Large-scale inference for the detection of sources in MUSE hyperspectral data. Towards robust error control.



F. Chatelain Joint work with R. Bacher, C. Meillier, O. Michel



JATIA, Strasbourg, January 25, 2019

MUSE instrument

Instrument for ESO, VLT, Chili (First light in 2014) :

• $[2D + \lambda \equiv 3D]$ imager = Integral field spectrograph



Observation of distant galaxies (thus, very young), and their possible halos

- dramatically faint except on a few characteristic lines
- understanding of universe, galaxy formation...

MUSE Data



Data Cube

Stack of \sim 3600 monochromatic images covering 60 \times 60 arcsec

- spatial resolution : .2 × .2 arcsec (300 × 300 pixels)
- spectral resolution : .14nm (spectral range : 465 – 930 nm)

Data Cube 300 \times 300 \times 3600

Redshift and detection

We want to detect 1) faint galaxies, or 2) galatic halos (hydrogen gas surrounding galaxies)

- Emission limited to a few wavelengths : Lyman- α emission line
- ... of unknown spectral position because of redshift

Redshift : during its trip to Earth, light emitted by a galaxy moving away from us (Universe expansion...) is shifted to the red (remember the ambulance !).



Calls for detection methods adapted to these large datasets.

1) Detection of faint galaxies : C. Meillier's PhD

Problem

Detect faint galaxies whose position, shape, spectrum, power, number... are unknown.



Bayesian Nonparametric approach : (marked) point process¹

- ▶ Object (galaxy) = a point (position) + marks (geometric ≈ elliptical object, and spectral parameters)
- Object configuration = realization of a marked point process
- naturally sparse representation of massive data fields : configuration of marked points + noise

^{1.} Meillier et al, IEEE TSP (2015)

1) Detection of faint galaxies : C. Meillier's PhD (Cont'd)

SELFI Results on HDFS data $^{\rm 2}$: comparison with MUSE and Hubble (HST) catalog

Total number of detected objects	298
Number of detected objects belonging to MUSE catalog	166 / 189
Number of detected objects belonging to HST catalog	(166+78)
Number of detected objects not belonging to any catalog	54
including potential galaxies	6

How to assess the significance of the detection list?

- no ground truth to assert the detection performance !
- need for a robust error control for these multiple inferences

^{2.} Meillier et al, A&A (2016)

2) Detection of galactic halo : R. Bacher's PhD

We have *n* pixels (e.g. n = 2500 for a 50 \times 50 neighborhood) to test for :

Which pixels have signal? / Which pixels belong to the galactic halo?



How to have guarantees on the detection results?

- no ground truth to assert the detection performance !
- need for a robust control, e.g. to guaranty the proportion of pixels among the detected set that are really part of the target ("purity" of the detection)

Outline

Introduction and Motivations MUSE instrument

Two detection problems

Multiple inference and Global error control

Multiple comparisons False Discovery Rate FDR BH Procedure

Detection of galatic sources : CGM

CGM multiple testing COMET procedure COMET Results

Conclusion and perspectives

Multiplicity problem and chance correlation

Lottery



- Winning probability for a given ticket is very low...
- But among the huge number of tickets, the probablity that there is at least one winning ticket is quite high !

Paul the octopus



- Paul predicts eight of the 2010 FIFA World Cup matches with a perfect score !
- Does it really means that Paul is an Oracle?
- Large-scale experiments : multiplying the comparisons dramatically increases the probability to obtain a good match by pure chance

Multiplicity problem for statistical testing

- T is the test statistics,
- \mathcal{R}_{α} is the region of rejection at level α : if H_0 is true, $\Pr(T \in \mathcal{R}_{\alpha}) = \alpha$

