Concomitant Lasso with Repetitions (CLaR): beyond averaging multiple realizations of heteroscedastic noise

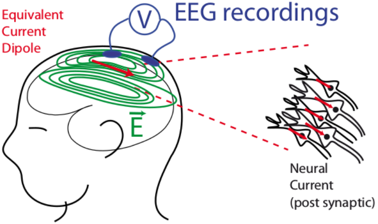
Joseph Salmon
http://josephsalmon.eu
IMAG, Univ Montpellier, CNRS
Montpellier, France

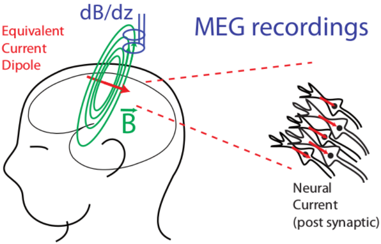
Joint works with:
Quentin Bertrand (INRIA, Parietal Team)
Mathurin Massias (INRIA, Parietal Team)
Olivier Fercoq (Institut Polytechnique de Paris)
Alexandre Gramfort (INRIA, Parietal Team)

Montpellier: come, visit, work, etc.

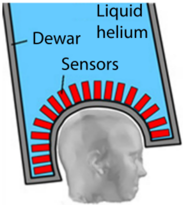
M/EEG inverse problem for brain imaging

- sensors: magneto- and electro-encephalogram measurements during a cognitive experiment
- sources: brain locations





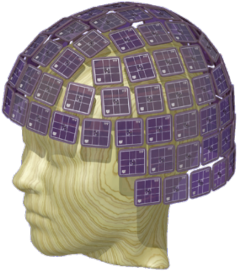
First EEG recordings in 1929 by H. Berger



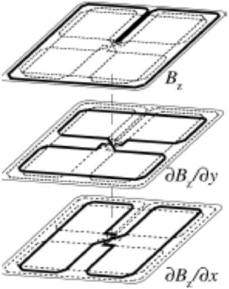
Hôpital La Timone
Marseille, France

MEG elements: magnometers and gradiometers

Device

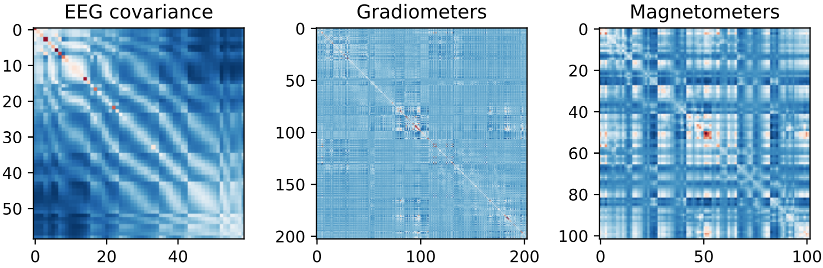


Sensors



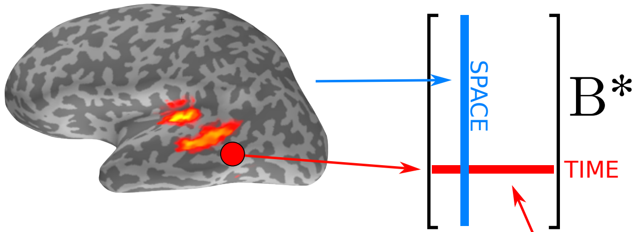
Detail of a sensor

Noise is different for EEG / MEG (magnometers and gradiometers)

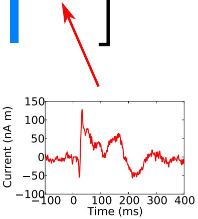


- 3 different sensors $\Longrightarrow$ 3 different noise structures

Source modeling

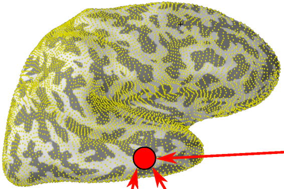


Position a few thousands candidate sources over the brain (*e.g.*, every 5mm)



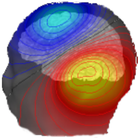
$$\mathrm{B}^* \in \mathbb{R}^{p \times q}$$

Design matrix - Forward operator

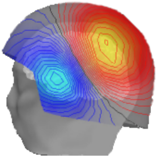


$$X = \left[\begin{array}{c} X_{\text{EEG}} \\ \hdashline X_{\text{MEG}} \end{array}\right] \in \mathbb{R}^{n \times p}$$

EEG:
Forward field of the electrodes

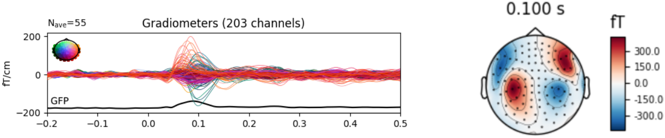


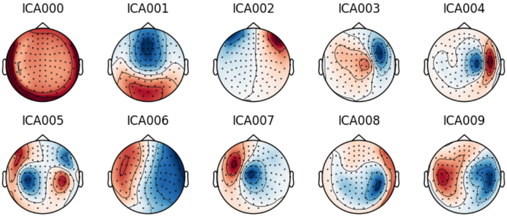
MEG:
Forward field of sensor



X : gain matrix / forward operator obtained by Maxwell's equations

Sparsity assumption: cortical sources produce dipolar patterns well modelled by focal sources



