Non asymptotic detection of two component mixtures

B. Laurent 1, C. Marteau 2 and Cathy Maugis-Rabusseau 1 .

Colloque ANR MixStatSeq - Toulouse 2016

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Outline

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Unknown mean under H₀
 The dense regime
 The sparse regime

4 Numerical simulation

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The mixture model

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We have at our disposal a sample $S = (X_1, \ldots, X_n)$ of i.i.d. random variables $(X_i \in \mathbb{R}^d)$, having a common density f.

In an unsupervised classification context, f can be considered of the form

$$f = \sum_{j=1}^{K} \pi_j \phi(.-\mu_j),$$

where ϕ is a known density, $\pi_j \in [0, 1]$, $\mu_j \in \mathbb{R}^d$ and K are unknown parameters.

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Classical statistical issues

- estimation of the sequences (π_j) and $(\mu_j)_j$ (EM algorithms),
- estimation of the component number K (model selection task).

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In this talk, we want to assess the component number ${\cal K}.$ Our aim is to test

$$H_0: f \in \mathcal{F}_0 = \left\{ x \in \mathbb{R} \mapsto \phi(x - \mu); \mu \in \mathbb{R}^d \right\}.$$

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against

$$\begin{aligned} H_1 &: f \in \mathcal{F}_1 = \left\{ x \in \mathbb{R} \mapsto (1 - \varepsilon)\phi(x - \mu_1) + \varepsilon\phi(x - \mu_2); \\ \varepsilon \in]0, 1[\text{ and } \mu_1, \mu_2 \in \mathbb{R}^d \right\}. \end{aligned}$$

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In particular, we want to

- construct a test,
- control the first kind error by a fixed level α ,
- find condition on (ϵ, μ_1, μ_2) for which the two hypotheses can be separated with a prescribed error.

This question has already been addressed in the literature

- Test based on the likelihood ratio,
- Seminal contribution by Y. Ingster.
- The Higher-Criticism proposed by Donoho and Jin (2004).

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In all these contributions, it is assumed that $\mu = \mu_1 = 0$ is a known parameter and d = 1.

We want to adopt a non-asymptotic point of view.

In this talk, we will focus on the Gaussian case ($\phi = \phi_G$, the density of a standard Gaussian random variable).

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In particular, the mean under H_0 is supposed to be known (and is the same in the first component of H_1).

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Lemme

Let $\mathcal{F} \subset \mathcal{F}_1$ a subset of alternatives, and π a probability measure on \mathcal{F} . Then

$$\inf_{\psi_{\alpha}} \sup_{f \in \mathcal{F}} \mathbb{P}_{f}(\psi_{\alpha} = 0) \geq 1 - \alpha - \frac{1}{2} \left(\mathbb{E}_{\mathcal{H}_{0}}[L^{2}_{\pi}(\mathbf{X})] - 1 \right)^{1/2},$$

where $L^2_{\pi}(\mathbf{X})$ the likelihood ratio $d\mathbb{P}_{\pi}/d\mathbb{P}_0$ and the infimum is taken over all α -level tests.

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where $L^2_{\pi}(\mathbf{X})$ the likelihood ratio $d\mathbb{P}_{\pi}/d\mathbb{P}_0$ and the infimum is taken over all α -level tests.

In particular, for some appropriate constant $C(\alpha, \beta)$,

$$\mathbb{E}_{H_0}[L^2_{\pi}(\mathsf{X})] \leq C(\alpha,\beta) \Rightarrow \inf_{\psi_{\alpha}} \sup_{f \in \mathcal{F}} \mathbb{P}_f(\psi_{\alpha}=0) \geq \beta.$$

See, e.g., Ingster (1995) or Baraud (2002) for more details.

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$$\mathbb{E}_{H_0} L^2_{\pi}(\mathbf{X}) \leq \mathbb{E}\left(1 + \epsilon^2 \left(\exp\left[\frac{\|\mu\|^2}{d}\sum_{j=1}^d Z_j\right] - 1\right)\right)^n,$$

where the Z_j denote i.i.d. Rademacher random variables (with param. 1/2).

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In particular

- If $\epsilon >> 1/\sqrt{n}$, $\|\mu\|$ is allowed to tends to 0 with n.
- If $\epsilon << 1/\sqrt{n}$, we can only deal with the case where $\|\mu\| \to +\infty$ with n.

