: Choose T such that

$$\mathsf{P}_{\widehat{G}}\Big\{\mathsf{FDP}^*(T) \le c\Big\} \ge 1-\alpha.$$

- This fails. The problem is an additional bias term:

$$\begin{aligned} 1-\alpha &= \mathsf{P}_{\widehat{G}}\Big\{\mathsf{FDP}^*(T) \le c\Big\} \\ &\approx \mathsf{P}_{G}\Big\{\mathsf{FDP}(T) \le c + (Q(T) - \widehat{Q}(T))\Big\} \\ &\neq \mathsf{P}_{G}\Big\{\mathsf{FDP}(T) \le c\Big\}, \end{aligned}$$

  where $Q = (1-a)U/G$ and $\widehat{Q} = (1-a)U/\widehat{G}$.

- Can fix this with double bootstrap (harder) or DKW correction (easier).

Bootstrap Confidence Thresholds (cont'd)

- Let $\beta = \alpha/2$ and $\epsilon_m \equiv \epsilon_m(\beta) = \sqrt{\frac{1}{2m} \log\left(\frac{2}{\beta}\right)}$.
- Procedure
  1. Draw $H_1^* \ldots, H_m^*$ iid Bernoulli$\langle a \rangle$
  2. Draw $P_i^* | H_i^*$ from $(1 - H_i^*)U + H_i^* \widehat{F}$.
  3. Define $\Omega_c^*(t) = \sum_i 1\left\{P_i^* \leq t\right\}(1 - H_i^* - c)$.
  4. Use threshold defined by

$$T_C = \max\left\{t\colon \mathsf{P}_{\widehat{G}}\left\{\Omega_c^*(t) \leq -c\,\epsilon_m\right\} \geq 1 - \beta\right\}.$$

- Then,

$$\mathsf{P}_G\left\{\mathsf{FDP}(T_C) \leq c\right\} \geq 1 - \alpha + O\left(\frac{1}{\sqrt{m}}\right).$$

Closed-Form Asymptotic Confidence Thresholds

- Let

$$t_0 = Q^{-1}(c) \qquad \hat{t}_0 = \widehat{Q}^{-1}(c).$$

- Then define

$$T_C = \hat{t}_0 + \frac{\widehat{\Delta}_{m,\alpha}}{\sqrt{m}},$$

where $\widehat{\Delta}_{m,\alpha}$ is depends on a density estimate of $g = G'$.

- Then,

$$\mathsf{P}_G\Big\{\mathsf{FDP}(T_C) \leq c\Big\} \geq 1 - \alpha + o(1).$$

Closed-Form Asymptotic Confidence Thresholds

- Details:

$$\widehat{\Delta}_{m,\alpha} = \frac{z_{\alpha/2}\left(\sqrt{\widehat{K}_{Q^{-1}}(\widehat{t_0},\widehat{t_0})} + \widehat{g}(\widehat{t_0})\right) + 2\sqrt{\log m}}{1 - \widehat{a} - c\widehat{g}(\widehat{t_0})}$$

$$\widehat{K}_{Q^{-1}}(s,t) = \frac{\widehat{K}_Q(\widehat{Q}^{-1}(s), \widehat{Q}^{-1}(t))}{\widehat{Q'}(\widehat{Q}^{-1}(s))\widehat{Q'}(\widehat{Q}^{-1}(t))}$$

$$\widehat{K}_Q(s,t) = \frac{(1-\widehat{a})^2 st}{\widehat{G}^2(s)\widehat{G}^2(t)}\left[\widehat{G}(s \wedge t) - \widehat{G}(s)\widehat{G}(t)\right].$$

- This requires no bootstrapping but does require density estimation.

  This is analogous to the situation faced when estimating the standard error of a median.

Exact Confidence Thresholds

- Let $\mathcal{M}_\beta$ be a $1-\beta$ confidence set for M_0, derived from the Binomial$\langle m, 1-a\rangle$.
- Define

$$S(t; h^m, p^m) = \frac{\sum_i 1\{p_i \le t\}(1-h_i)}{\sum_i (1-h_i)} \qquad \text{[EDF of null p-values]}$$

$$\mathcal{U}_\beta(p^m) = \left\{ h^m \colon \sum_i (1-h_i) \in \mathcal{M}_\beta \text{ and } \| S(\cdot; h^m, p^m) - U \|_\infty \le \epsilon_{m_0}(\beta) \right\},$$

where $m_0 = \sum_i (1-h_i)$ and $\epsilon_{m_0}(\beta) = \sqrt{\log(2/\beta)/2m_0}$.