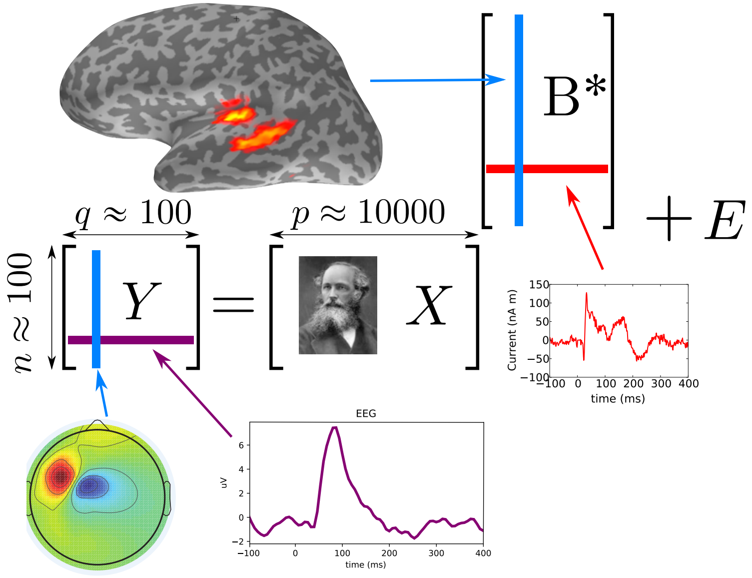


ICA : Blind source separation recovers dipolar patterns[1]

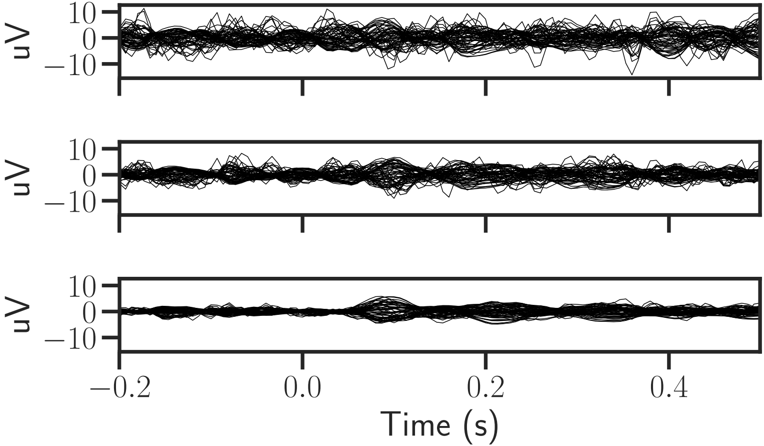
http://martinos.org/mne/stable/auto_tutorials/plot_visualize_evoked.html
http://martinos.org/mne/stable/auto_tutorials/plot_artifacts_correction_ica.html

[1] A. Delorme et al. "Independent EEG sources are dipolar". In: *PloS one* 7.2 (2012), e30135.

The M/EEG inverse problem: modeling



Multiple repetitions (r) of experiments: $r = 5$ (top), $r = 10$ (middle), $r = 50$ (bottom) repetitions



A multi-task framework

Multi-task regression notation:

- n observations (*e.g.*, number of sensors)
- q tasks (*e.g.*, temporal information)
- p features (*e.g.*, spatial description)
- r number of repetitions for the experiment
- $Y^{(1)}, \dots, Y^{(r)} \in \mathbb{R}^{n \times q}$ observation matrices; $\bar{Y} = \frac{1}{r} \sum_l Y^{(l)}$
- $X \in \mathbb{R}^{n \times p}$ forward matrix

$$\boxed{Y^{(l)} = X\mathrm{B}^* + S\mathrm{E}^{(l)}}, \quad \text{where}$$

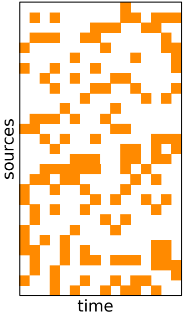
- $\mathrm{B}^* \in \mathbb{R}^{p \times q}$: true source activity matrix (**unknown**)
- $S \in \mathbb{S}^n_{++}$ co-standard deviation matrix[(2)] (**unknown**)
- $\mathrm{E}^{(1)}, \dots, \mathrm{E}^{(r)} \in \mathbb{R}^{n \times q}$: white Gaussian noise

[(2)] $S \succeq \underline{\sigma}$ means $S - \underline{\sigma}$ is Semi-Definite Positive

Multi-tasks penalties[3]

Popular convex penalties considered:

$$\hat{\mathrm{B}} \in \mathop{\arg\min}_{\mathrm{B}\in\mathbb{R}^{p\times q}} \left(\frac{1}{2nq}\left\|\bar{Y} - X\mathrm{B}\right\|^2 + \lambda\Omega(\mathrm{B})\right)$$



Parameter $\hat{\mathrm{B}} \in \mathbb{R}^{p\times q}$

Sparse support: no structure

Penalty: **Lasso type**

$$\Omega(\mathrm{B}) = \|\mathrm{B}\|_1 = \sum_{j=1}^{p}\sum_{k=1}^{q} |\mathrm{B}_{j,k}|$$

[3] G. Obozinski, B. Taskar, and M. I. Jordan. "Joint covariate selection and joint subspace selection for multiple classification problems". In: *Statistics and Computing* 20.2 (2010), pp. 231–252.

