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Variable selection for correlated data in high dimension using decorrelation methods

Emeline Perthame

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Joint work with

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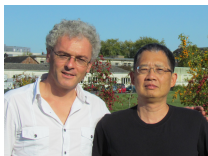
Agrocampus, Rennes

Ching-Fan Sheu

NCKU, Tainan, Taiwan

Chloé Friguet

UBS, Vannes

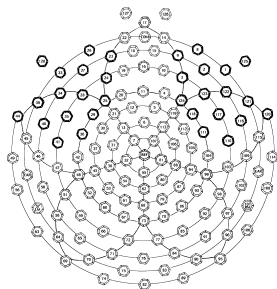


StatLearn, Vannes, April 2016

1. Introduction
2. Impact of dependence and dependence modeling
3. Disentangling signal from noise ...
 - ... for a multiple testing issue
 - ... for a supervised classification issue
4. Conclusion

The instrument: a 128-channel geodesic sensor net

- Electroencephalography (EEG) is the recording of electrical activity at scalp locations over time.
- The recorded EEG traces, which are time locked to external events, are averaged to form the event-related (brain) potentials (ERPs).



Auditory oddball experiment

A very commonly used experimental task

- Two auditory stimuli are presented to subjects
 - A stimulus (500Hz) occurring frequently
 - A stimulus (1000Hz) occurring infrequently
- ERPs are recorded on a 400 ms interval after the onset.

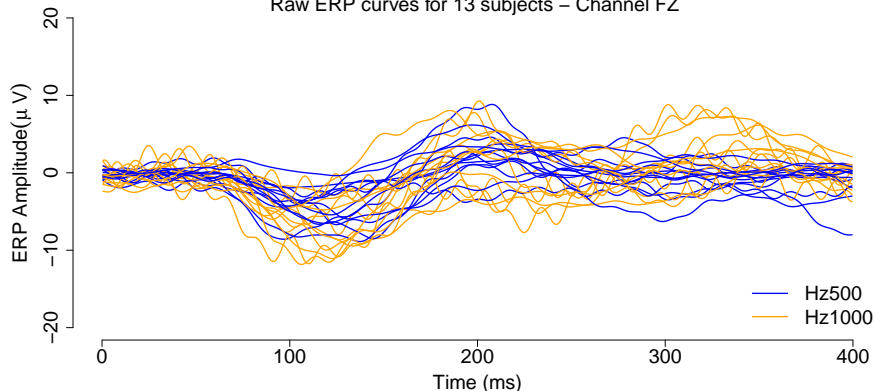
Motivations

- Auditory evoked potential (AEP): elicited by auditory stimulus
- Mismatch negativity (MMN): elicited by any change in the stimulus (odd/frequent)
- AEP and MMN are electrophysiological marker candidates for psychiatric disorders such as schizophrenia

ERP curves

Auditory ERP data – Kaohsiung Medical University

Raw ERP curves for 13 subjects – Channel FZ



- Signal detection: is there any difference between the two conditions?
- Signal identification: when does the difference occur?

At time t for subject i in condition j

- Multivariate analysis of variance model

$$Y_{ijt} = \mu_t + \alpha_{it} + \gamma_{jt} + \varepsilon_{ijt}$$

- Functional analysis of variance model

$$Y_{ijt} = \sum_{s=1}^S m_s \varphi_s(t) + \sum_{s=1}^S a_{is} \varphi_s(t) + \sum_{s=1}^S g_{js} \varphi_s(t) + \varepsilon_{ijt}$$

where $\varphi_s(\cdot)$, $s = 1, \dots, S$ are B-splines.

Linear model framework for ERP curves

At time t for subject i in condition j

$$Y_{ijt} = \mu_t + \alpha_{it} + \gamma_{jt} + \varepsilon_{ijt}$$

Signal detection

- Is there any difference between the two conditions?

$$H_0 : \text{for } t = 1, \dots, T \text{ and } j = 1, 2, \gamma_{jt} = 0$$

- Is it relevant to predict the label from ERP curves?

→ High dimension: need for variable selection

Signal identification

$$\text{For } t = 1, \dots, T, H_{0t} : \text{for } j = 1, 2, \gamma_{jt} = 0$$

Some approaches

Detection

- F-test for multivariate (or functional) ANOVA ¹
- Optimal detection (Higher Criticism ²)

Supervised classification

- Ignoring correlations: Naive approaches ³
- Introducing sparsity: Lasso, Sparse LDA ⁴

Identification

- FDR controlling: Benjamini-Hochberg ...

