

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

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Joint works with:

**Quentin Bertrand** (INRIA, Parietal Team)

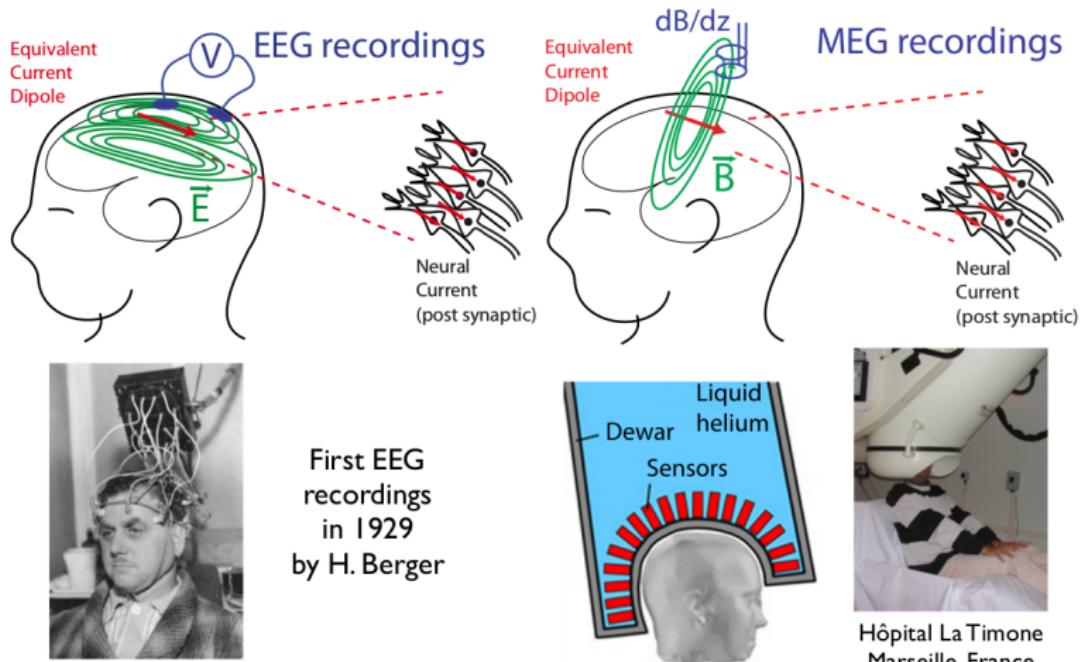
**Mathurin Massias** (INRIA, Parietal Team)

**Olivier Fercoq** (Institut Polytechnique de Paris)

**Alexandre Gramfort** (INRIA, Parietal Team)

# M/EEG inverse problem for brain imaging

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



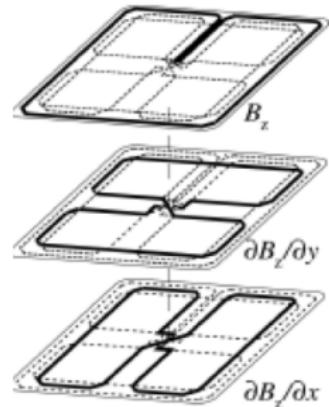
# MEG elements: magnometers and gradiometers