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Popular convex penalties considered: Multi-Task Lasso (MTL)

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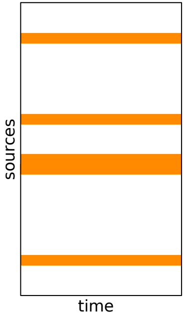

Parameter $\hat{\mathrm{B}} \in \mathbb{R}^{p \times q}$

Sparse support: group structure

Penalty: **Group-Lasso type**

$$\Omega(\mathrm{B}) = \|\mathrm{B}\|_{2,1} = \sum_{j=1}^{p} \|\mathrm{B}_{j,:}\|_2$$

where $\mathrm{B}_{j,:}$ the j-th row of B

[3] G. Obozinski, B. Taskar, and M. I. Jordan. "Joint covariate selection and joint subspace selection for multiple classification problems". In: *Statistics and Computing* 20.2 (2010), pp. 231–252.

Multi-tasks data-fitting term

- Classical multi-tasks estimator: use averaged signal

$$\hat{\mathrm{B}} \in \underset{\mathrm{B} \in \mathbb{R}^{p \times q}}{\arg\min} \left(\frac{1}{2nq} \left\| \bar{Y} - X\mathrm{B} \right\|_F^2 + \lambda \Omega(\mathrm{B}) \right)$$

- **How to take advantage of the number of repetitions ?**

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$$\hat{\mathrm{B}}^{\text{repet}} \in \underset{\mathrm{B}\in\mathbb{R}^{p\times q}}{\arg\min} \left(\frac{1}{2nqr} \sum_{l=1}^{r} \left\| Y^{(l)} - X\mathrm{B} \right\|_F^2 + \lambda \Omega(\mathrm{B}) \right)$$

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Table of Contents

Step back on the Lasso case ($q = 1$)

Sparse Gaussian model: $y = X\beta^* + \sigma_* \varepsilon$

- $y \in \mathbb{R}^n$: observation
- $X \in \mathbb{R}^{n \times p}$: design matrix
- $\beta^* \in \mathbb{R}^p$: signal to recover; **unknown**
- $\|\beta^*\|_0 = s^*$: sparsity level (small w.r.t. p); s^* **unknown**
- $\varepsilon \sim \mathcal{N}(0, \sigma_*^2 \,\mathrm{Id}_n)$; σ_* **unknown**

Lasso reminder : $$\boxed{\hat{\beta}^{(\lambda)} \in \mathop{\arg\min}_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|y - X\beta\|^2 + \lambda \|\beta\|_1}$$

Lasso theory[4],[5]

Theorem

For Gaussian noise model and X satisfying the "Restricted Eigenvalue" property, for $\lambda = 2\sigma_* \sqrt{\frac{2\log(p/\delta)}{n}}$, then

$$\frac{1}{n}\left\| X\beta^* - X\hat{\beta}^{(\lambda)} \right\|^2 \leq \frac{18}{\kappa_{s^*}^2} \frac{\sigma_*^2 s^*}{n} \log\left(\frac{p}{\delta}\right)$$

with probability $1-\delta$, where $\hat{\beta}^{(\lambda)}$ is a Lasso solution

Rem: optimal rate in the minimax sense (up to constant/log term)

Rem: $\kappa_{s^*}^2$ controls the conditioning of X when extracting the s^*columns of X associated to the true support

BUT σ_* is unknown in practice !

[4] P. J. Bickel, Y. Ritov, and A. B. Tsybakov. "Simultaneous analysis of Lasso and Dantzig selector". In: *Ann. Statist.* 37.4 (2009), pp. 1705–1732.

[5] A. S. Dalalyan, M. Hebiri, and J. Lederer. "On the Prediction Performance of the Lasso". In: *Bernoulli* 23.1 (2017), pp. 552–581.

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Joint estimation of β and σ

How to calibrate (theoretically) λ when σ_* is unknown?

Intuitive idea: initialize λ

- run Lasso with λ; get β
- estimate σ, *e.g.*, with residual $\sigma \leftarrow \frac{\|y-X\beta\|}{\sqrt{n}}$
- re-scale $\lambda \propto \sigma$, and run Lasso with it
- iterate (until convergence)

Rem: exactly the Concomitant Lasso[6] / Scaled-Lasso[7] implementation

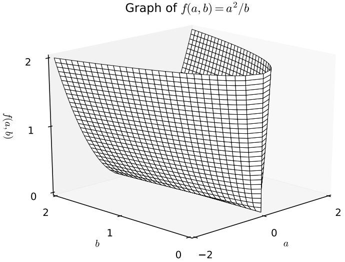
[6] A. B. Owen. "A robust hybrid of lasso and ridge regression". In: *Contemporary Mathematics* 443 (2007), pp. 59–72.

