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.

<table>
<thead>
<tr>
<th>Gene</th>
<th>1</th>
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<th>Subject</th>
<th>Condition 2</th>
<th>Subject</th>
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<td>$X_{212}$</td>
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- 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)
Sarkar (2002)
Storey & Tibshirani (2001)
Tusher, Tibshirani, Chu (2001)
The Multiple Testing Problem

- Perform $m$ simultaneous hypothesis tests.

Classify results as follows:

<table>
<thead>
<tr>
<th></th>
<th>$H_0$ Retained</th>
<th>$H_0$ Rejected</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_0$ True</td>
<td>$M_{0</td>
<td>0}$</td>
<td>$M_{1</td>
</tr>
<tr>
<td>$H_0$ False</td>
<td>$M_{0</td>
<td>1}$</td>
<td>$M_{1</td>
</tr>
<tr>
<td>Total</td>
<td>$m - R$</td>
<td>$R$</td>
<td>$m$</td>
</tr>
</tbody>
</table>

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:

\[
FDP = \begin{cases} 
\frac{M_{1|0}}{R} & \text{if } R > 0, \\
0 & \text{if } R = 0.
\end{cases}
\]

\[
FNP = \begin{cases} 
\frac{M_{0|1}}{m - R} & \text{if } R < m, \\
0 & \text{if } R = m.
\end{cases}
\]

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

\[
\text{FDR} = \mathbb{E}(FDP) \quad \text{FNR} = \mathbb{E}(FNP).
\]
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:

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

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$(0, 1)$ cdf and

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

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

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

• 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 $[0, 1]^m \rightarrow [0, 1]$, 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 $T_U(P^m) = \alpha$
  - Bonferroni $T_B(P^m) = \frac{\alpha}{m}$
  - Fixed threshold at $t$ $T_t(P^m) = t$
  - First $r$ $T_{(r)}(P^m) = P_{(r)}$
  - Benjamini-Hochberg $T_{BH}(P^m) = \sup\{t: \hat{G}(t) = t/\alpha\}$
  - Oracle $T_{O}(P^m) = \sup\{t: G(t) = (1 - a)t/\alpha\}$
  - Plug In $T_{PI}(P^m) = \sup\{t: \hat{G}(t) = (1 - \hat{a})t/\alpha\}$
  - Regression Classifier $T_{Reg}(P^m) = \sup\{t: \hat{P}\{H_1=1|P_1=t\} > 1/2\}$
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

\[
FDP(t) \equiv FDP(t; P^m, H^m) = \frac{\sum \mathbb{1}\{P_i \leq t\} (1 - H_i)}{\sum \mathbb{1}\{P_i \leq t\} + \mathbb{1}\{\text{all } P_i > t\}}
\]

\[
FNP(t) \equiv FNP(t; P^m, H^m) = \frac{\sum \mathbb{1}\{P_i > t\} H_i}{\sum \mathbb{1}\{P_i > t\} + \mathbb{1}\{\text{all } P_i \leq t\}}.
\]

- For procedure \(T\), the FDP and FNP are obtained by evaluating these processes at \(T(P^m)\).
Both these processes converge to Gaussian processes outside a neighborhood of 0 and 1 respectively.

For example, define

\[ Z_m(t) = \sqrt{m} (\text{FDP}(t) - Q(t)), \quad \delta \leq t \leq 1, \]

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, \(Z_m \sim Z\).
Plug-in Procedures

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

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

as Storey (2002) first noted.

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

$$u^*(a, G) = \max \left\{ t : G(t) = \frac{t}{\alpha} \right\} = \max \left\{ t : F(t) = \beta t \right\},$$

where $\beta = (1 - \alpha + \alpha a)/\alpha a$. 
Asymptotic Behavior of BH Procedure

This yields the following picture:

![Graph showing the asymptotic behavior of BH Procedure](image-url)
Optimal Thresholds

- Under the mixture model and in the continuous case,
  \[ E(\text{FDP}(T_{BH}(P^m))) = (1 - a)\alpha. \]

- The BH procedure overcontrols FDR and thus will not in general minimize FNR.