- Take $\beta = 1 - \sqrt{1-\alpha}$.

Exact Confidence Thresholds (cont'd)

- Let

$$T_C = \text{sup}\left\{t: \text{ FDP}(t; h^m, P^m) \leq c \text{ and } h^m \in \mathcal{U}_\beta(P^m)\right\}$$
$$\mathcal{G} = \left\{\text{FDP}(\cdot; h^m, P^m)\text{: } h^m \in \mathcal{U}_\beta(P^m)\right\}.$$

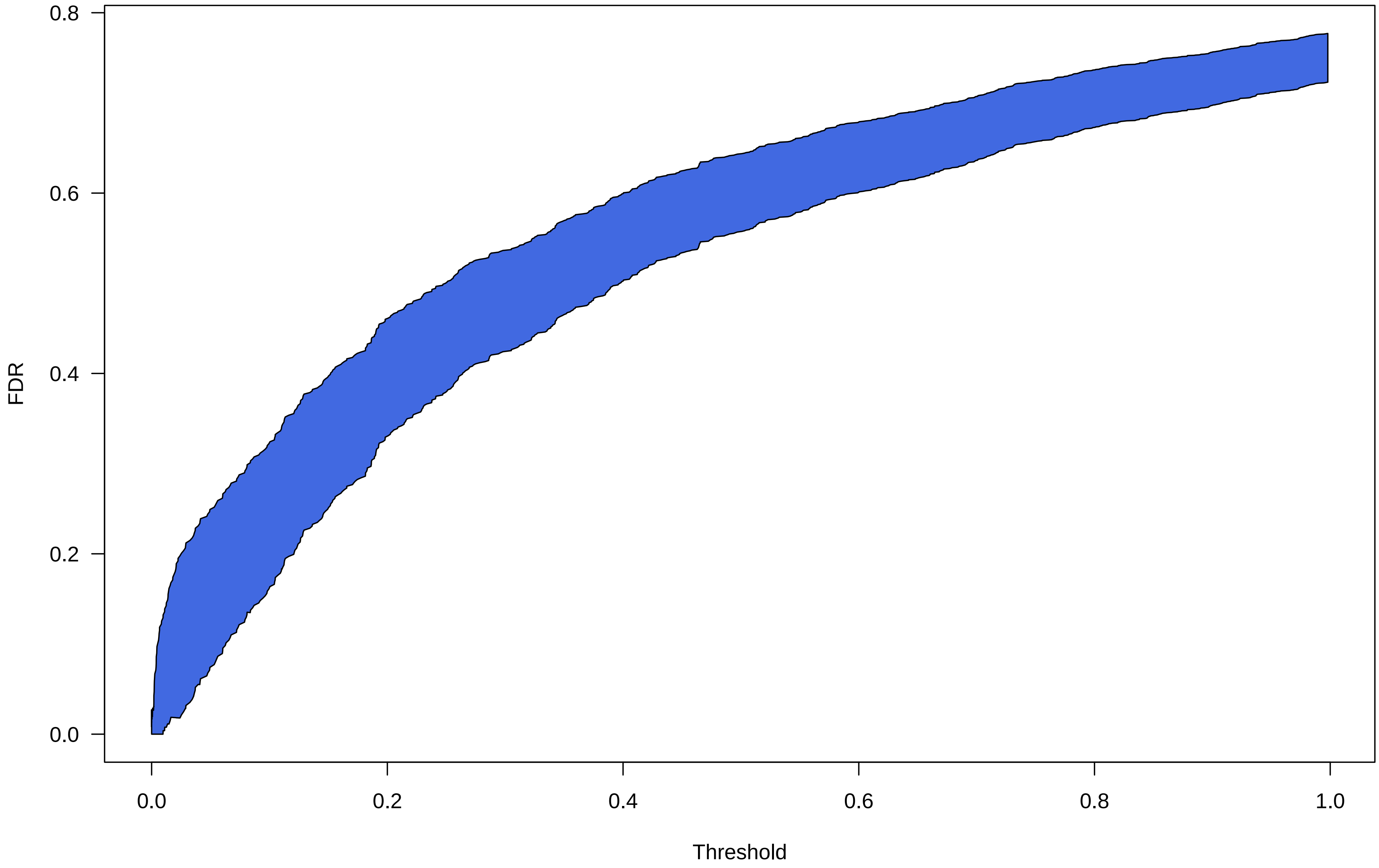
- Then,

$$\text{P}_G\left\{H^m \in \mathcal{U}_\beta(P^m)\right\} \geq 1 - \alpha,$$
$$\text{P}_G\left\{\text{FDP}(\cdot; H^m, P^m) \in \mathcal{G}\right\} \geq 1 - \alpha,$$
$$\text{P}_G\left\{\text{FDP}(T_C) \leq c\right\} \geq 1 - \alpha.$$

Hence, T_C is a $(1 - \alpha, c)$ confidence threshold procedure.