[7] T. Sun and C.-H. Zhang. "Scaled sparse linear regression". In: *Biometrika* 99.4 (2012), pp. 879–898.

Concomitant Lasso

$$\boxed{(\beta^{(\lambda)}, \sigma^{(\lambda)}) \in \underset{\beta \in \mathbb{R}^p, \sigma > 0}{\arg\min} \left(\frac{\|y - X\beta\|^2}{2n\sigma} + \frac{\sigma}{2} + \lambda \|\beta\|_1 \right)}$$

- $\frac{\sigma}{2}$: penalty on noise level, roots in robust estimation[8],[9]
- jointly convex program: $(a, b) \mapsto a^2/b$ is convex



[8] P. J. Huber and R. Dutter. "Numerical solution of robust regression problems". In: *Compstat 1974 (Proc. Sympos. Computational Statist., Univ. Vienna, Vienna, 1974)*. Physica Verlag, Vienna, 1974, pp. 165–172.

[9] P. J. Huber. *Robust Statistics*. John Wiley & Sons Inc., 1981.

Concomitant performance

Theorem[10],[11]

For Gaussian noise model and X satisfying the "Restricted Eigenvalue" property and $\lambda = 2\sqrt{\frac{2\log(p/\delta)}{n}}$, then

$$\frac{1}{n}\left\|X\beta^* - X\hat{\beta}^{(\lambda)}\right\|^2 \leq \frac{18}{\kappa_{s^*}^2}\frac{\sigma_*^2 s_*}{n}\log\left(\frac{p}{\delta}\right)$$

with high probability, where $\hat{\beta}^{(\lambda)}$ is a Concomitant Lasso solution

Rem: provide same rate as Lasso, **without knowing** σ_*

Rem: λ has no dimension, but calibration still needed in practice...

[10] T. Sun and C.-H. Zhang. "Scaled sparse linear regression". In: *Biometrika* 99.4 (2012), pp. 879–898.

[11] C. Giraud. *Introduction to high-dimensional statistics*. Vol. 138. CRC Press, 2014.

Link with $\sqrt{\text{Lasso}}$[12]

- Independently, $\sqrt{\text{Lasso}}$ analyzed to get "σ free" choice of λ

$$\boxed{\hat{\beta}^{(\lambda)}_{\sqrt{\text{Lasso}}} \in \mathop{\arg\min}_{\beta \in \mathbb{R}^p} \left(\frac{1}{\sqrt{n}} \|y - X\beta\| + \lambda \|\beta\|_1 \right)}$$

- Connections with Concomitant Lasso:
  $\left(\hat{\beta}^{(\lambda)}_{\sqrt{\text{Lasso}}}, \hat{\sigma}^{(\lambda)}_{\sqrt{\text{Lasso}}}\right)$ is solution of the Concomitant Lasso when

$$\hat{\sigma}^{(\lambda)}_{\sqrt{\text{Lasso}}} = \frac{\left\| y - X\hat{\beta}^{(\lambda)}_{\sqrt{\text{Lasso}}} \right\|}{\sqrt{n}} \neq 0$$

Rem: non-smooth data fitting term with non-smooth regularization

[12] A. Belloni, V. Chernozhukov, and L. Wang. "Square-root Lasso: pivotal recovery of sparse signals via conic programming". In: *Biometrika* 98.4 (2011), pp. 791–806.

The Smoothed Concomitant Lasso[14]

$$\boxed{(\hat{\beta}^{(\lambda)}, \hat{\sigma}^{(\lambda)}) \in \mathop{\arg\min}_{\beta \in \mathbb{R}^p, \sigma \geq \underline{\sigma}} \frac{\|y - X\beta\|^2}{2n\sigma} + \frac{\sigma}{2} + \lambda \|\beta\|_1}$$

- useful for optimization with small λ
- with prior information on the minimal noise level, one can set $\underline{\sigma}$ as this bound (recovers Concomitant Lasso)
- setting $\underline{\sigma} = \epsilon$, smoothing theory asserts that $\frac{\epsilon}{2}$-solutions for the smoothed problem provide ϵ-solutions for the $\sqrt{\mathrm{Lasso}}$[13]

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[13] Y. Nesterov. "Smooth minimization of non-smooth functions". In: *Math. Program.* 103.1 (2005), pp. 127–152.

[14] E. Ndiaye et al. "Efficient Smoothed Concomitant Lasso Estimation for High Dimensional Regression". In: *Journal of Physics: Conference Series* 904.1 (2017), p. 012006.