Multiple testing issue

- N independent statistics T_1, \ldots, T_N obtained under the null H_0
- Probability to reject at least one of the N null hypotheses :

$$\Pr\left(\exists T_i \in \mathcal{R}_\alpha\right) = 1 - \Pr\left(T_1, \dots, T_N \notin \mathcal{R}_\alpha\right) = 1 - \prod_{i=1}^N \Pr\left(T_i \notin \mathcal{R}_\alpha\right),$$
$$= 1 - \prod_{i=1}^N (1 - \alpha) = 1 - (1 - \alpha)^N$$

- For a usual significative level $\alpha = 0.05$, performing N = 20 tests gives a probability 0.64 to find a 'significative' discovery by pure chance...
- \mathbb{P} Pr (at least one false positive) \gg Pr (the *i*-th is a false positive)

Multiplicity problem in science

The Economist, 2013, "Unreliable research"



Many published research findings in top-ranked journals are not, or poorly, reproducible [loannidis, 2005]

Source: The Economist

if the test power is only 0.4, 40 true positives in average for 45 false positives. Is this significant?

Large-Scale Hypothesis Testing [Efron, 2010]

Era of Massive Data Production

- "omics" revolution, e.g. microarrays measures expression levels of tens of thousands of genes for hundreds of subjects
- ▶ astrophysics, e.g. MUSE spectro-imager delivers cubes of 300×300 images for 3600 wavelengths : detecting faint sources leads to $N \approx 3 \times 10^8$ tests in a pixelwise approach

Large-Scale methodology

- statistical inference and hypothesis testing theory devolopped in the early 20th century (Pearson, Fisher, Neyman, ...) for small-data sets collected by individual scientist
- corrections are needed to assess significancy in large-scale experiments

P-values : an universal language for hypothesis testing

Intuitive definition

p-value \equiv probability of obtaining a result as extreme or "more extreme" than the observed statistics, under H_0

One-sided test example

- ► *T* is the test statistic, *t*_{obs} an observed realization of *T*
- H_0 rejected when t_{obs} is too large : $\mathcal{R}_{\alpha} = \{t : t \ge \eta_{\alpha}\}$

$$p(t_{obs}) = \Pr_{H_0} (T \ge t_{obs})$$



Mathematical definition

Smallest value of α such that $t_{obs} \in \mathcal{R}_{\alpha}$

$$p(t_{\rm obs}) = \inf_{\alpha} \{ t_{\rm obs} \in \mathcal{R}_{\alpha} \}$$

Property of *p*-values

Let P = p(T) be the random variable. If H_0 is true

$$\operatorname{Pr}_{H_0}(P \leq u) = \operatorname{Pr}_{H_0}(T \in \mathcal{R}_u) = u,$$

so p-value \equiv transformation of the test statistics to be uniformly distributed under the null (whatever the distribution of *T*)

Statistical hypothesis test based on p-value

- H_0 : p-value has a uniform distribution on [0, 1]: $P \sim U([0, 1])$
- H_1 : p-value is stochastically lower than $\mathcal{U}([0,1])$: $\Pr_{H_1}(P \le u) = \Pr_{H_1}(T \in \mathcal{R}_u) > u$,
 - regions the smaller is $p \equiv p(t_{obs})$, the more decisevely is H_0 rejected
 - so for a given α , H_0 is rejected at level α if $p \leq \alpha$

Counting the errors in multiple testing

N hypothesis tests with a common procedure

		Decision			
		H ₀ retained	H ₀ rejected	Total	
Actual	H ₀ true	V	U	N ₀	
	H ₀ false	S	Т	<i>N</i> ₁	
	Total	N-R	R	N	

- $N_0 = \#$ true nulls, $N_1 = \#$ true alternatives
- ► U = # False Positives ← Type I Errors
- T = # True Positives,
- R = # Rejections

How to define, and control, a global Type I Error rate/criterion?