- This suggests using \( T_{PI} \), the plug-in estimator for

  \[
  t^*(a, G) = \max \left\{ t : \ G(t) = \frac{(1 - a)t}{\alpha} \right\}
  = \max \left\{ t : \ F(t) = (\beta - 1/\alpha)t \right\},
  \]

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

- Note that \( t^* \geq u^* \).
Optimal Thresholds (cont’d)

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

$$E(\text{FDP}(t)) = \frac{(1-a)t}{G(t)} + O((1-t)^m)$$

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

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

- GW (2002) show that

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

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

$$P_G\{\text{FDP}(T_C) > c\} \leq \alpha$$

for some specified $c$ and $\alpha$.

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 $\alpha$ 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
  \[ P_G\{ \text{FDP}^*(T) \leq c \} \geq 1 - \alpha. \]

• This fails. The problem is an additional bias term:
  \[ 1 - \alpha = P_G\{ \text{FDP}^*(T) \leq c \} \]
  \[ \approx P_G\{ \text{FDP}(T) \leq c + (Q(T) - \hat{Q}(T)) \} \]
  \[ \neq P_G\{ \text{FDP}(T) \leq c \}, \]

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

• 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$(a)$
2. Draw $P_i^* | H_i^*$ from $(1 - H_i^*) U + H_i^* \hat{F}$.
3. Define $\Omega_c^*(t) = \sum_i 1\{P_i^* \leq t\} (1 - H_i^* - c)$.
4. Use threshold defined by

$$T_C = \max \left\{ t : \Pr[\hat{G}] \{ \Omega_c^*(t) \leq -c \epsilon_m \} \geq 1 - \beta \right\}.$$

Then,

$$\Pr[G] \{ \text{FDP}(T_C) \leq c \} \geq 1 - \alpha + O \left( \frac{1}{\sqrt{m}} \right).$$
Closed-Form Asymptotic Confidence Thresholds

- Let
  \[ t_0 = Q^{-1}(c) \quad \hat{t}_0 = \hat{Q}^{-1}(c). \]
- Then define
  \[ T_C = \hat{t}_0 + \frac{\hat{\Delta}_{m,\alpha}}{\sqrt{m}}, \]
  where \( \hat{\Delta}_{m,\alpha} \) is depends on a density estimate of \( g = G' \).
- Then,
  \[ P_G\{ \text{FDP}(T_C) \leq c \} \geq 1 - \alpha + o(1). \]
Closed-Form Asymptotic Confidence Thresholds

Details:

\[ \hat{\Delta}_{m, \alpha} = \frac{z_{\alpha/2} \left( \sqrt{\hat{K}_{Q^{-1}}(\hat{t}_0, \hat{t}_0)} + \hat{g}(\hat{t}_0) \right) + 2\sqrt{\log m}}{1 - \hat{a} - c\hat{g}(\hat{t}_0)} \]

\[ \hat{K}_{Q^{-1}}(s, t) = \frac{\hat{K}_Q(\hat{Q}^{-1}(s), \hat{Q}^{-1}(t))}{\hat{Q}'(\hat{Q}^{-1}(s))\hat{Q}'(\hat{Q}^{-1}(t))} \]

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

- 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$(m, 1 - a)$.
- Define
  \[
  S(t; h^m, p^m) = \frac{\sum_i 1\{p_i \leq t\} (1 - h_i)}{\sum_i (1 - h_i)} \quad \text{[EDF of null p-values]}
  \]
  \[
  \mathcal{U}_\beta(p^m) = \left\{ h^m: \sum_i (1 - h_i) \in \mathcal{M}_\beta \text{ and } \|S(\cdot; h^m, p^m) - U\|_\infty \leq \epsilon_{m_0}(\beta) \right\},
  \]
  where $m_0 = \sum_i (1 - h_i)$ and $\epsilon_{m_0}(\beta) = \sqrt{\log(2/\beta)/2m_0}$.
- Take $\beta = 1 - \sqrt{1 - \alpha}$. 
Let

$$T_C = \sup \{ t : \text{FDP}(t; h^m, P^m) \leq c \text{ and } h^m \in U_\beta(P^m) \}$$

$$G = \{ \text{FDP}(\cdot; h^m, P^m) : h^m \in U_\beta(P^m) \}.$$ 

Then,

$$P_G\{ H^m \in U_\beta(P^m) \} \geq 1 - \alpha,$$

$$P_G\{ \text{FDP}(\cdot; H^m, P^m) \in G \} \geq 1 - \alpha,$$

$$P_G\{ \text{FDP}(T_C) \leq c \} \geq 1 - \alpha.$$

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 $\alpha$ and $F$

- Recall that the p-value distribution $G = (1 - \alpha)U + \alpha F$ where $\alpha$ and $F$ are unknown.