→ Efficient under independence

-
1. Bugli and Lambert, 2006, Stat Med
 2. Donoho and Jin, 2004, AOS
 3. Bickel and Levina, 2004, Bernoulli; Tibshirani et al., 2003, Stat Sc
 4. Tibshirani, 1996, JRSS; Clemmensen et al., 2011, Technometrics

- Assumes an auto-regressive process with auto-correlation ρ
- Distribution of L_ρ under the null

$$L_\rho = \#\{t, p_t \leq \alpha\}$$

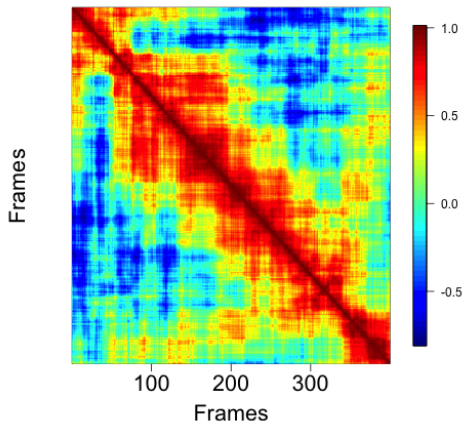
where (p_1, \dots, p_T) are p-values and α is a preset level

- A time interval is rejected if it is significant at the preset level and longer than usual time intervals

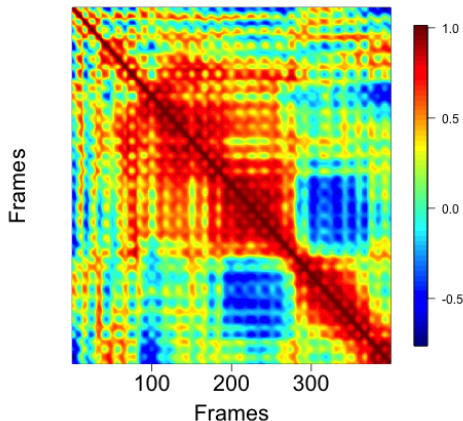
5. Guthrie and Buchwald, 1991, Psychophysiology

Strong and complex temporal dependence structure

Time correlations of an AR(1) process



Time correlations of ERP data



→ Dependence affects the stability of selection procedures

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Rare and Weak paradigm⁶

- Two components mixture for test statistics

$$\mathcal{T} = \mu + \varepsilon, \varepsilon \sim \mathcal{N}(0, \mathbb{I}_T)$$

- Where signal is
 - Rare

$$\eta = T^{-\beta}, \beta \in \left(\frac{1}{2}, 1\right)$$

- Weak

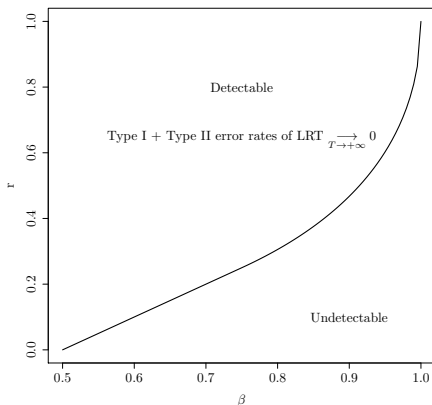
$$A = \sqrt{2r \log(T)}, r \in (0, 1)$$

6. Donoho and Jin, 2004, AOS ; 2008, PNAS

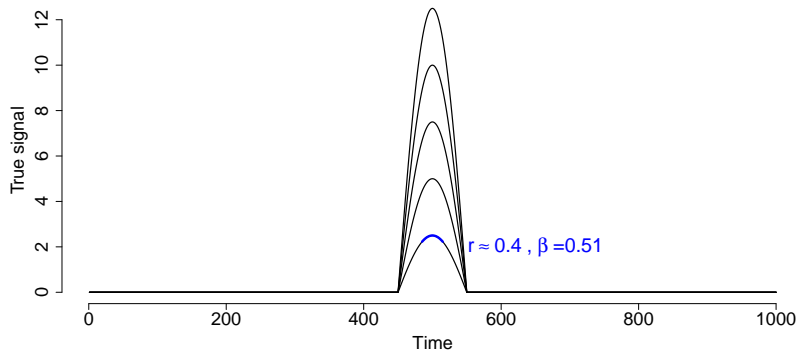
Phase diagram under independence⁷

- Signal is detectable when $r > \rho^*(\beta)$:

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

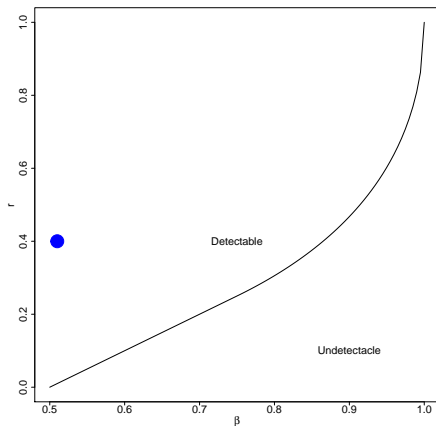


Impact of dependence - Signal identification



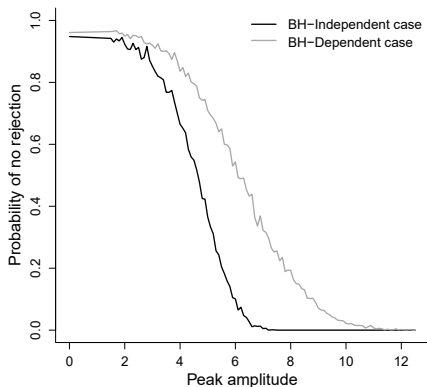
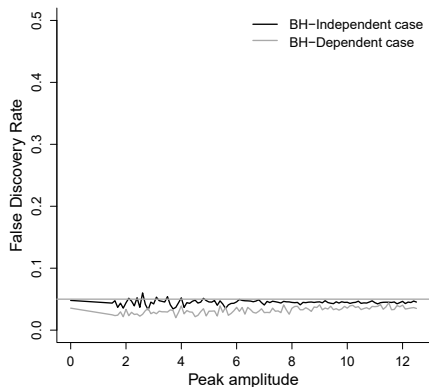
- Independence and ERP time dependence pattern
- 1000 datasets for each amplitude
- Benjamini Hochberg correction

Impact of dependence - Signal identification



- Independence and ERP time dependence pattern
- 1000 datasets for each amplitude
- Benjamini Hochberg correction

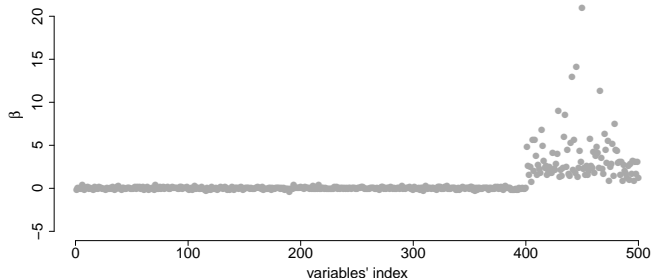
Impact of dependence - Signal identification



- Instability of multiple testing procedures

$$\text{FDR} = \text{pFDR}(1-\text{PNR})$$

Impact of dependence - Variable selection

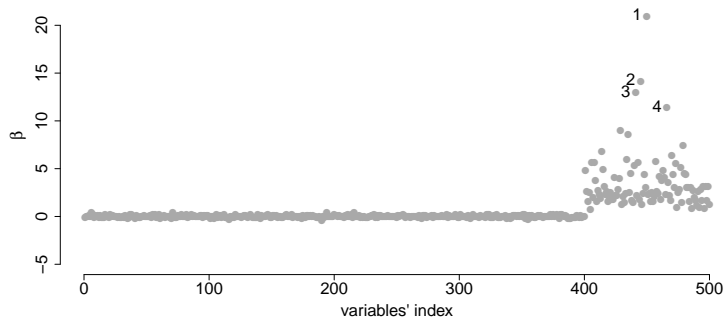


$$\log \frac{\mathbb{P}(Y = 2|X)}{\mathbb{P}(Y = 1|X)} = \beta_0 + \beta'x$$

- Independence and ERP time dependence pattern
- 1000 datasets for each dependence structure
- Variable selection performed by Lasso⁸

8. `glmnet` R package, Friedman et al., 2010, JSS

Impact of dependence - Variable selection

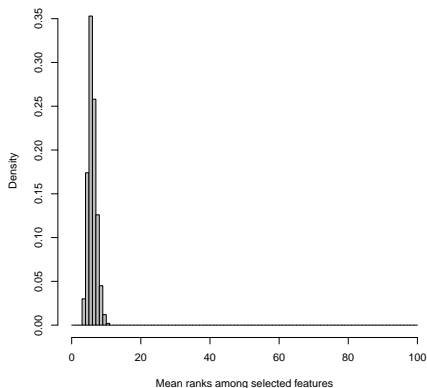


- Predictor X_t is assessed by its rank r_t deduced from its regression coefficient
- Relevance of a selected set \mathcal{S} is given by the mean rank in