False Discovery Rate FDR [Benjamini and Hochberg, 1995]

"Discovery" terminology

- $R \equiv$ # Discoveries (Detections or Positives)
- ► $U \equiv \#$ False Discoveries (False Positives) \leftarrow Type I errors,
- $T \equiv$ # True Discoveries (True Positives),

	Decision			
		H ₀ retained	H ₀ rejected	Total
Actual	H ₀ true	V	U	N ₀
Actual	H ₀ false	S	Т	N ₁
	Total	N - R	R	N
Definition				
FDP $\equiv \frac{U}{R \lor 1}$, where $R \lor 1 \equiv \max(R, 1) \leftarrow$ False Discovery Proportion				
$FDR \equiv E [FDP] = E \left\lfloor \frac{U}{R \lor 1} \right\rfloor \leftarrow False Discovery Rate$				

- single test errors (e.g. PFA controls in average the U/N₀ ratio), or power, are calculated horizontally in the table
- False Discovery Rate is calculated vertically (Bayesian flavor)

False Discovery Rate FDR [Benjamini and Hochberg, 1995]

"Discovery" terminology

- $R \equiv$ # Discoveries (Detections or Positives)
- ► $U \equiv \#$ False Discoveries (False Positives) \leftarrow Type I errors,
- $T \equiv$ # True Discoveries (True Positives),

		Decision			
		H ₀ retained	H ₀ rejected	Total	
Actual	H ₀ true	V	U	N ₀	
Actual	H ₀ false	S	Т	N ₁	
	Total	N - R	R	N	
Definition					
$FDP \equiv \frac{U}{R \lor 1}, \text{ where } R \lor 1 \equiv \max(R, 1) \leftarrow \text{False Discovery Proportion}$ $FDR \equiv E [FDP] = E \left[\frac{U}{R \lor 1}\right] \leftarrow \text{False Discovery Rate}$					

- single test errors (e.g. PFA controls in average the U/N_0 ratio), or power, are calculated horizontally in the table
- False Discovery Rate is calculated vertically (Bayesian flavor)

False Discovery Rate FDR [Benjamini and Hochberg, 1995]

"Discovery" terminology

- ► R = # Discoveries (Detections or Positives)
- ▶ $U \equiv \#$ False Discoveries (False Positives) \leftarrow Type I errors,
- ▶ $T \equiv$ # True Discoveries (True Positives),

		Decision			
		H_0 retained	H ₀ rejected	Total	
Actu	H_0 true	V	U	N ₀	
Acit	H_0 false	S	Т	N ₁	
	Total	N - R	R	N	
Definition					
$FDP \equiv \frac{U}{R \lor 1}, \text{ where } R \lor 1 \equiv \max(R, 1) \leftarrow \text{False Discovery Proportion}$ $FDR \equiv E [FDP] = E \left[\frac{U}{R \lor 1}\right] \leftarrow \text{False Discovery Rate}$					

- single test errors (e.g. PFA controls in average the U/N_0 ratio), or power, are calculated horizontally in the table
- False Discovery Rate is calculated vertically (Bayesian flavor)

Source detection example

Multiple testing problem

Statistical linear model (source + noise) for each i = 1, ..., N

$$X_i = \mu r_i + \epsilon_i$$

with $\mu > 0$, $r_i \in \{0, 1\}$, $\epsilon_i \sim \mathcal{N}(0, 1)$

- H_0 : null hypothesis \equiv absence of signal, i.e. $r_i = 0$
- H_1 : alternative hypothesis \equiv presence of signal, i.e. $r_i = 1$

Test statistics

for each i

- X_i is the test statistics
- ▶ $p_i = 1 \Phi(X_i)$, where Φ is the standard normal cdf, is the associated p-value

How to choose a good threshold *t* to reject the tests s.t. $p_i \le t$?