Device

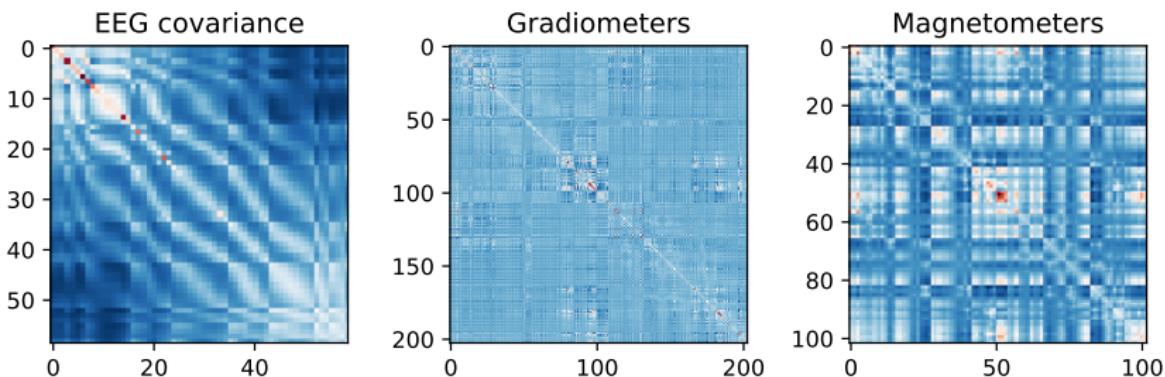


Sensors



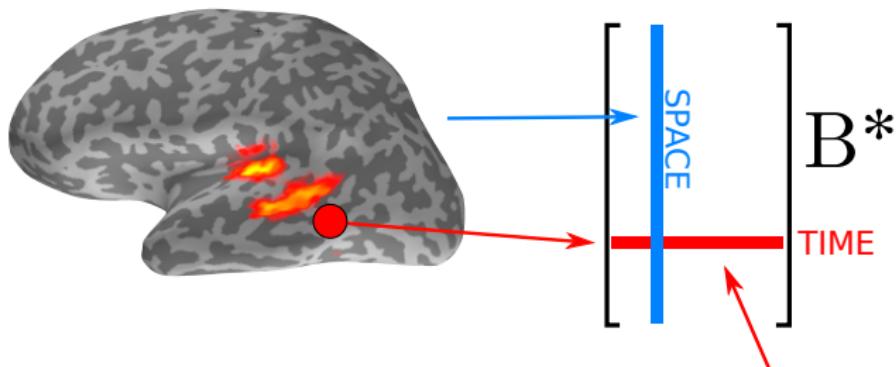
Detail of a sensor

# Noise is different for EEG / MEG (magnetometers and gradiometers)

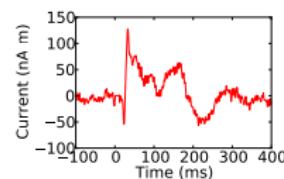


- ▶ 3 different sensors  $\implies$  3 different noise structures

# Source modeling

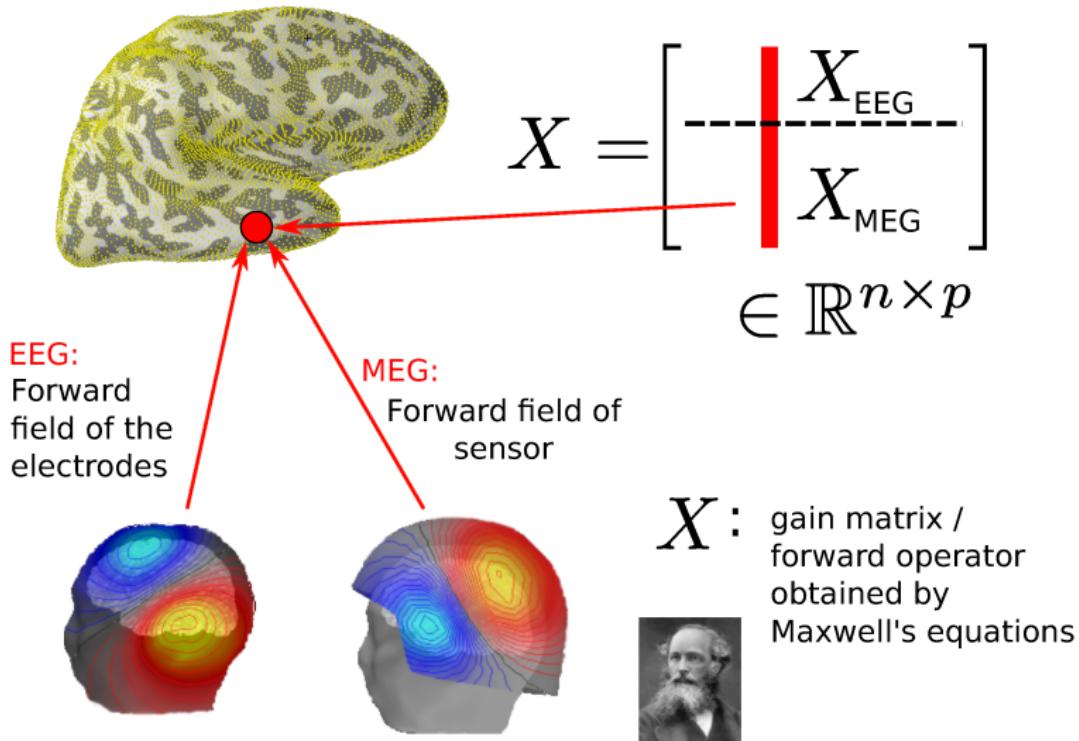


Position a few thousands  
candidate sources over the brain  
(e.g., every 5mm)