Exact Confidence Thresholds (cont'd)

$\mathcal{G}$ gives a confidence envelope for FDP(t) sample paths.



Estimating a and F

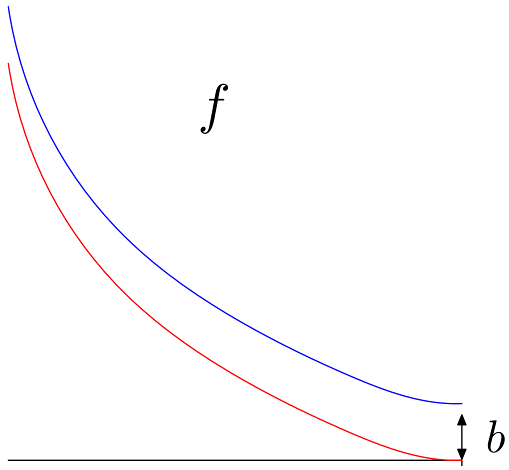
- Recall that the p-value distribution $G = (1 - a)U + aF$ where a and F are unknown.
- We need a good estimate of a for plug-in estimates,

$$T_{\mathrm{PI}}(P^m) = \max\left\{t\colon\ \widehat{G}(t) = \frac{(1-\widehat{a})t}{\alpha}\right\},$$

  that approximate the optimal threshold.
- We need good estimates of a and F for confidence thresholds.

Estimating a and F (cont'd)

- Identifiability and Purity



If $\min f = b > 0$, can write $F = (1-b)U + bF_0$,
$\mathcal{O}_G = \{(\widetilde{a}, \widetilde{F}) : \widetilde{F} \in \mathcal{F}, G = (1-\widetilde{a})U + \widetilde{a}\widetilde{F}\}$
may contain more than one element.

If $f = F'$ is decreasing with $f(1) = 0$, then (a, F) is identifiable.

- In general, let $\underline{a} \leq a$ be the smallest mixing weight in the orbit: $\underline{a} = 1 - \min_t g(t)$. This is identifiable.

  Storey (2002) notes that $0 \leq \sup_{0<t<1} \dfrac{G(t) - t}{1 - t} \leq \underline{a} \leq a \leq 1$.

- $a - \underline{a}$ is typically small: $a - \underline{a} = ae^{-n\theta^2/2}$ in the two-sided test of $\theta = 0$ versus $\theta \neq 0$ in the Normal$\langle\theta, 1\rangle$ model.

Estimating a and F (cont'd)

- Parametric Case
  - Derived a $1-\beta$ one-sided conf. int. for $\underline{a}$ and thus a. (a,θ) typically identifiable even if $a > \underline{a}$; use MLE.
- Non-parametric case:
  - Derived a $1-\beta$ one-sided conf. int. for $\underline{a}$ and thus a.
  - When F concave, get $\widehat{a}_{\mathrm{LCM}} = \underline{a} + O_P(m^{-1/3})$.
  - When F smooth enough, get $\widehat{a}_{\mathrm{S}} = \underline{a} + O_P(m^{-2/5})$.
  - Consistent estimate for F_0 if $\widehat{a}$ consistent for $\underline{a}$:

$$\widehat{F}_m = \operatorname*{argmin}_{H \in \mathcal{F}} \|\widehat{G} - (1-\widehat{a})U - \widehat{a}H\|_\infty.$$

Estimating a and F (cont'd)

- $\widehat{a}_{\mathrm{S}}$ uses "spacings" estimator (Swanepoel, 1999) to estimate $\min g(t)$. This yields

$$\frac{m^{2/5}}{(\log m)^{\delta}}(\widehat{a} - \underline{a}) \rightsquigarrow \text{Normal}\langle 0, (1 - \underline{a})^2 \rangle$$

- In the concave case, take $\widehat{g} = G'_{LCM}$ and $\widehat{a}_{\mathrm{LCM}} = 1 - \widehat{g}(1)$. A $1 - \alpha$ confidence interval for a is

$$\widehat{a}_{\mathrm{LCM}} \pm 4 q_{\alpha} \, |\widehat{g}(1)|^{1/3} \, n^{-1/3}$$

where $\mathsf{P}\left\{ \text{argmax}_h (W(h) - h^2) \geq q_{\alpha} \right\} = \alpha$ and W_h is a 2-sided Brownian motion tied down at 0.