Smoothing aparté[15],[16]

Motivation: smooth a non-smooth function f to ease optimization

Smoothing: for $\mu > 0$, a "smoothed" version of f is f_μ

$$f_\mu = \mu\omega\left(\frac{\cdot}{\mu}\right)\Box f, \quad \text{where} \quad f\Box g(x) = \inf_u\{f(u) + g(x-u)\}$$

- ω is a predefined smooth function (s.t. $\nabla\omega$ is Lipschitz)

	Fourier: $\mathcal{F}(f)$	Fenchel/Legendre: f^*
	convolution: $\star$	**inf-convolution**: $\Box$
Kernel smoothing analogy:	$\mathcal{F}(f \star g) = \mathcal{F}(f) \cdot \mathcal{F}(g)$	$(f\Box g)^* = f^* + g^*$
	Gaussian : $\mathcal{F}(g) = g$	$\omega = \frac{\|\cdot\|^2}{2}$: $\quad \omega^* = \omega$
	$f_h = \frac{1}{h}g\left(\frac{\cdot}{h}\right) \star f$	$f_\mu = \mu\omega\left(\frac{\cdot}{\mu}\right)\Box f$

[15] Y. Nesterov. "Smooth minimization of non-smooth functions". In: *Math. Program.* 103.1 (2005), pp. 127–152.

[16] A. Beck and M. Teboulle. "Smoothing and first order methods: A unified framework". In: *SIAM J. Optim.* 22.2 (2012), pp. 557–580.

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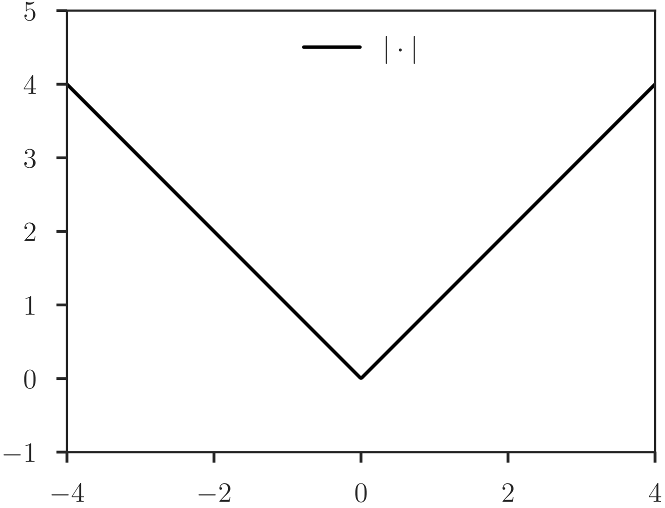
Huber function: $\omega(t) = \frac{t^2}{2}$



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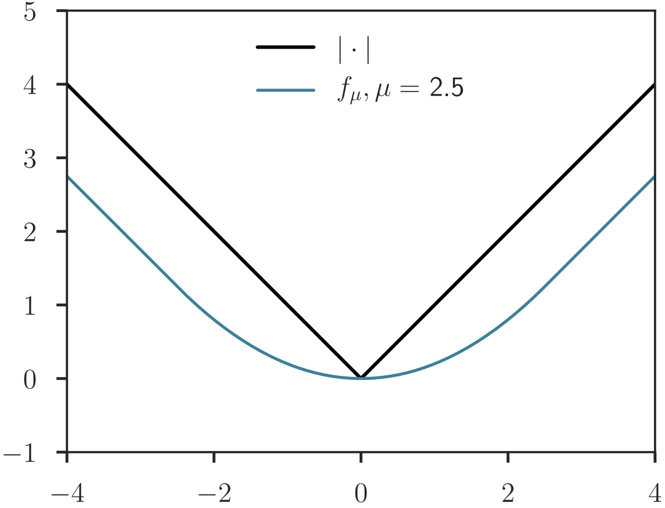

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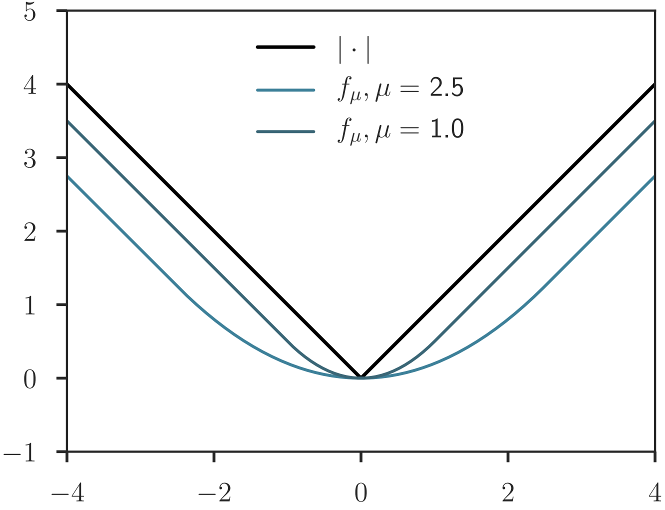

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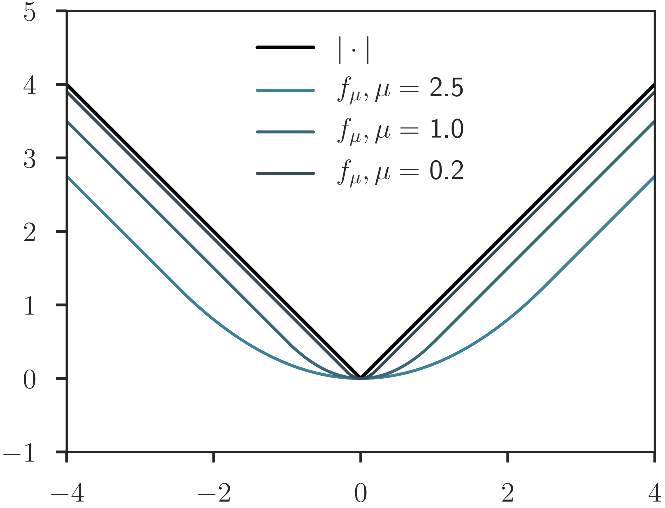