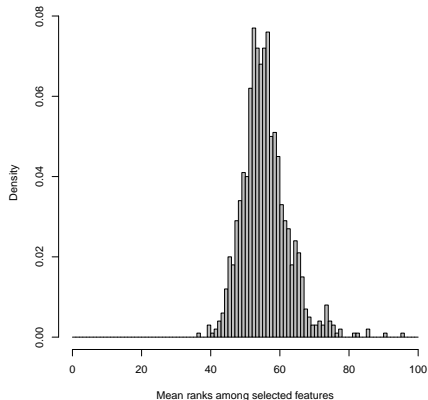
$$\mathcal{S}: r_{\mathcal{S}} = \frac{1}{\#\mathcal{S}} \sum_{t \in \mathcal{S}} r_t$$

Impact of dependence - Variable selection

Under independence



Under dependence



- Relevance: the most predictive variables are not selected under dependence
- Stability: selected subsets are not reproducible

Impact of dependence - Improving stability

- Bootstrap
 - Bolasso⁹
 - Stability selection¹⁰
- Dependence modeling
 - Surrogate variable analysis¹¹
 - Latent effect adjustment after primary projection¹²
 - Factor analysis for multiple testing¹³

9. Bach, 2008, Proceedings ICML

10. Meinshausen and Bühlmann, 2010, JRSS

11. Leek and Storey, 2007, PLoS Genetics

12. Sun, Zhang and Owen, 2012, AOAS

13. Friguet, Kloareg and Causeur, 2009, JASA

Factor modeling of dependence

- Distribution of ERP curves

$$X = (X_1, \dots, X_T) | Y = y \sim \mathcal{N}_T(\mu_y, \Sigma)$$

- Latent factor modeling

$$X = \mu_y + BZ + e \text{ with } e \sim \mathcal{N}_T(0, \Psi)$$

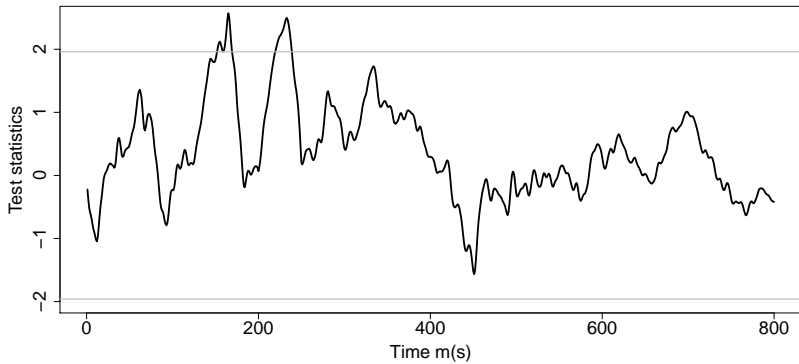
$$\Psi \text{ diagonal, } \text{rank}(B) = q,$$

$$Z \sim \mathcal{N}_q(0, \mathbb{1}_q),$$

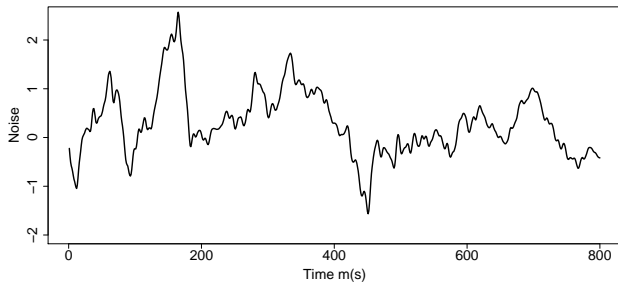
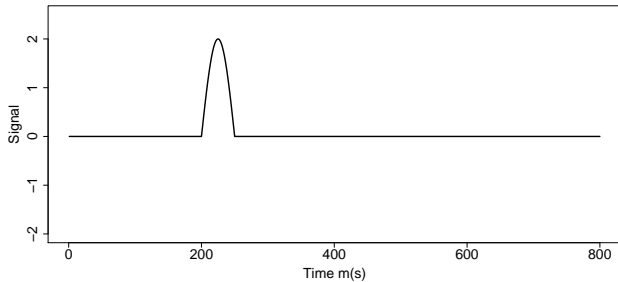
- Decomposition of covariance matrix