Estimating a and F (cont'd)

- Confidence interval for a given by

$$\mathcal{A}_m = \left[\max_t \frac{\widehat{G}_m(t) - t - \epsilon_m(\alpha)}{1-t}, 1\right],$$

where $\widehat{G}_m$ is EDF and $\epsilon_m(\alpha) = \sqrt{\log(2/\alpha)/2m}$.

Then,

$$1 - \alpha \leq \inf_{a,F} \mathsf{P}\left\{a \in A_m\right\} \leq 1 - \alpha + R_m$$

where

$$R_m = \sum_j (-1)^j \frac{\alpha^{j^2}}{2^{j^2-1}} + O\left(\frac{(\log m)^2}{\sqrt{m}}\right)$$

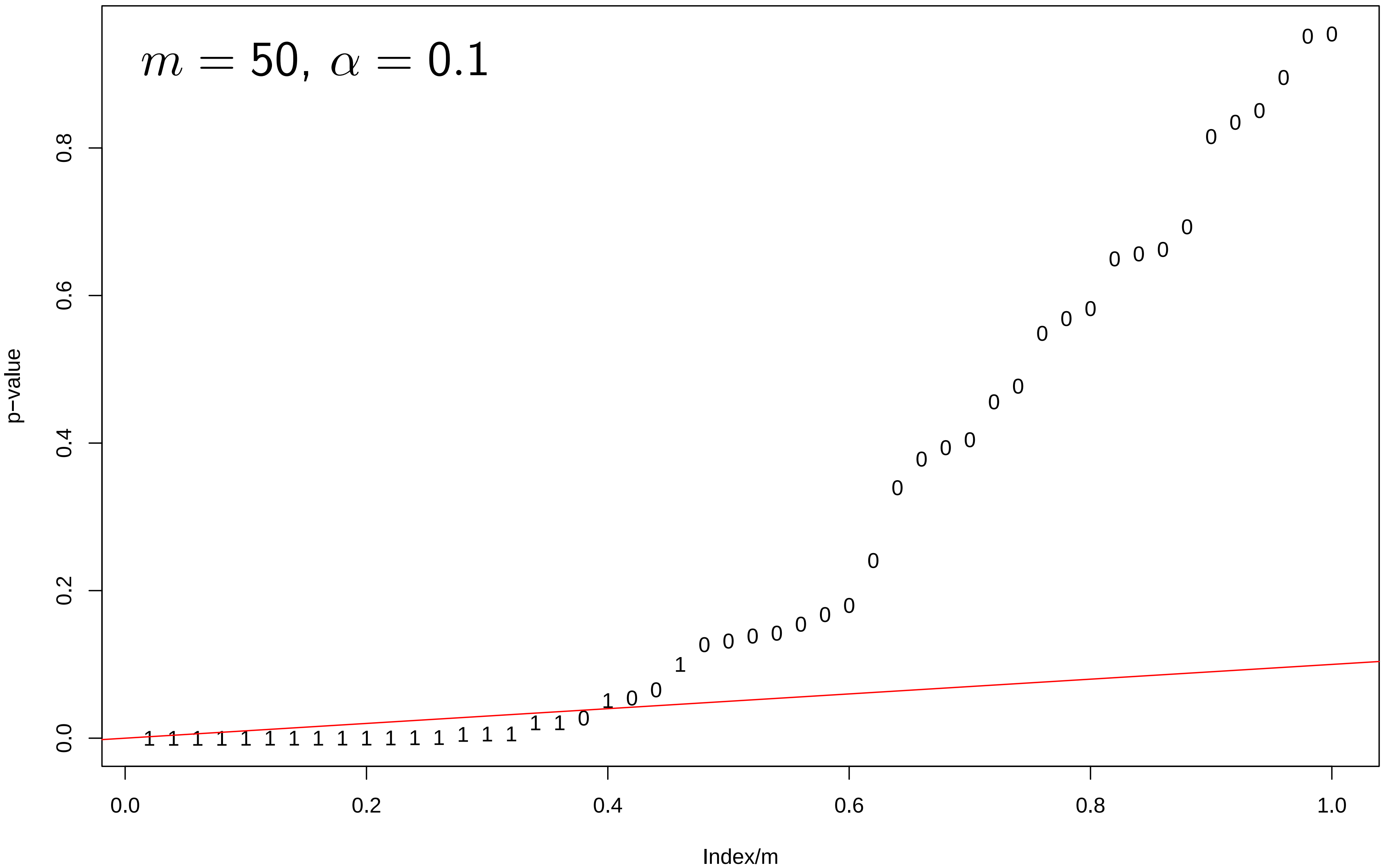
Take-Home Points

- Asymptotic view motivated by particular applications, but asymptotics appear to kick in rather quickly.
- Confidence thresholds address a question that collaborating scientists frequently raise.
- Helpful to think of FDP (FDR) and FNP (FNR) as stochastic processes.