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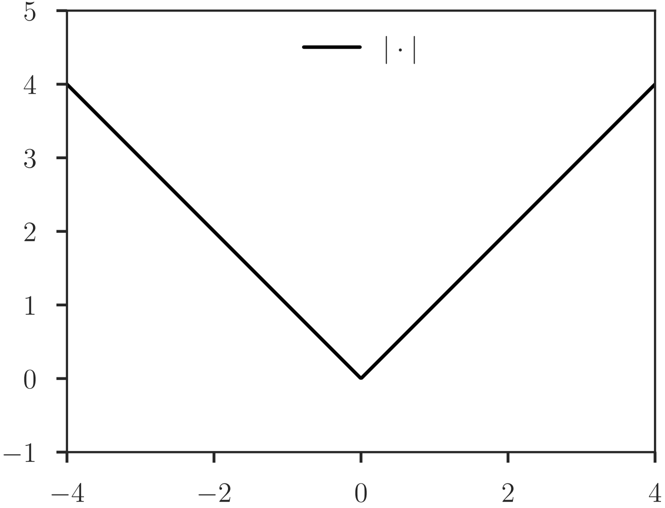

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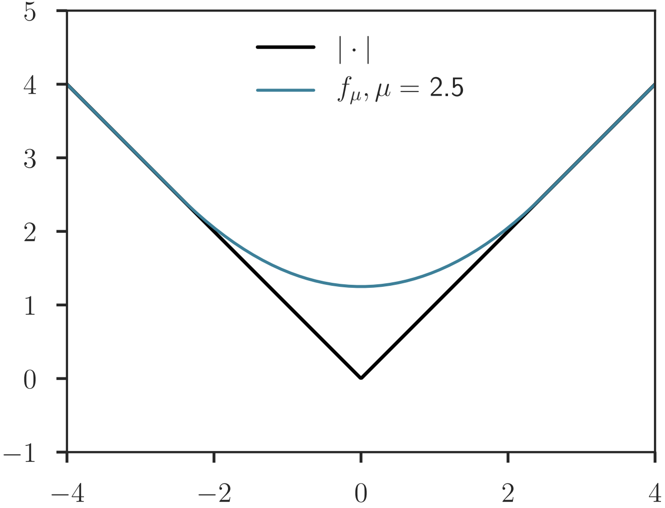

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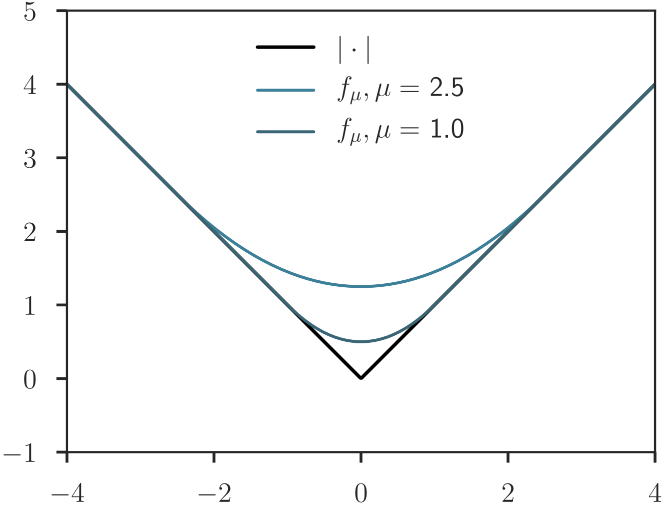

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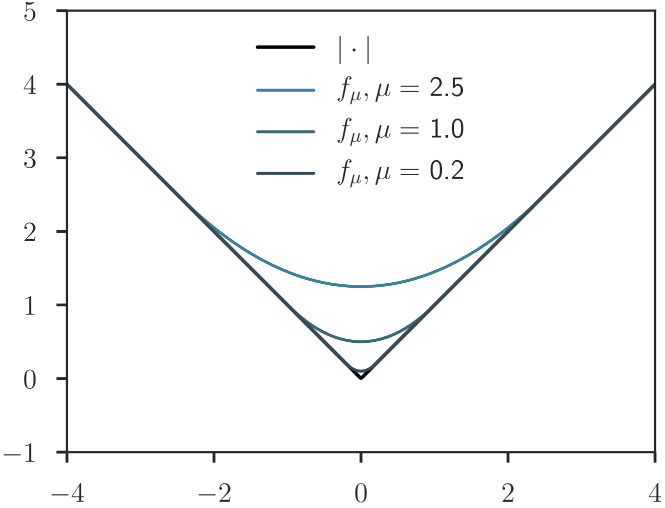