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Proposition Let $\alpha, \beta \in]0, 1[$ be fixed. Then,

$$\inf_{\Psi_{\alpha}} \sup_{f \in \mathcal{F}_{1}, \ \epsilon \parallel \mu \parallel \geq \rho} \mathbb{P}_{f}(\Psi_{\alpha} = 0) \geq \beta,$$

for all

$$\rho < \rho^{\dagger} := c_{\alpha,\beta} \frac{d^{1/4}}{\sqrt{n}}.$$

In some sense, testing is impossible if $\epsilon \|\mu\| \leq c_{\alpha,\beta} d^{1/4} n^{-1/2}$. We recover the asymptotic bound obtained by Cai et al. (2011) for d = 1.

Question : Is this bound optimal in dimension d?

A testing procedure

The sample **X** is splited in two different parts $A = (A_1, \ldots, A_{n/2})$ and $Y = (Y_1, \ldots, Y_{n/2})$ (we assume w.l.o.g. *n* is even and write n/2 = n in the sequel). Set

$$Z_i = \left\langle Y_i, \frac{\bar{A}_n}{\|A_n\|} \right\rangle := \left\langle Y_i, v_n \right\rangle \quad \forall i \in \{1, \dots, n\}.$$

Conditionally to A,

- the Z_i are i.i.d. standard Gaussian random variables under H_0 .
- $Z_j \sim (1 \epsilon)\mathcal{N}(0, 1) + \epsilon \mathcal{N}(\langle \mu, v_n \rangle, 1)$ under H_1 .

Provided v_n is a 'good' approximation of μ , we retrieve the classical uni-dimensional setting investigated in e.g. Cai et al. (2011).

In the following define $Z_{(1)} \leq \cdots \leq Z_{(n)}$ the ordered sample.

Our test statistics is defined as

$$\Psi_{\alpha} := \sup_{k \in \mathcal{K}_n} \left\{ \mathbf{1}_{Z_{(n-k+1)} > q_{\alpha_n,k}} \right\},$$

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Assume that $n \ge 2$ and consider the subset \mathcal{K}_n of $\{1, 2, \ldots, n/2\}$ defined as

$$\mathcal{K}_n = \{2^j, 0 \le j \le [\log_2(n/2)]\}.$$

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where, for all $u \in]0, 1[$, $q_{u,k}$ is the (1 - u)-quantile of $Z_{(n-k+1)}$ under the null hypothesis and

$$\alpha_n = \sup\left\{u\in]0,1[,\mathbb{P}_{H_0}\left(\exists k\in\mathcal{K}_n,Z_{(n-k+1)}>q_{u,k}\right)\leq\alpha\right\}.$$

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The terms $q_{\alpha_n,k}$ and α_n can be approximated (via Monte-Carlo simulations for instance) under the assumption that the X_i 's have common density ϕ .

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In some sense, we can 'play' with the spacing k and adapt to the possible values of $\|\mu\|$ (see below).

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Proposition

Let $\alpha, \beta \in]0, 1[$ be fixed. Then, the testing procedure Ψ_{α} introduced above is of level α . Moreover, there exists a positive constant $C_{\alpha,\beta}$

$$\sup_{\overline{\epsilon}\in\mathcal{F}_{1}, \ \epsilon \parallel \mu \parallel \geq \rho} \mathbb{P}_{f}(\Psi_{\alpha} = \mathbf{0}) \leq \beta,$$

for all $\rho \in \mathbb{R}^+$ such that

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$$\rho \ge \rho^{\star} := C_{\alpha,\beta} \frac{d^{1/4}}{\sqrt{n}} \sqrt{\ln \ln(n)}.$$

We recover the lower bound obtained above up to a logarithmic term.

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The parameters $\epsilon, \mu, \mu_1, \mu_2$ are unknown.

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- the distribution of the variables $X_{(l)} X_{(k)}$ is known under H_0 .

• it has a different behavior under *H*₁, provided *k* and *l* are well-chosen.

Our testing procedure is based on theses properties.

Our test statistics is defined as

$$\Psi_{\alpha} := \sup_{k \in \mathcal{K}_n} \left\{ \mathbf{1}_{X_{(n-k+1)} - X_{(k)} > q_{\alpha_n, k}} \right\},$$

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Assume that $n \ge 2$ and consider the subset \mathcal{K}_n of $\{1, 2, \ldots, n/2\}$ defined as

$$\mathcal{K}_n = \{2^j, 0 \le j \le [\log_2(n/2)]\}.$$

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where, for all $u \in]0, 1[$, $q_{u,k}$ is the (1 - u)-quantile of $X_{(n-k+1)} - X_{(k)}$ under the null hypothesis and

$$\alpha_n = \sup\left\{u \in]0, 1[, \mathbb{P}_{H_0}\left(\exists k \in \mathcal{K}_n, X_{(n-k+1)} - X_{(k)} > q_{u,k}\right) \leq \alpha\right\}.$$

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The terms $q_{\alpha_n,k}$ and α_n can be approximated (via Monte-Carlo simulations for instance) under the assumption that the X_i 's have common density ϕ .