$$\Sigma = \Psi + BB'$$

Signal is hidden by noise



Signal is hidden by noise



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Multiple testing issue

- ERP measure at time t , for subject i ,

$$Y_{ijt} = \mu_t + \alpha_{it} + \gamma_{jt} + \varepsilon_{ijt}$$

- In matrix notations

$$Y_t = \mu_t + X_0\alpha_t + X\gamma_t + \varepsilon_t$$

with $\mathbb{V}(\varepsilon_1, \dots, \varepsilon_T) = \Sigma$

- Multiple testing for $t = 1, \dots, T$

$$H_{0,t} : \gamma_t = 0$$

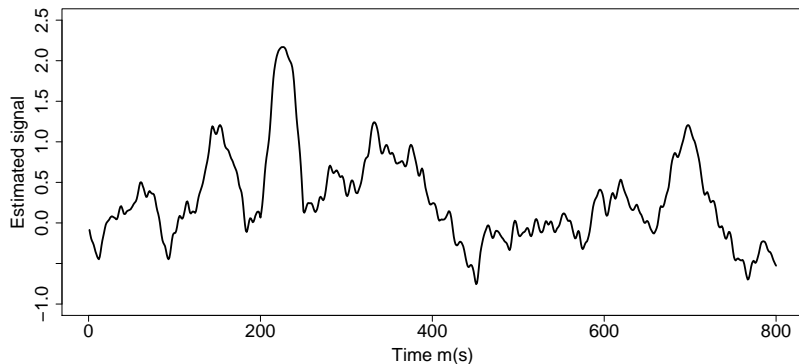
- Dependence among tests

A prior knowledge of the signal

- OLS signal estimation of $\gamma = (\gamma_1, \dots, \gamma_T)$

$$\hat{\gamma} = \gamma + \delta$$

with $\delta \sim \mathcal{N}(0, \tilde{\Sigma})$ and $\tilde{\Sigma} \propto \Sigma$

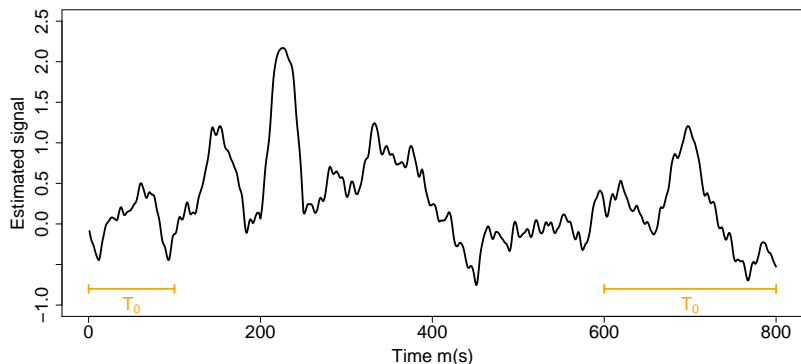


A prior knowledge of the signal

- OLS signal estimation of $\gamma = (\gamma_1, \dots, \gamma_T)$

$$\hat{\gamma} = \gamma + \delta$$

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A prior knowledge of the signal

- OLS signal estimation of $\gamma = (\gamma_1, \dots, \gamma_T)$

$$\hat{\gamma} = \gamma + \delta$$

with $\delta \sim \mathcal{N}(0, \tilde{\Sigma})$ and $\tilde{\Sigma} \propto \Sigma$

- Noise is somewhere observed **without** signal

$$\begin{pmatrix} \delta_0 \\ \delta_{-0} \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \tilde{\Sigma}_{0,0} & \tilde{\Sigma}'_{-0,0} \\ \tilde{\Sigma}_{-0,0} & \tilde{\Sigma}_{-0,-0} \end{pmatrix} \right]$$

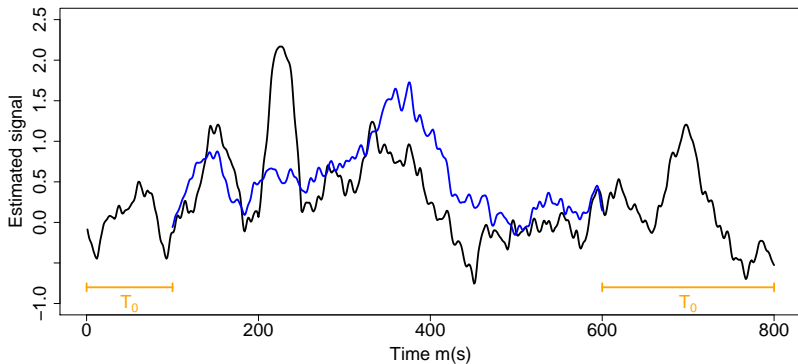
- And can be estimated elsewhere

$$\hat{\delta}_{-0} = \hat{\Sigma}_{-0,0} \hat{\Sigma}_{0,0}^{-1} \hat{\delta}_0$$