Ordered p-values plot for N = 100, $N_0 = 80$, $\mu = 3$, $\alpha = 0.1$

Try something between Bonferroni and single test control : choose $t_i = q \frac{i}{N}$ (here $q = \alpha = 0.1$)



Benjamini-Hochberg (BH) procedure

BH procedure ³

- ▶ Ordered p-values $p_{(1)} \le p_{(2)} \le \ldots \le p_{(N)}$, let $p_{(0)} = 0$ by convention
- ▶ For a given FDR control level $0 \le q \le 1$:
 - find the largest \hat{k} s.t. $p_{(k)} \leq q \frac{k}{N}$
 - reject H_0 for all $p_{(i)}$, $i = 1, \ldots, \hat{k}$

Theorem

Under the independence assumption (or specific positive dependence) among the tests, BH procedure controls the FDR at level q.

- learning from the other experiments idea
- "testimation problem": blurs the line between testing and estimation

^{3.} Benjamini and Hochberg, JRSS, Series B (1995)

Popularity of FDR and BH procedure



Historical context and citations⁴ of the seminal paper [Benjamini and Hochberg, 1995]

FDR for Big Data

Large-scale hypothesis testing in many fields

- DNA microarray, genomics, fMRI data,....
- Several works with astronomical imaging applications since the early 2000s

^{4.} thanks to Marine Roux for the picture

Outline

Introduction and Motivations

MUSE instrument Two detection problems

Multiple inference and Global error control

Multiple comparisons False Discovery Rate FDR BH Procedure

Detection of galatic sources : CGM

CGM multiple testing COMET procedure COMET Results

Conclusion and perspectives

Detection of galactic halo : CGM

We want to explore the gas halo surrounding a galaxy : Circum galactic medium or CGM).

Galaxy properties

- Spatially limited (quasi-punctual)
- Lyman emission line + spectral continuum (+ other lines)
- Known spatial and spectral (redshift) positions

Halo properties

- Hydrogen gas
- Emission only in Lyman line
- Spatial extension around the galaxy
- Lyman emission similar (in first approx.) to the galaxy one

multiple testing : need to explore a great number of pixels around the galaxy in search of the Lyman signature.

CGM detection problem

Goal : Detect a quasi-connected multipixel target, while ensuring global control of errors

On each pixel *i*, detection of a positive signal using a one-sided test :

$$\begin{cases} H_0: \boldsymbol{y}_i = \boldsymbol{\epsilon}, \\ H_1: \boldsymbol{y}_i = \alpha_i \boldsymbol{d} + \boldsymbol{\epsilon}, \quad \text{with } \alpha_i > \boldsymbol{0}, \end{cases}$$

- ▶ $\epsilon \in \mathbb{R}^{l}$: noise vector of unknown distribution but assumed **symmetrical**
- $\boldsymbol{d} \in \mathbb{R}^{l}$: known reference (Lyman signature)
- $\boldsymbol{y}_i \in \mathbb{R}^l$: spectrum vector
- set extension to sparse representation with multiple atoms d_k , k = 1, ..., K.

Application of BH procedure to our case

Simple but generalizable approach : matched filter test statistics $\{w_i \equiv d^T y_i\}_{1 \le i \le n}$

spatial, or spectral, or 3D (spatial+spectral) templates d

Example : spatial matched filter



FDR control for matched filter test statistics

Testing problem

For each pixel *i*,

$$\begin{cases} H_0: \boldsymbol{y}_i = \boldsymbol{\epsilon}, \\ H_1: \boldsymbol{y}_i = \alpha_i \boldsymbol{d} + \boldsymbol{\epsilon}, \quad \text{with } \alpha_i > \mathbf{0}, \end{cases}$$

Exact FDR control

Assuming

- A Gaussian noise ε ∼ N(0, Σ), with positive (component) covariance Σ ≥ 0
- a positive template $d \ge 0$,

Then BH procedure apllied to matched filter statistics ensures a FDR control at specified level q

Issue : Misspecification of the null distribution

Deviation from the theoretical null

BH procedure requires so little : only the choice of the test statistics and its specification when the null hypothesis is true

- theoretical null hypothesis usually derived in an idealized framework, (e.g. does not account for complex spatial/spectral correlations, spatial inhomogeneities, standardization...)
- unlikely to be correctly specified in large-scale testing !
- Iarge-scale testing : possibility to detect and to correct possible miss-specification of the null hypothesis

Empirical null distribution⁵

Estimation of the H_0 distribution : based on the observations that are the most likely under theoretical H_0

^{5.} Efron, B., Cambridge University Press, 2010

Learning the null distribution

Key assumptions

- noise distribution is symmetrical;
- source contribution is positive.