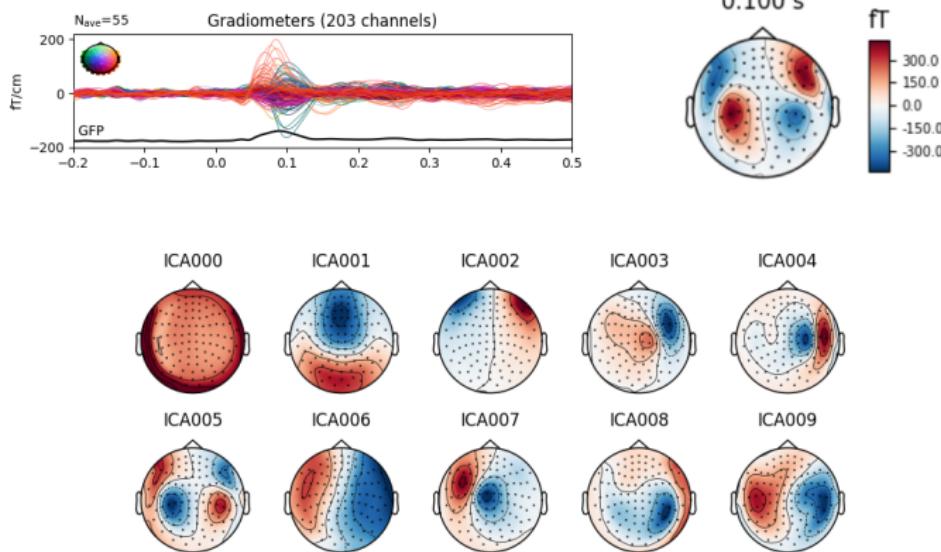


$$B^* \in \mathbb{R}^{p \times q}$$

# Design matrix - Forward operator



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

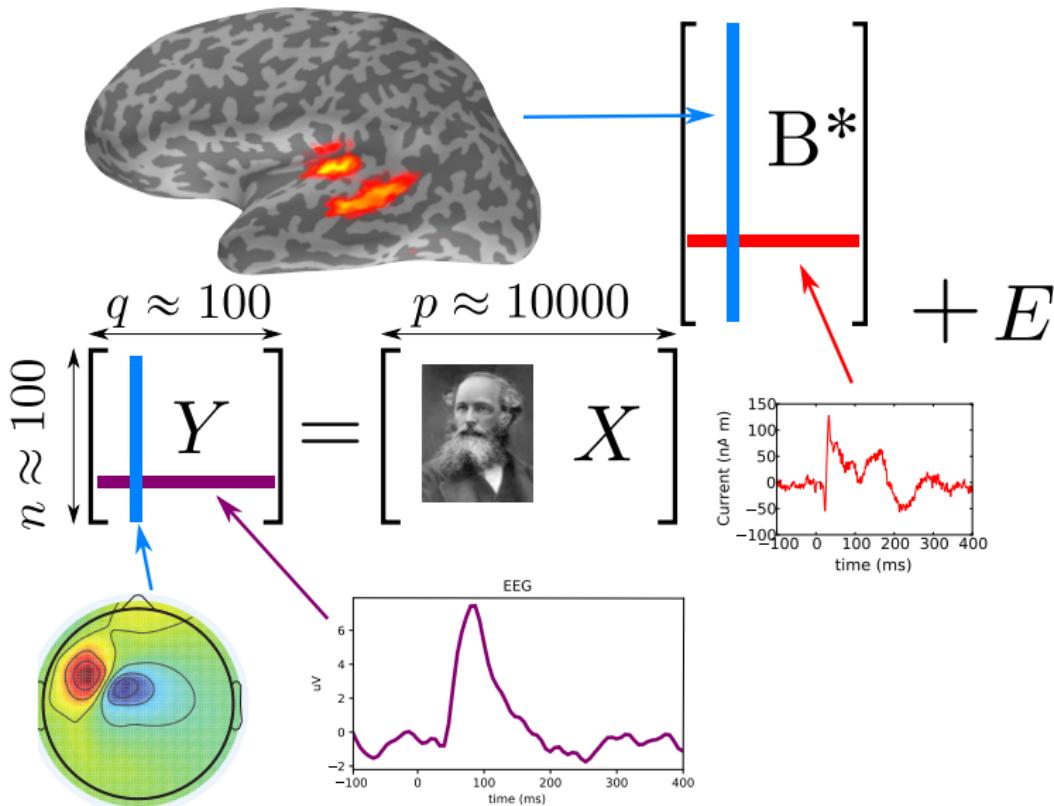


ICA : Blind source separation recovers dipolar patterns<sup>(1)</sup>

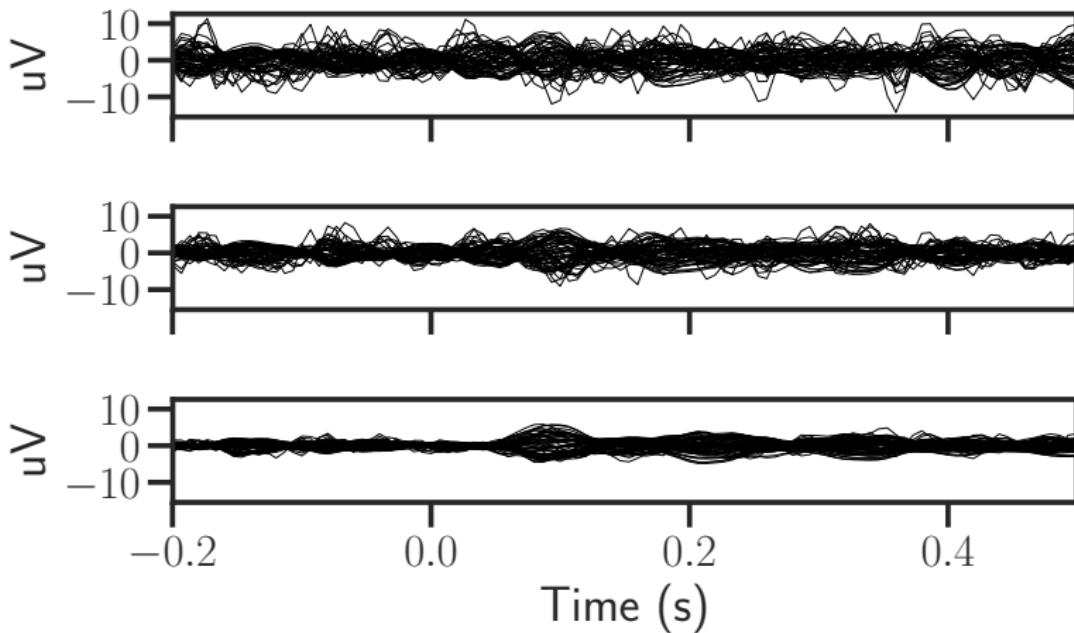
[http://martinos.org/mne/stable/auto\\_tutorials/plot\\_visualize\\_evoked.html](http://martinos.org/mne/stable/auto_tutorials/plot_visualize_evoked.html)  
[http://martinos.org/mne/stable/auto\\_tutorials/plot\\_artifacts\\_correction\\_ica.html](http://martinos.org/mne/stable/auto_tutorials/plot_artifacts_correction_ica.html)