Huberization of the $\sqrt{\text{Lasso}}$

"**Huberization**": $f(z) = \|z\|$, $\mu = \underline{\sigma}$, $\omega(z) = \frac{\|z\|^2}{2} + \frac{1}{2}$

$$\|\cdot\| \,\square_{\underline{\sigma}} \omega\left(\frac{\cdot}{\underline{\sigma}}\right)(z) = \begin{cases} \frac{\|z\|^2}{2\underline{\sigma}} + \frac{\underline{\sigma}}{2}, & \text{if } \|z\| \leq \underline{\sigma} \\ \|z\|, & \text{if } \|z\| > \underline{\sigma} \end{cases}$$

$$= \min_{\sigma \geq \underline{\sigma}} \left(\frac{\|z\|^2}{2\sigma} + \frac{\sigma}{2}\right)$$

Leads to the Smoothed Concomitant Lasso formulation:

$$\boxed{(\hat{\beta}^{(\lambda)}, \hat{\sigma}^{(\lambda)}) \in \mathop{\arg\min}_{\beta \in \mathbb{R}^p, \sigma \geq \underline{\sigma}} \left(\frac{\|y - X\beta\|^2}{2n\sigma} + \frac{\sigma}{2} + \lambda \|\beta\|_1\right)}$$

Solving the Smooth Concomitant Lasso

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Jointly convex formulation : can be optimized by alternate minimization w.r.t. β and σ (gradient Lipschitz)

Alternate iteratively:

- Fix σ: (approximatively) solve a Lasso problem to update β

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Back to multi-task : $Y^{(l)} = X\mathrm{B}^* + S\mathrm{E}^{(l)}$

General case: $Y \in \mathbb{R}^{n \times q}$, $\mathrm{B} \in \mathbb{R}^{p \times q}$, and the noise $\mathrm{E} \in \mathbb{R}^{n \times q}$ might have some structure evolving along the n samples (sensors)

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$$\left\|\cdot\right\|_F \Box \underline{\sigma}\omega\left(\frac{\cdot}{\underline{\sigma}}\right)(Z) = \begin{cases} \frac{\|Z\|_F^2}{2\underline{\sigma}} + \frac{\underline{\sigma}}{2}, & \text{if } \|Z\| \leq \underline{\sigma} \\ \|Z\|_F, & \text{if } \|Z\| > \underline{\sigma} \end{cases}$$

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and similar efficient algorithms.

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$$\|\cdot\|_{s,1} \,\square\, \omega_{\underline{\sigma}}(Z) = \begin{cases} \frac{1}{2\underline{\sigma}} \sum_i \gamma_i^2 - (\gamma_i \wedge \underline{\sigma} - \gamma_i)^2, & \text{if } \|Z\|_{s,1} \leq \underline{\sigma} \\ \|Z\|_F\,, & \text{if } \|Z\|_{s,1} > \underline{\sigma} \end{cases}$$
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γ_i: singular values of Z
$\|Z\|_{S^{-1}}^2 := \mathrm{Tr}(Z^\top S^{-1} Z)$ **Mahalanobis distance**

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Smoothing of the nuclear/trace norm

Smoothed Generalized Concomitant Lasso (SGCL)[17]:

$$\boxed{(\hat{\mathrm{B}}^{\mathrm{SGCL}}, \hat{S}^{\mathrm{SGCL}}) \in \underset{\substack{\mathrm{B} \in \mathbb{R}^{p \times q} \\ S \in \mathbb{S}^n_{++}, S \succeq \underline{\sigma}}}{\arg\min} \frac{\left\| \bar{Y} - X\mathrm{B} \right\|^2_{S^{-1}}}{2nq} + \frac{\mathrm{Tr}(S)}{2n} + \lambda \left\| \mathrm{B} \right\|_{2,1}}$$

Concomitant Lasso with Repetitions (CLaR)[18]:

$$\boxed{(\hat{\mathrm{B}}^{\mathrm{CLaR}}, \hat{S}^{\mathrm{CLaR}}) \in \underset{\substack{\mathrm{B} \in \mathbb{R}^{p \times q} \\ S \in \mathbb{S}^n_{++}, S \succeq \underline{\sigma}}}{\arg\min} \frac{\sum_{l=1}^{r} \left\| Y^{(l)} - X\mathrm{B} \right\|^2_{S^{-1}}}{2nqr} + \frac{\mathrm{Tr}(S)}{2n} + \lambda \left\| \mathrm{B} \right\|_{2,1}}$$

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Efficient solvers for SGCL and CLaR

General case: $Y^{(l)} \in \mathbb{R}^{n\times q}$, $\mathrm{B} \in \mathbb{R}^{p\times q}$, and the noise $\mathrm{E}^{(l)} \in \mathbb{R}^{n\times q}$

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- jointly convex formulation (=nuclear norm smoothing[19])
- noise penalty on the sum of the eigenvalues of S ($S^* = {\Sigma^*}^{\frac{1}{2}}$)

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SGCL and CLaR computations: B update

Jointly convex formulation: alternate minimization still converging

B **Update** - S **fixed**:

"smooth + non-smooth" optimization; use Block Coordinate Descent (Iterative Block Soft-Thresholding) to update B row-wise

Possible refinements:

- (Gap) safe screening rules[20],[21]
- Strong rules[22]
- Active sets methods[23] etc.