Empirical *p*-values

Big picture : to have \widehat{F}_0 , the empirical distribution law of the w_i under \mathcal{H}_0 , it is sufficient to symmetrize the negative part of the empirical distribution of the data



- *p*-value associated to the pixel $i : p_i = 1 \hat{F}_0(w_i)$.
- $^{\mbox{\tiny ES}}$ We can then apply the BH procedure to the empirical $p\mbox{-values} \to empirical\,{\rm BH}$ (EBH) 6

^{6.} Bacher, R. et al. in IEEE TSP (2017)

Barber and Candes procedure (BC)

BH procedure : the most well known but not always the most relevant.

A recent alternative : the BC procedure⁷

Build control statistics w_i that are

- ▶ symmetrical under \mathcal{H}_0 , i.e. $\mathbb{P}(w_i > t | i \in \mathcal{H}_0) = \mathbb{P}(w_i < -t | i \in \mathcal{H}_0)$,
- ▶ stochastically greater under \mathcal{H}_1 , i.e. $\mathbb{P}(w_i > t | i \in \mathcal{H}_1) > \mathbb{P}(w_i > t | i \in \mathcal{H}_0)$.

We sort w_i by absolute decreasing order : $|w_{(1)}| \ge |w_{(i)}| \ge |w_{(n)}|$.

We control at level q by rejecting $|w_{(1)}|, \ldots, |w_{(\widehat{k})}|$ where :

$$\widehat{k} = \max\left\{k : \frac{1 + \#\{w_{(i), i \le k} < 0\}}{1 \lor \#\{w_{(i), i \le k} > 0\}} < q\right\}$$

^{7.} Barber and Candes, Ann. Stat. (2015)

Control statistics

Knockoff issue

In (BC 2015) construction of the control statistics using knockoffs

Iow power and high computational cost in high dimension.

Here we already have the following hypothesis :

- noise distribution is symmetrical.
- sources have a positive contribution
- **Easy** build of the control statistics $\{w_i \equiv \boldsymbol{d}^T \boldsymbol{y}_i\}_{1 \le i \le n}$.

Estimate of the False Discovery Proportion FDP (among the $w_i > 0$ discovered in a set A) :

$$\widehat{FDP} = \frac{1 + \#\{i \in \mathcal{A}, w_i < 0\}}{1 \lor \#\{i \in \mathcal{A}, w_i > 0\}}$$

With these control statistics, and BC procedures can be shown to be equivalents. How can we now gain in power?

COMET idea

The BC procedure sort statistics by absolute value before looking at the signs. BUT ... we can sort the statistics in another way, for ex. here to promote connectivity.

Algorithm

Region growth :

- start from an already detected region (galactic core)
 - add to the area the new pixels of interest from the neighborhood (cf next slide)
 - estimate the \widehat{FDP} on the pixels of this area
 - iterate onto the new neighborhood of the extended area
- stop onto the largest set of selection with \widehat{FDP} inferior to the given FDR
- ▶ in this set of exploration A we only keep as detection pixels *i* with $w_i \ge 0$

To control FDR, the selection procedure must follow [P1] :

Post-selection symmetry [P1]

For any *selected* pixel *j* corresponding to a true null hypothesis, the control statistic w_j is symmetrically distributed.