<sup>(1)</sup> A. Delorme et al. "Independent EEG sources are dipolar". In: *PLoS one* 7.2 (2012), e30135.

# The M/EEG inverse problem: modeling



**Multiple repetitions structure:**  
 $r = 5$  (**top**),  $r = 10$  (**middle**), and  $r = 50$  (**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
- ▶  $r$  number of repetitions
- ▶  $Y^{(1)}, \dots, Y^{(r)} \in \mathbb{R}^{n \times q}$  observation matrices;  $\bar{Y} = \frac{1}{r} \sum_l Y^{(l)}$
- ▶  $X \in \mathbb{R}^{n \times p}$  forward matrix

$$Y^{(l)} = XB^* + SE^{(l)}$$

where

- ▶  $B^* \in \mathbb{R}^{p \times q}$  : true source activity matrix (**unknown**)
- ▶  $S \in \mathbb{S}_{++}^n$  co-standard deviation matrix<sup>(2)</sup> (**unknown**)
- ▶  $E^{(1)}, \dots, E^{(r)} \in \mathbb{R}^{n \times q}$  : white Gaussian noise

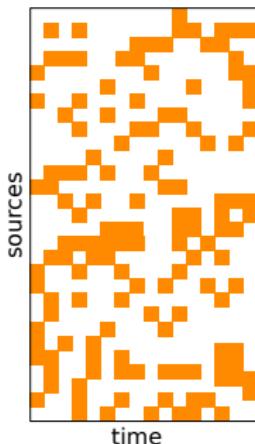
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<sup>(2)</sup>  $S \succeq \underline{\sigma}$  means  $S - \underline{\sigma}$  is Semi-Definite Positive

# Multi-tasks penalties<sup>(3)</sup>

Popular convex penalties considered:

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



Sparse support: no structure

Penalty: **Lasso type**

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

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

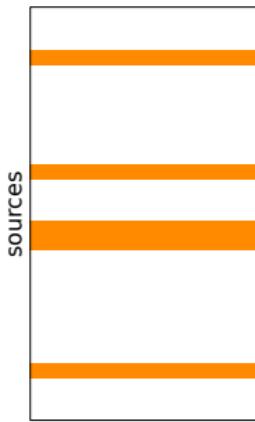
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<sup>(3)</sup> G. Obozinski, B. Taskar, and M. I. Jordan. "Joint covariate selection and joint subspace selection for multiple classification problems". In: *Statistics and Computing* 20.2 (2010), pp. 231–252.

## Multi-tasks penalties<sup>(3)</sup>

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

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



Sparse support: group structure

Penalty: **Group-Lasso type**

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

where  $B_{j,:}$ : the  $j$ -th row of  $B$

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

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## Multi-tasks data-fitting term

- ▶ Classical multi-tasks estimator: use averaged signal

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

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

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

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# Table of Contents

Calibrating  $\lambda$  and noise level estimation

Multi-task case and noise structure

Experiments

## 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**
- ▶  $\varepsilon \sim \mathcal{N}(0, \sigma_*^2 \text{Id}_n)$ ;  $\sigma_*$  **unknown**

Lasso reminder :

$$\hat{\beta}^{(\lambda)} \in \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|y - X\beta\|^2 + \lambda \|\beta\|_1$$

# Lasso theory<sup>(4), (5)</sup>

## Theorem

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

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

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**  $\sigma_*$  is unknown in practice !

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<sup>(4)</sup>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.

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## Joint estimation of $\beta$ and $\sigma$

How to calibrate (theoretically)  $\lambda$  when  $\sigma_*$  is unknown?

Intuitive idea: initialize  $\lambda$

- ▶ run Lasso with  $\lambda$ ; get  $\beta$
- ▶ estimate  $\sigma$ , 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)

N.B.: exactly the Concomitant Lasso<sup>(6)</sup> / Scaled-Lasso<sup>(7)</sup> implementation

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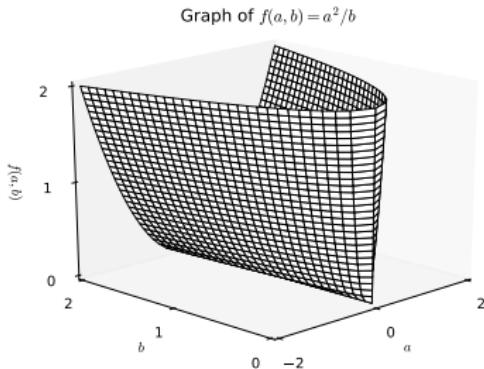
<sup>(6)</sup>A. B. Owen. "A robust hybrid of lasso and ridge regression". In: *Contemporary Mathematics* 443 (2007), pp. 59–72.