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For SGCL and CLaR the problem can be reformulated as

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Closed-form solution (**Spectral clipping**):

if $U^\top \mathrm{diag}(s_1, \dots, s_n) U$ is the spectral decomposition of $Z Z^\top$:

$$\hat{S} = U^\top \mathrm{diag}(\max(\underline{\sigma}, \sqrt{s_1}), \dots, \max(\underline{\sigma}, \sqrt{s_n})) U$$

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Main drawbacks

- Statistically[24]: $\mathcal{O}(n^2)$ parameters to estimate for S
  - SGCL case: only nq observations (need q large w.r.t. n)
  - CLaR case: only nqr observations
- Computationally: S update cost is $\mathcal{O}(n^3)$ too slow in general (SVD computation)
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More structure can easily be incorporated to estimate S, *e.g.*, block diagonal, etc.

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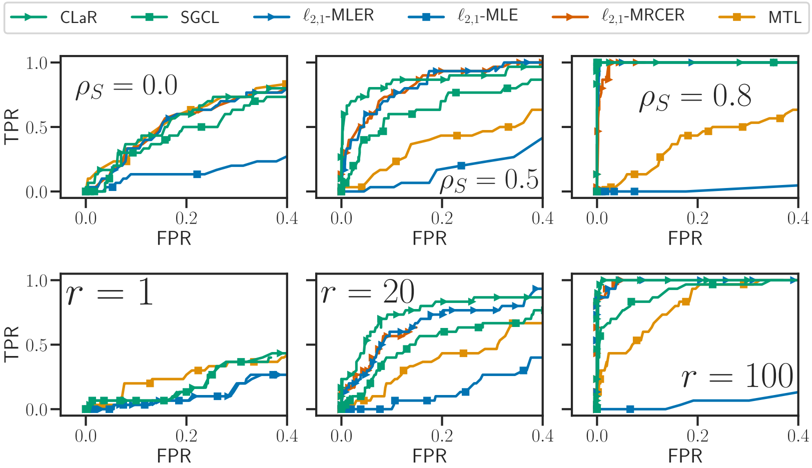
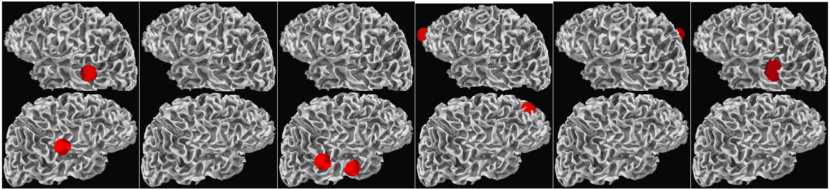
Simulated scenarios

- $n = 150$, $p = 500$, $q = 100$
- X Toeplitz-correlated: $\mathrm{Cov}(X_i, X_j) = \rho^{|i-j|}$, $\rho_X \in]0, 1[$
- S^* Toeplitz matrix: ${S^*}_{i,j} = \rho_{S^*}^{|i-j|}$, $\rho_{S^*} \in]0, 1[$



Real data



(a) CLaR (ours) (b) SGCL (c) MLER (d) MLE (e) MRCER (f) MTL

Figure: *Real data, left auditory stimulations ($n = 102$, $p = 7498$, $q = 76$, $r = 63$)* Sources found in the left hemisphere (top) and the right hemisphere (bottom) after left auditory stimulations.

- expected: 2 sources (one in each auditory cortex)
- λ chosen such that $\|\hat{\mathrm{B}}\|_{2,0} = 2$
- deep sources for SGCL and $\ell_{2,1}$-MRCER (not visible)

Conclusion and perspectives

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Merci!

"*All models are wrong but some come with good open source implementation and good documentation so use those.*"

A. Gramfort

- Paper: arXiv / personal webpage[25],[26]
- Python code online for CLaR https://github.com/QB3/CLaR
- Python code online for SGCL https://github.com/mathurinm/SHCL

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Competitors

- (smoothed) $\ell_{2,1}$-MLE

$$(\hat{\mathrm{B}}, \hat{\Sigma}) \in \mathop{\arg\min}_{\substack{\mathrm{B}\in\mathbb{R}^{p\times q} \\ \Sigma \succeq \underline{\sigma}^2/r^2}} \left\| \bar{Y} - X\mathrm{B} \right\|^2_{\Sigma^{-1}} - \log\det(\Sigma^{-1}) + \lambda \left\| \mathrm{B} \right\|_{2,1} \quad ,$$

- and its repetitions version ($\ell_{2,1}$-MLER):

$$(\hat{\mathrm{B}}, \hat{\Sigma}) \in \mathop{\arg\min}_{\substack{\mathrm{B}\in\mathbb{R}^{p\times q} \\ \Sigma \succeq \underline{\sigma}^2}} \sum_1^r \left\| Y^{(l)} - X\mathrm{B} \right\|^2_{\Sigma^{-1}} - \log\det(\Sigma^{-1}) + \lambda \left\| \mathrm{B} \right\|_{2,1} \quad .$$

- $\ell_{2,1}$-MLE and $\ell_{2,1}$-MLER are bi-convex but not jointly convex