- We need a good estimate of $\alpha$ for plug-in estimates,

$$T_{PI}(P^m) = \max \left\{ t: \hat{G}(t) = \frac{(1 - \hat{\alpha})t}{\alpha} \right\},$$

that approximate the optimal threshold.

- We need good estimates of $\alpha$ and $F$ for confidence thresholds.
Estimating \( a \) and \( F \) (cont’d)

- **Identifiability and Purity**

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

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

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

  Storey (2002) notes that
  \[ 0 \leq \sup_{0 < t < 1} \frac{G(t) - t}{1 - t} \leq a \leq a \leq 1. \]

- \( a - a \) is typically small: \( a - a = ae^{-n\theta^2/2} \) 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 $a$ and thus $a$. $(a, \theta)$ typically identifiable even if $a > \underline{a}$; use MLE.

- **Non-parametric case:**
  - Derived a $1 - \beta$ one-sided conf. int. for $a$ and thus $a$.
  - When $F$ concave, get $\hat{a}_{\text{LCM}} = a + O_P(m^{-1/3})$.
  - When $F$ smooth enough, get $\hat{a}_S = a + O_P(m^{-2/5})$.
  - Consistent estimate for $F_0$ if $\hat{a}$ consistent for $\underline{a}$:
    \[
    \hat{F}_m = \arg\min_{H \in \mathcal{F}} \| \hat{G} - (1 - \hat{a})U - \hat{a}H \|_{\infty}.
    \]
Estimating $a$ and $F$ (cont’d)

- $\hat{a}_S$ uses “spacings” estimator (Swanepoel, 1999) to estimate $\min g(t)$. This yields

$$\frac{m^{2/5}}{(\log m)^\delta} (\hat{a} - a) \sim \text{Normal}(0, (1 - a)^2)$$

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

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

where $P\{ \arg\max_h (W(h) - h^2) \geq q_\alpha \} = \alpha$ 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

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

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

Then,

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

where

$$R_m = \sum (-1)^j \frac{\alpha j^2}{2j^2 - 1} + O \left( \frac{(\log m)^2}{\sqrt{m}} \right)$$
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 alternative
- $H^m = (H_1, \ldots, H_m)$: 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 $P_i$
- $\hat{G}_m$: 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 $\|\hat{G}_k - G\|_\infty$
\( m = 50, \alpha = 0.1 \)
Bayesian Thresholds

- Bayesian Threshold bounds posterior FDR:

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

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

\[ T_{\text{Bayes}, c} = \sup \{ t : \ P\{\text{FDP}(t) \leq c \mid P^m\} \leq \alpha \} \]
EBT (Empirical Bayes Testing)

- Efron et al (2001) note that

\[
P\{H_i = 0 \mid P^m\} = \frac{(1 - a)}{g(P_i)} \equiv q(P_i)
\]

- Reject whenever \( q(p) \leq \alpha \)?

- For \( a, f \) unknown, \( f \geq 0 \) implies that

\[
a \geq 1 - \min_p g(p) \implies \hat{a} = 1 - \min_p \hat{g}(p).
\]

- Then,

\[
\hat{q}(p) = \frac{1 - \hat{a}}{\hat{g}(p)} = \frac{\min_s \hat{g}(s)}{\hat{g}(p)}
\]
EBT versus FDR

- If we reject when $P\{H_i = 0 \mid P^m\} \leq \alpha$, 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 $\hat{q}$

**Theorem.** Let $\hat{q}(t) = \frac{(1-a)}{g(t)}$. Suppose that

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

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

$$m^\alpha (\hat{q}(t) - q(t)) \rightsquigarrow Z$$

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 $\tilde{q}$ (cont’d)

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

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

- **Nonparametric Case**

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

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

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