  In general, the threshold and the FDP are coupled, and these correlations can have a large effect.
- Dependence

Recurring Notation

$m, M_0, M_{1\|0}$	# of tests, true nulls, false discoveries
a	Mixture weight on $a$lternative
$H^m = (H_1, \ldots, H_m)$	Unobserved true classifications
$P^m = (P_1, \ldots, P_m)$	Observed p-values
U	CDF of Uniform$\langle 0, 1\rangle$
F, f	Alternative CDF and density
$G = (1-a)U + aF$	Marginal CDF of P_i
$g = G'$	Marginal density of P_i
$\widehat{G}_m$	Estimate of G (e.g., empirical CDF of P^m)
$\epsilon_k(\beta) = \sqrt{\frac{1}{2k}\log\left(\frac{2}{\beta}\right)}$	DKW bound $1-\beta$ quantile of $\lVert \widehat{G}_k - G \rVert_\infty$



$m = 50,\ \alpha = 0.1$
p−value
Index/m
0.0
0.2
0.4
0.6
0.8
1.0

Bayesian Thresholds

- Bayesian Threshold bounds posterior FDR:

$$T_{\text{Bayes}} = \mathsf{sup}\{t : \ \mathsf{E}(\mathsf{FDP}(t) \mid P^m) \leq \alpha\}$$

- Similarly, can construct a posterior (c, α) confidence threshold $T_{\text{Bayes},c}$ by

$$T_{\text{Bayes},c} = \mathsf{sup}\{t : \ \mathsf{P}\Big\{\mathsf{FDP}(t) \leq c \mid P^m\Big\} \leq \alpha\}$$

EBT (Empirical Bayes Testing)

- Efron et al (2001) note that

$$\mathsf{P}\left\{H_i = 0 \mid P^m\right\} = \frac{(1-a)}{g(P_i)} \equiv q(P_i)$$

- Reject whenever $q(p) \leq \alpha$?
- For a, f unknown, $f \geq 0$ implies that

$$a \geq 1 - \min_p g(p) \Longrightarrow \widehat{a} = 1 - \min_p \widehat{g}(p).$$

- Then,

$$\widehat{q}(p) = \frac{1-\widehat{a}}{\widehat{g}(p)} = \frac{\min_s \widehat{g}(s)}{\widehat{g}(p)}$$

EBT versus FDR

- If we reject when $\mathsf{P}\Big\{H_i = 0 \mid P^m\Big\} \leq \alpha$, how many errors are we making?

- Under weak conditions, can show that

$$q(t) \leq \alpha \;\; \text{implies} \;\; Q(t) < \alpha$$

So EBT is conservative.

Behavior of $\widehat{q}$

- THEOREM. Let $\widehat{q}(t) = \frac{(1-a)}{\widehat{g}(t)}$. Suppose that

$$m^{\alpha}(\widehat{g}(t) - g(t)) \rightsquigarrow W$$

for some $\alpha > 0$, where W is a mean 0 Gaussian process with covariance kernel $\tau(v, w)$. Then

$$m^{\alpha}\left(\widehat{q}(t) - q(t)\right) \rightsquigarrow Z$$

where Z is a Gaussian process with mean 0 and covariance kernel

$$K_q(v, w) = \frac{(1-a)^2 \tau(v, w)}{g(v)^4 g(w)^4}.$$

Behavior of $\widehat{q}$ (cont'd)

- Parametric Case: $g \equiv g_\theta = (1-a) + a f_\theta(v)$ Then,

$$\text{rel}(v) = \frac{\widehat{\text{se}}(\widehat{q}(v))}{q(v)} \approx O\left(\frac{1}{\sqrt{m}}\right) \left|\frac{\partial \log g_\theta}{\partial d\theta}\right| = O\left(\frac{1}{\sqrt{m}}\right) |v-\theta| \quad \text{Normal case}$$

- Nonparametric Case

$$\widehat{g}(t) = \frac{1}{m}\sum_{i=1}^{m} \frac{1}{h_m} K\left(\frac{t-P_i}{h_m}\right)$$

$h_m = cm^{-\beta}$ where $\beta > 1/5$ (undersmooth). Then

$$\text{rel}_v = \frac{c}{m^{(1-\beta)/2}\sqrt{g(v)}}.$$