A prior knowledge of the signal

- And can be estimated elsewhere

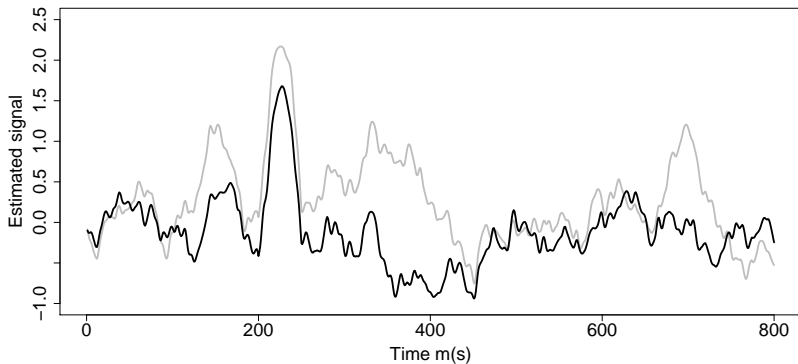
$$\hat{\delta}_{-0} = \hat{\Sigma}_{-0,0} \hat{\Sigma}_{0,0}^{-1} \hat{\delta}_0$$



A prior knowledge of the signal

- New estimation of the signal

$$\hat{\gamma}^{\text{new}} = \hat{\gamma} - \hat{\delta}$$



Iterative algorithm

- New estimation of the signal

$$\hat{\gamma}^{\text{new}} = \hat{\gamma} - \hat{\delta}$$

- Update of residual errors $\hat{\varepsilon}^{\text{new}} = Y_t - (\hat{\mu}_t + \hat{\alpha}_{it} + \hat{\gamma}_t^{\text{new}})$
- New estimation of covariance matrix
- Alternates estimation of signal and covariance structure
- Until convergence of test statistics
- Update of T_0

Prior knowledge

- ERP: psychologists may know that signal does not occur before/after some time points
- Genomics: biologists may know that some genes are not involved in a biological process

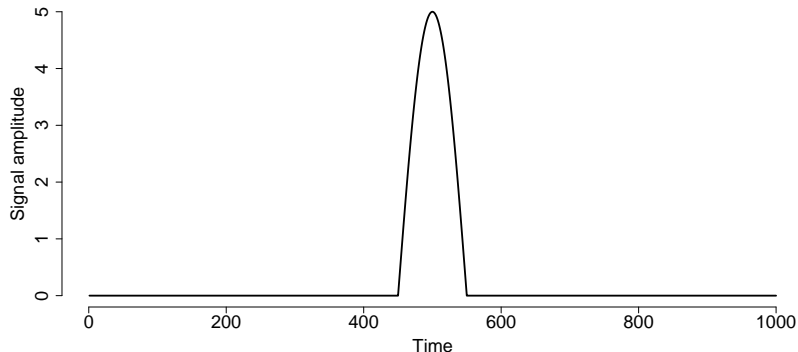
No prior knowledge

- Conservative approach

$$T_0 = \{t, p_t \geq t_0\}$$

where (p_1, \dots, p_T) are p-values

Simulations - Adaptive factor analysis procedure



- Dependence structure of ERP experiment
- 1000 generated datasets

Simulations - Adaptive factor analysis procedure

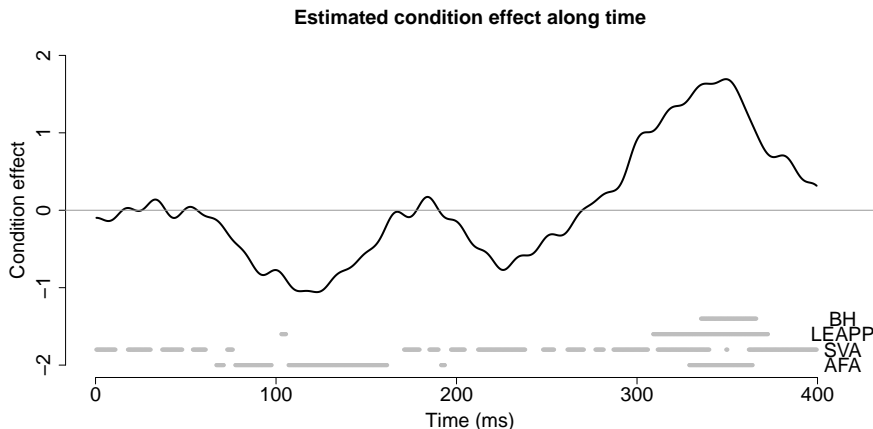
Method	FDR ¹⁴	TDR ¹⁵	PD ¹⁶
Benjamini-Hochberg	0.031	0.057	0.281
Benjamini-Yekutieli	0.009	0.011	0.101
Guthrie-Buchwald	0.086	0.233	0.538
SVA	0.088	0.151	0.599
LEAPP	0.151	0.304	0.847
AFA	0.034	0.498	1.000