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

# Concomitant Lasso

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

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



<sup>(8)</sup>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.

<sup>(9)</sup>P. J. Huber. *Robust Statistics*. John Wiley & Sons Inc., 1981.

# Concomitant performance

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**Theorem**<sup>(10), (11)</sup>

---

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

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

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

---

Rem: provide same rate as Lasso, **without knowing**  $\sigma_*$

Rem:  $\lambda$  has no dimension, but calibration still needed in practice...

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<sup>(10)</sup> T. Sun and C.-H. Zhang. “Scaled sparse linear regression”. In: *Biometrika* 99.4 (2012), pp. 879–898.

<sup>(11)</sup> 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 “ $\sigma$  free” choice of  $\lambda$

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

- ▶ Connections with Concomitant Lasso:

$(\hat{\beta}_{\sqrt{\text{Lasso}}}^{(\lambda)}, \hat{\sigma}_{\sqrt{\text{Lasso}}}^{(\lambda)})$  is solution of the Concomitant Lasso when

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

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

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<sup>(12)</sup> 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<sup>(14)</sup>

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

- ▶ useful for optimization with small  $\lambda$
- ▶ 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  $\epsilon$ -solutions for the  $\sqrt{\text{Lasso}}$ <sup>(13)</sup>

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

<sup>(14)</sup> E. Ndiaye et al. "Efficient Smoothed Concomitant Lasso Estimation for High Dimensional Regression". In: *NCMIP*. 2017.