Outline

In the following, we will concentrate our attention on two different schemes :

- The dense regime : the term $|\mu_1 \mu_2|$ is supposed to be bounded under H_1 . In some sense, it will be impossible to detect mixtures where $\epsilon < 1/\sqrt{n}$.
- The sparse regime : the term $|\mu_2 \mu_1|$ is allow to grow as $\epsilon \rightarrow 0$ (asymptotic setting)... which allows to consider smaller values for ϵ .

Main aim : Find *optimal* separation conditions on these parameters.

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Guideline

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We suppose in this section that $\mu_2 > \mu_1$ and

$$\mu_2-\mu_1\leq M,$$

for some constant M. We will

- establish a lower bound (in the Gaussian case),
- propose a consider upper bound associated to a variance-based test,
- prove that our procedure is optimal (up to a log term).

Lower bound

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Lemme

Let $\alpha, \beta \in]0, 1[$ be fixed and assume that $|\mu_2 - \mu_1| \le M$ for some constant M > 0. Then, there exists $C = C(\alpha, \beta, M) > 0$ such that

$$\inf_{\psi_{\alpha}} \sup_{\epsilon(\mu_{2}-\mu_{1})^{2} > C/\sqrt{n}} P_{f}(\psi_{\alpha}=0) \geq \beta.$$

Lower bound

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Some remarks

- testing is impossible if $\epsilon(\mu_2 \mu_1)^2$ is smaller than C/\sqrt{n} .
- different result in the case where the mean μ under ${\it H}_{\rm 0}$ is available.

Upper bound (heuristic)

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Under H_1 , the X_i can be writen as

$$X_i = (\mu_2 - \mu_1)V_i + \eta_i, \ \forall i \in \{1 \dots n\},$$

where $V_i \sim Ber(\epsilon)$ and η_i has density $\phi(. - \mu_1)$.

Upper bound (heuristic)

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$$\operatorname{Var}(X_i) = \operatorname{Var}(\eta_i) + \epsilon (1-\epsilon)(\mu_2 - \mu_1)^2.$$

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$$\operatorname{Var}(X_i) = \operatorname{Var}(\eta_i) + \epsilon (1-\epsilon)(\mu_2 - \mu_1)^2.$$

Let $\sigma^2 = \operatorname{Var}(\eta_i)$ and $\Psi_{V,\alpha}$ the test defined as

$$\Psi_{V,\alpha} = \mathbf{1}_{\{S_n^2 > \sigma^2 + c_\alpha/\sqrt{n}\}},$$

where c_{α} is s.t. $\mathbb{P}_{H_0}(S_n^2 - \sigma^2 > c_{\alpha}/\sqrt{n}) \leq \alpha$.

This test reaches the lower bound presented above (up to a constant).

Upper bound for our procedure

Proposition

There exists $C_{\alpha,\beta}$ s.t.

$$\sup_{\epsilon(\mu_2-\mu_1)^2>C_{\alpha,\beta}\sqrt{\log\log n}/\sqrt{n}}P_f(\Psi_\alpha=0)\leq\beta.$$

Remarks

- The proof is based on a control of the deviation of the ordered statistics and associated quantiles.
- The logarithmic loss is due to the adaptation step.
- This results holds for all symmetric and derivable density ϕ .

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The asymptotic setting

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$$\varepsilon \underset{n \to +\infty}{\sim} n^{-\delta} \text{ and } \mu_2 - \mu_1 \underset{n \to +\infty}{\sim} n^{-r}$$

avec $0 < \delta \leq \frac{1}{2}$ et $0 < r < \frac{1}{2}$.

Proposition

The detection boundary in the *dense* regime is $r^*(\delta) = \frac{1}{4} - \frac{\delta}{2}$

- the detection is possible when $r < r^*(\delta) = \frac{1}{4} \frac{\delta}{2}$ (for *n* large enough, the power of our test is greater than $1 - \beta$)
- the detection is impossible if $r > r^*(\delta)$.

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Proof.

$$\epsilon(\mu_2-\mu_1)^2 > \frac{C}{\sqrt{n}} \quad \Leftrightarrow \quad \frac{1}{n^\delta} \frac{1}{n^{2r}} \gtrsim \frac{1}{\sqrt{n}}.$$

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Sparse mixtures : asymptotic setting

In this section, we consider mixtures for which

$$\epsilon \ll \frac{1}{\sqrt{n}}$$
 quand $n \to +\infty$.