14. False Discovery Rate

15. True Discovery Rate

16. Probability of Detecting the peak

Application to auditory data



80 - 120 ms: Auditory evoked potential

100 - 200 ms: Mismatch negativity for the difference curve

- Adaptive estimation of signal and factor model parameters
- Designed for strong dependence
- Efficient multiple testing procedure
 - FDR is controlled
 - Good detection power
- ERP package available on CRAN¹⁷

17. Causeur and Sheu, 2014, R package version 1.0.1

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Supervised classification issue

- Prediction of a label \rightarrow Hz500 or Hz1000 frequency
- From ERP curves profiles $X = (X_1, \dots, X_T)$

$$(X|Y = y) \sim \mathcal{N}_p(\mu_y, \Sigma)$$

- Among linear classification rule

$$LR(x) = \log \frac{\mathbb{P}(Y = 2|X)}{\mathbb{P}(Y = 1|X)} = \beta_0 + x'\beta$$

- The best one is Bayes' rule

$$\begin{aligned}\beta &= \Sigma^{-1}(\mu_2 - \mu_1) \\ \beta_0 &= \log \frac{p_2}{p_1} - 0.5(\mu_2 + \mu_1)'\Sigma^{-1}(\mu_2 - \mu_1)\end{aligned}$$

- Theoretical misclassification rate π

Logistic regression

- Minimizing the deviance

$$(\hat{\beta}_0, \hat{\beta}) = \operatorname{argmin}_{\beta_0, \beta} - 2 \sum_{i=1}^n \log[1 + \exp(-V_i(\beta_0 + x_i' \beta))]$$

where $V_i = \pm 1$

- High dimension
 - ℓ_2 -penalization: Ridge¹⁸
 - ℓ_1 -penalization: Lasso¹⁹

18. Hoerl and Kennard, 1970, Technometrics

19. Tibshirani, 1996, JRSS

Linear Discriminant Analysis

- OLS estimate \rightarrow Method of moments

$$(\hat{\beta}_0, \hat{\beta}) = \operatorname{argmin}_{\beta_0, \beta} \sum_{i=1}^n [V_i - (\beta_0 + x_i' \beta)]^2, \text{ where } V_i = \pm 1$$

- High dimension
 - Ignoring correlations: Diagonal Discriminant Analysis (DDA)¹⁸, Nearest Shrunken Centroids¹⁹
 - Shrinkage Discriminant Analysis²⁰ (SDA)
 - Sparse linear discriminant analysis²¹ (SLDA)

18. Bickel and Levina, 2004, Bernoulli

19. Tibshirani et al., 2003, Stat Sc

20. Ahdesmäki and Strimmer, 2010, AOAS

21. Clemmensen et al., 2011, Technometrics

Conditional classification rule

- Under factor model assumption ($\Sigma = \Psi + BB'$)

$$\begin{pmatrix} X \\ Z \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} \mu_y \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma & B \\ B' & I_q \end{pmatrix} \right]$$

- Among classification rules linear in (x, z)
- The best one is the **conditional Bayes' classifier**

$$LR(x, z) = \log \frac{\mathbb{P}(Y = 2|X, Z)}{\mathbb{P}(Y = 1|X, Z)} = \beta_0^* + (x - Bz)' \beta^*$$

$$\text{with } \beta^* = \Psi^{-1}(\mu_2 - \mu_1)$$

$$\beta_0^* = \log \frac{p_2}{p_1} - 0.5(\mu_2 + \mu_1)' \Psi^{-1}(\mu_2 - \mu_1)$$

- Analytical expression of misclassification rate π_Z^*

Conditional classification rule

- Bayes rule error π
- Under factor model assumption

$$\begin{pmatrix} X \\ Z \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} \mu_y \\ 0 \end{pmatrix}, \begin{pmatrix} \Sigma & B \\ B' & I_q \end{pmatrix} \right]$$

- Conditional Bayes rule error π_Z^*
- One can show that $\pi \geq \pi_Z^*$

→ Theoretical superiority of conditional approach based on decorrelated data $\tilde{X} = X - BZ$