# Smoothing aparté<sup>(15), (16)</sup>

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

Smoothing: for  $\mu > 0$ , a “smoothed” version of  $f$  is  $f_\mu$

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

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

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

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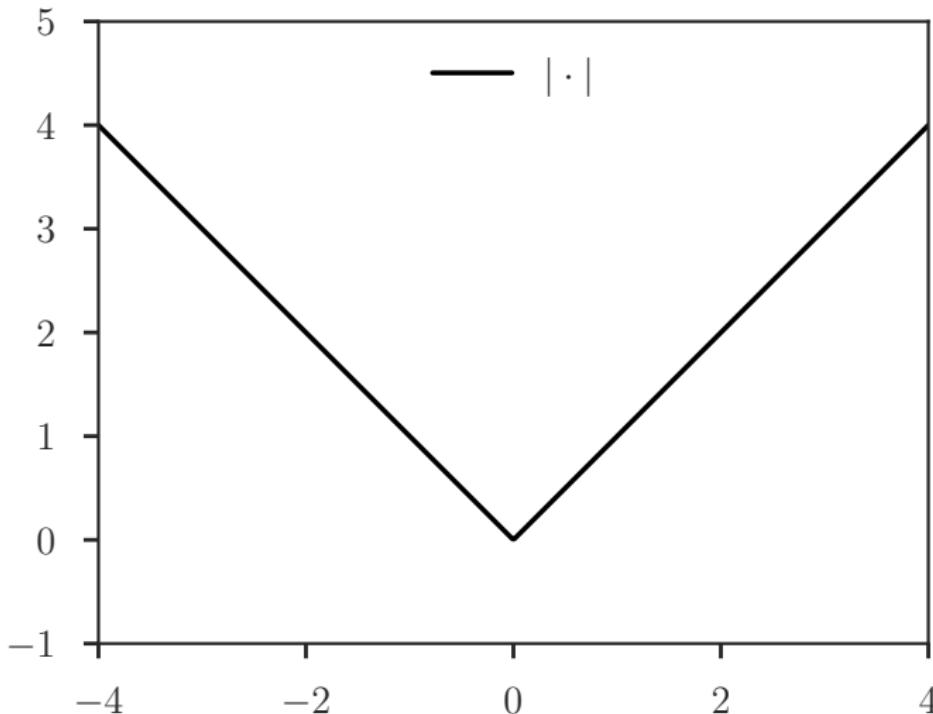
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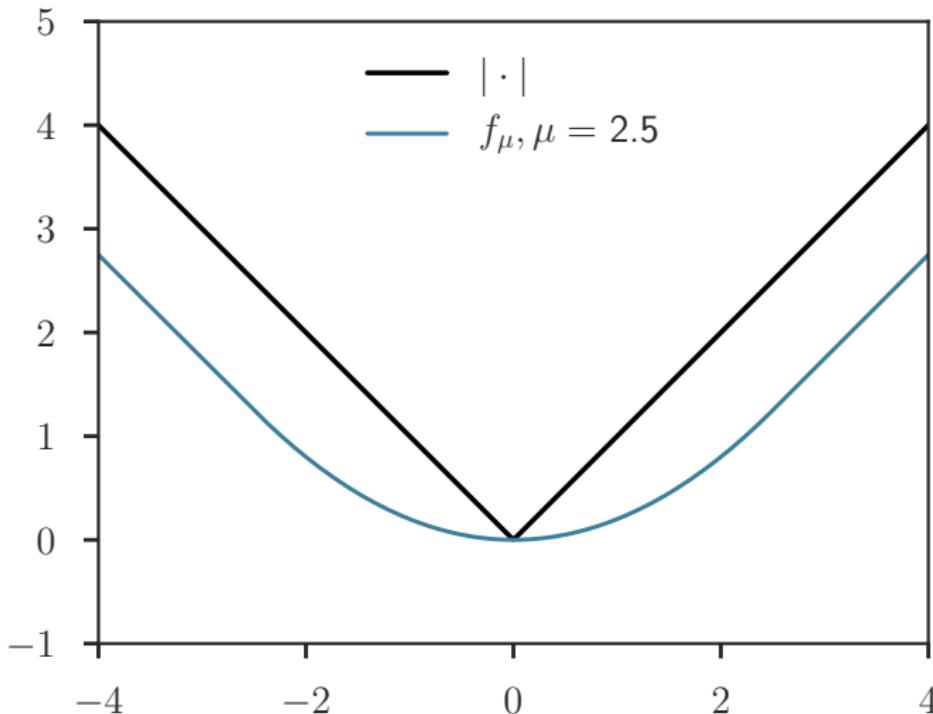
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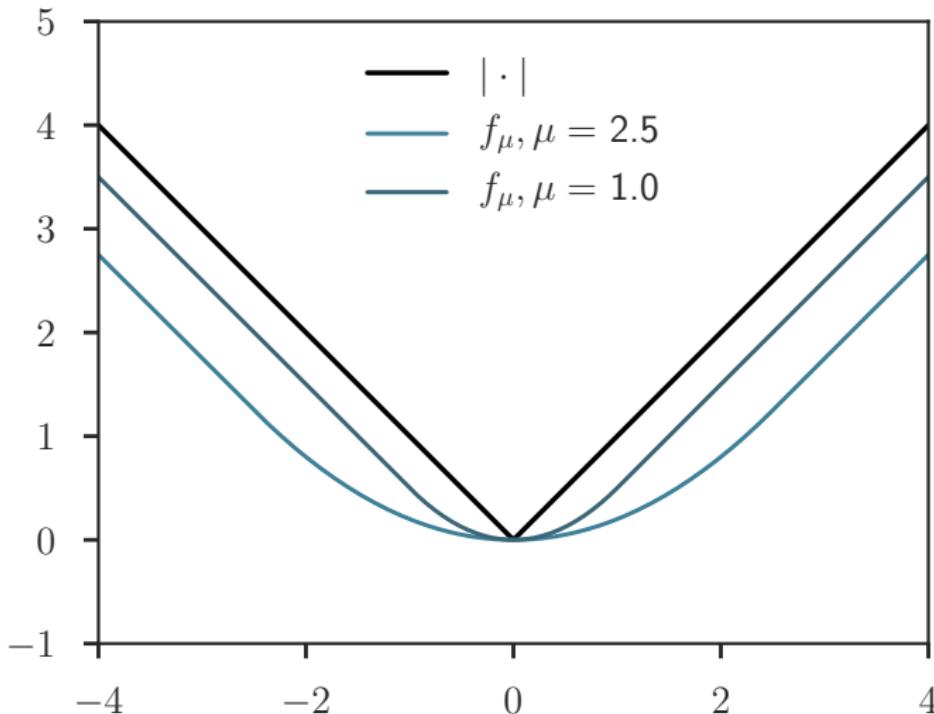
**Huber function:**  $\omega(t) = \frac{t^2}{2}$