Proposition (Reminder)

Let $\alpha, \beta \in]0, 1[$ be fixed and assume that $\mu_2 - \mu_1 \leq M$ for some given constant M > 0. Then there exists $C = C(\alpha, \beta, M) > 0$ such that

$$\inf_{\psi_{\alpha}} \sup_{\epsilon(\mu_{2}-\mu_{1})^{2} > C/\sqrt{n}} P_{f}(\psi_{\alpha}=0) \geq \beta.$$

According to this result, it is 'necessary to consider situations for which

$$|\mu_1 - \mu_2| \to +\infty \text{ as } n \to +\infty.$$

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Gaussian asymptotic setting

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Assume that

$$\phi(x) = \phi_G(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad \forall x \in \mathbb{R}.$$

In the literature, the sparse asymptotic regime is expressed as

$$\varepsilon \underset{n \to +\infty}{\sim} n^{-\delta} \text{ and } \mu_2 - \mu_1 \underset{n \to +\infty}{\sim} \sqrt{2r \log(n)}$$

where $\frac{1}{2} < \delta < 1$ and 0 < r < 1.

The sparse case

Proposition

Assume that $r > r^*(\delta)$ with

Then, setting $f(.) = (1 - \varepsilon)\phi_G(. - \mu_1) + \varepsilon\phi_G(. - \mu_2)$, we have, for *n* large enough,

$$\mathbb{P}_f(\Psi_{\alpha}=0)\leq\beta.$$

In such a case, the separation 'conditions' are the same when the mean μ under H_0 is known (see e.g. Donoho and Jin (2004) for a description of this rate)

The 'adaptive' scheme appears to be necessary in this context.

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• the Kolmogorov-Smirnov test.

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- the Kolmogorov-Smirnov test.
- the Higher Criticism Let $\hat{p}_i = \mathbb{P}(Z \bar{X} > X_i)$ where $Z \sim \mathcal{N}(0, 1)$ for all $i \in \{1, \dots, n\}$ and $\hat{p}_{(1)} \leq \hat{p}_{(2)} \leq \dots \leq \hat{p}_{(n)}$.

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$$\widehat{HC} = \max_{1 \le i \le n} \frac{\sqrt{n} \left(\frac{i}{n} - \hat{p}_{(i)}\right)}{\sqrt{\hat{p}_{(i)}(1 - \hat{p}_{(i)})}}.$$

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Then, define $\hat{\psi}_{HC,\alpha} = \mathbf{1}_{\widehat{HC} > \hat{q}_{HC,\alpha}}$ where $\hat{q}_{HC,\alpha}$ is the $(1 - \alpha)$ -quantile of \widehat{HC} under H_0 .

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We used N = 100000 Monte-Carlo replications of size n = 100 for a Gaussian mixture with $\varepsilon \in \{0.05, 0.15, 0.25, 0.35\}$ and $\mu \in [0, 10]$.

Numerical study (Gaussian case)



Figure : Power function of the three considered testing procedures (continuous line for our test Ψ_{α} , dashed line for Higher Criticism and dotted line for the Kolmogorov-Smirnov test) according to μ , for $\varepsilon = 0.05$ (top-left), 0.15 (top right), 0.25 (middle left) and 0.35 (middle right).

Numerical study (Laplace case)



Figure : Power function of the three considered testing procedures (continuous line for our test Ψ_{α} , dashed line for Higher Criticism and dotted line for the Kolmogorov-Smirnov test) according to μ , for $\varepsilon = 0.05$ (top-left), 0.15 (top right), 0.25 (middle left) and 0.35 (middle right).

Conclusion

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Possible extensions

- Complete the investigations for the general case $d \neq 1$ (sparse regime and unknown mean under the null).
- generalization to the cases where $K \ge 2$,
- take into account a possible heteroscedasticity,

B. Laurent, C. Marteau and C. Maugis-Rabusseau. Non-asymptotic detection of mixtures with unknown mean. Bernoulli, 22 (2016), pp. 242-274.

B. Laurent, C. Marteau and C. Maugis-Rabusseau. Multidimensional two component Gaussian mixtures detection. *Arxiv* :1509.09129

Non asymptotic detection of two component mixtures

B. Laurent ³, C. Marteau ⁴ and Cathy Maugis-Rabusseau¹ .

Colloque ANR MixStatSeq - Toulouse 2016

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