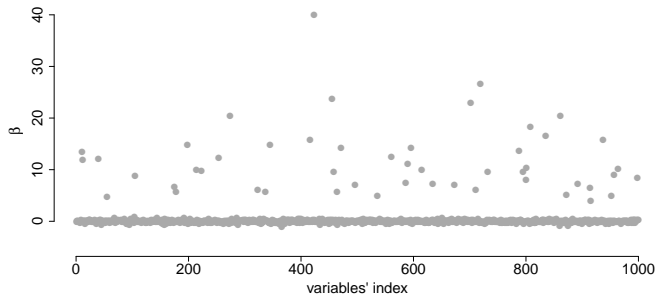
- Estimation of μ_1 and μ_2
- Computation of centered profiles
- Estimation of factor model parameters²² (Ψ, B)
- Decorrelation of data using generalized Thompson's formula

$$\tilde{x} = x - \hat{B}\hat{z}'$$

Generalized Thompson's formula

$$\hat{Z} = \mathbb{E}_X(Z) = (I_q + B'\Psi^{-1}B)^{-1}B'\Psi^{-1}\left(x - [\mu_1\mathbb{P}_X(1) + \mu_2\mathbb{P}_X(2)]\right)$$

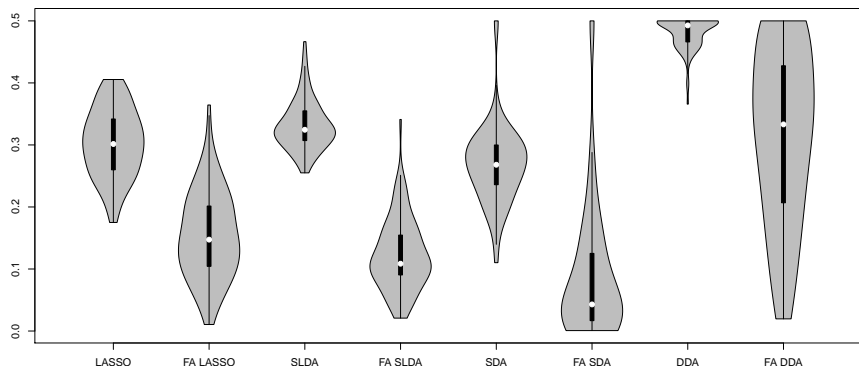
22. Friguet, Kloareg and Causeur, 2009, JASA



- $n_0 = n_1 = 13$
- Various dependence structures²³
- 1000 learning datasets
- 1 testing dataset

23. Meinshausen and Bühlmann, JRSS, 2010

Simulations - Prediction error rates



→ Variable selection methods compared to their factor-adjusted version

Simulations - Selection accuracy

Method	Nb of selected var.	Accuracy
LASSO ²⁴	13.10	62.36
Factor-adjusted LASSO	8.03	93.02
SLDA ²⁵	10.00	62.50
FA SLDA	10.00	90.90
SDA ²⁶	57.20	75.07
FA SDA	68.22	67.93
DDA ²⁷	149.42	15.58
FA DDA	97.65	48.76

24. Tibshirani, 1996, JRSS ; Friedman et al., 2010, JSS

25. Clemmensen et al., 2011, Technometrics

26. Ahdesmäki and Strimmer, 2010, AOAS

27. Bickel and Levina, 2004, Bernoulli

- Decorrelation method designed for prediction issues
- Preprocessing of the data which enables the use of usual selection methods
- FADA package available on CRAN²⁸
- Application in genomics
- Adjustment for batch effect²⁹

28. Perthame, Friguet and Causeur, 2014, R package version 1.2

29. Hornung, Boulesteix and Causeur, submitted

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→ Whatever the statistical analysis, it would be efficient to account for dependence because it is a *blessed* situation³⁰

→ Accounting for dependence introduces hyper-parameters

- Risk of overfitting
- Results depend on the estimation of the dependence model
 - Need for robust models
 - With few parameters
 - To guarantee reproducible results

30. Hall and Jin, 2010, AOS

References

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ERP: Significance analysis of Event-Related Potentials data, 2014.

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E. Perthame, C. Friguet, and D. Causeur.

FADA: Variable selection for supervised classification in high dimension, 2014.

R package version 1.2.

E. Perthame, C. Friguet, and D. Causeur.

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Statistics and Computing, pages 1–14, 2015.

C. Sheu, E. Perthame, D. Causeur, and Y. Lee.

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AOAS, 10(1):219–245, 2016.