Greedy approach proposed

At each step, the greatest statistic (in absolute value) among the neighbors is selected.

COMET in action



To summarize : EBH

FDR control using EBH : thresholding of *p*-values pondered by the number of tests



To summarize : BC

FDR control using BC : sort statistics control by absolute value



To summarize : COMET

FDR control by COMET : sort statistics control using region growth



COMET properties

Exact control of FDR if independence of the noise

Let the noise vectors $\epsilon_1, \ldots, \epsilon_n$ be symmetrically distributed and independent. Then the COMET procedure ensures an exact control of FDR :

$$\mathbb{E}\left[\frac{U}{R\vee 1}\right]\leq q$$

Asymptotic control if correlated noise

Under the assumption of weakly dependent noise, if the control statistics are symmetrically distributed under \mathcal{H}_0 , COMET ensures an asymptotic control of FDR

Rk 1 : MUSE data follow this second case (short-range correlations). Rk 2 : Note that these results do not require any stationarity of the noise.

Results (simulation)





- Same error control
- Increase in detection power
- Power independent of total number of tests (i.e. size of explored region)

1.0

Application to real data

Preprocessing

- continuum subtraction
- SNR enhancement

Spectral variability

Detection over a dictionary of spectral signatures

- ► **d**₀ : spatial mean of galaxy core spectra.
- **D** : dictionary of shifts of **d**₀.
- Spectral Angular Distance (SAD) .

$$SAD(\boldsymbol{d}_0, \boldsymbol{x}) = rac{\langle \boldsymbol{d}_0, \boldsymbol{x}
angle}{||\boldsymbol{d}_0||||\boldsymbol{x}||}$$

• Test statistics : max over all atoms $\boldsymbol{w}_i = \max_k SAD(\boldsymbol{d}_k, \boldsymbol{x}_i)$

Demo time !



 \rightarrow https://phd.rbacher.fr/these-app/realDetect

Outline

Introduction and Motivations

MUSE instrument Two detection problems

Multiple inference and Global error control

Multiple comparisons False Discovery Rate FDR BH Procedure

Detection of galatic sources : CGM

CGM multiple testing COMET procedure COMET Results

Conclusion and perspectives

Conclusion

- Empirical approaches : no need to specify the law under H₀ (~ non parametric learning)
- Robust control of errors using this learning
- Simple hypotheses : noise symmetry and positivity of the source
- Take into account a spatial connectivity prior
- Generic detection method under FDR control with constraints
- Meaningful notion of "connected FDR" ("purity" of the detection)

Thank you !



References

- Benjamini, Y. and Hochberg, Y. (1995), "Controlling the false discovery rate : a practical and powerful approach to multiple testing," *Journal of the Royal Statistical Society*, Series B (Methodological), 289-300
- Barber, R. F. and Candes, E. (2015). "Controlling the False Discovery Rate via Knockoffs," Ann. Statist. 43 (2015), no. 5, 2055–2085.
- Efron, B. (2010), "Large-scale inference : empirical Bayes methods for estimation, testing, and prediction," (Vol. 1), Cambridge University Press
- Meillier, C. *et al.*, "Nonparametric Bayesian extraction of object configurations in massive data", in IEEE TSP, 2015, vol. 63(8).
- Meillier, C. et al., "SELFI : an object-based, Bayesian method for faint emission line source detection in MUSE deep field data cubes", in A&A 588, A140 (2016)
- Meillier, C. et al., "Error control for the detection of rare and weak signatures in massive data", in Proc. of EUSIPCO, 2015, Nice, France, pp. 1974-1978
- Bacher, R. et al., "Robust Control of Varying Weak Hyperspectral Target Detection With Sparse Nonnegative Representation," in IEEE TSP, 65 (13), pp. 3538-3550 (2017)
- Bacher, R. et al., "Global error control procedure for spatially structured targets," in Proc. of EUSIPCO, 2017, Kos, Greece, pp. 206-210