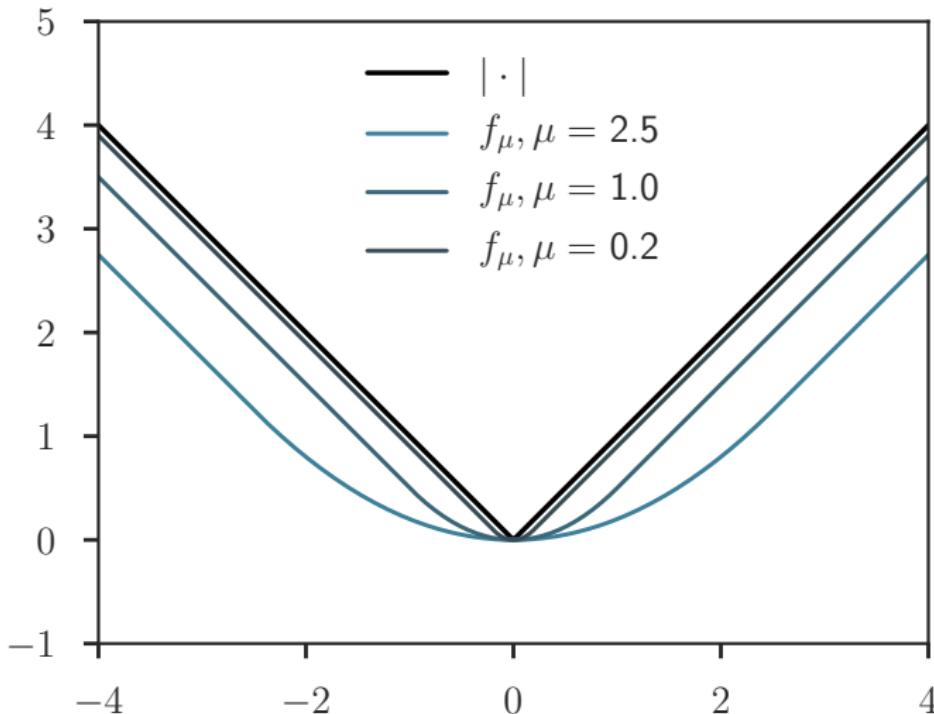
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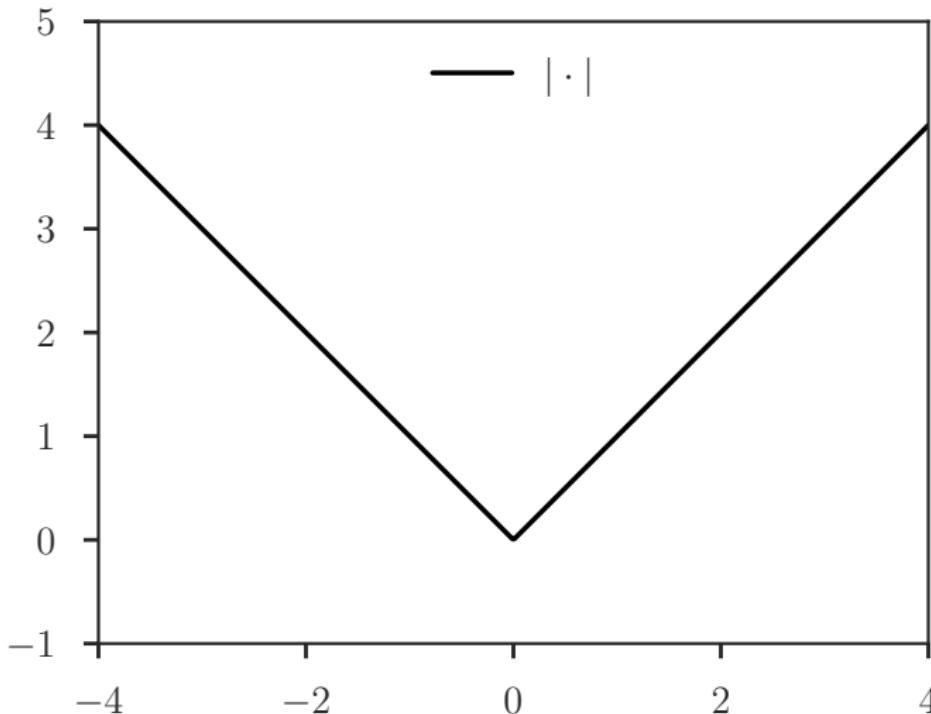
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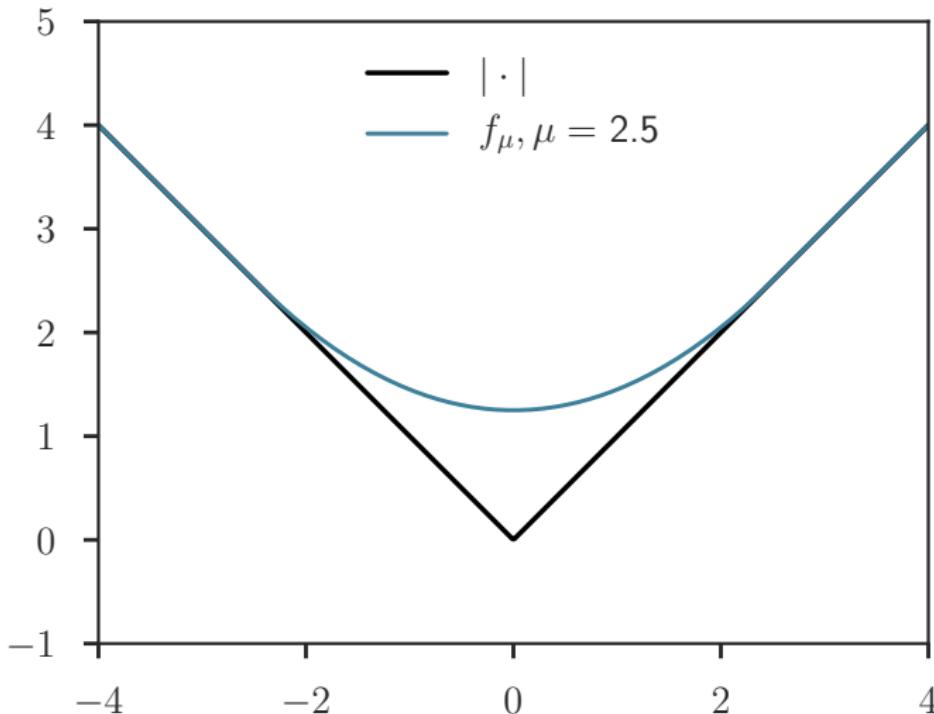
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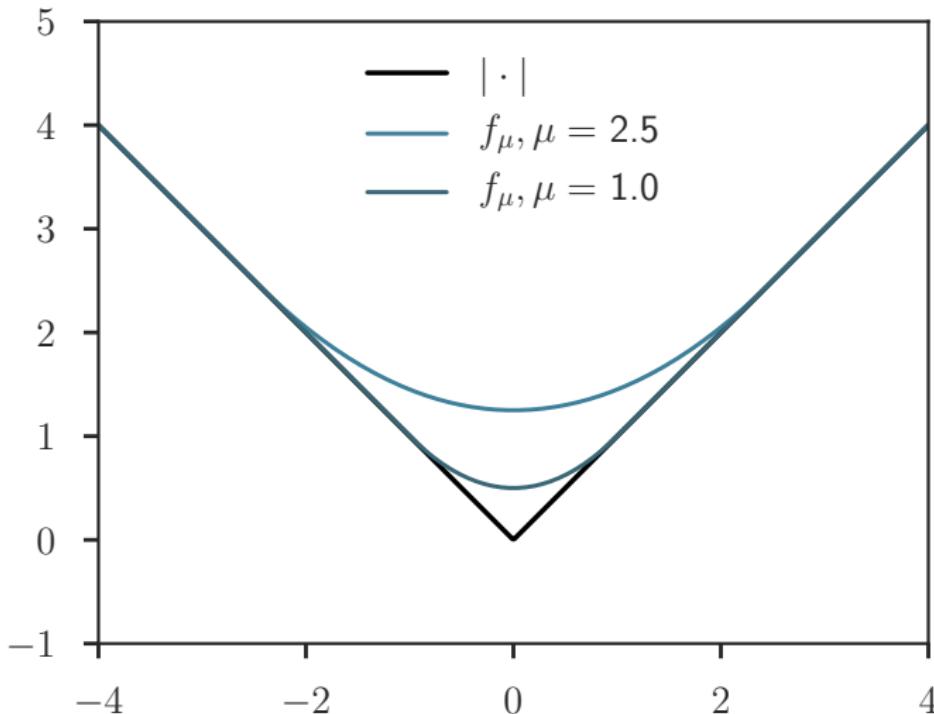
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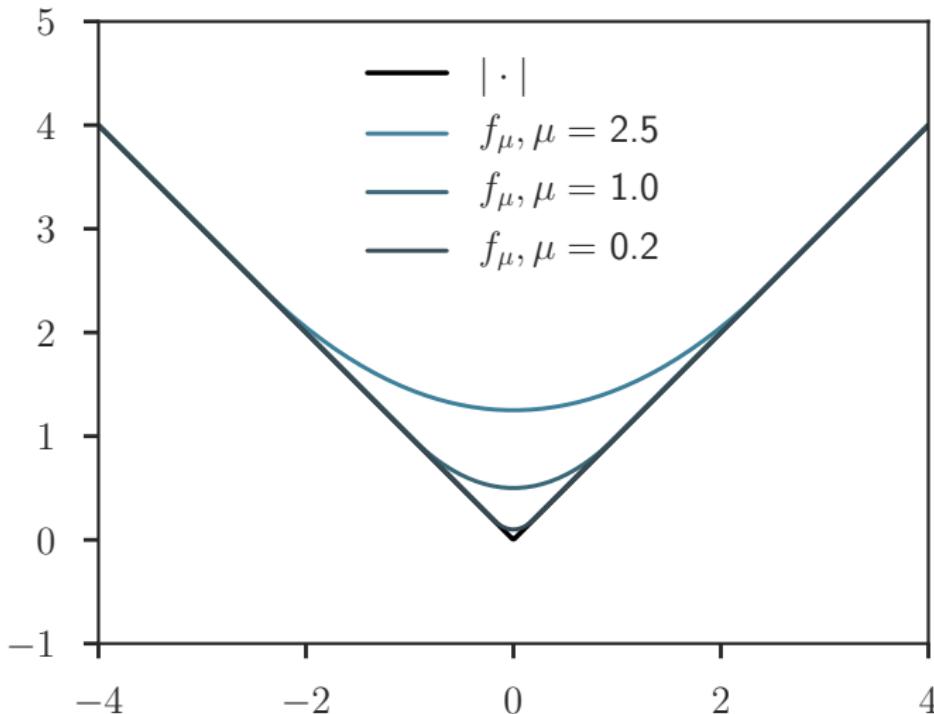
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# Huberization of the $\sqrt{\text{Lasso}}$

“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:

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

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**Jointly convex** formulation : can be optimized by alternate minimization w.r.t.  $\beta$  and  $\sigma$  (gradient Lipschitz)

Alternate iteratively:

- ▶ Fix  $\sigma$ : (approximatively) solve a Lasso problem to update  $\beta$

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

“Huberization of the Frobenius norm”

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

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$$\begin{aligned}\|\cdot\|_{s,1} \square \omega_{\underline{\sigma}} (Z) &= \begin{cases} \frac{1}{2\underline{\sigma}} \sum_i \gamma_i^2 - (\gamma_i \wedge \underline{\sigma} - \gamma_i)^2, & \text{if } \|Z\|_{s,1} \leq \underline{\sigma} \\ \|Z\|_F, & \text{if } \|Z\|_{s,1} > \underline{\sigma} \end{cases} \\ &= \min_{S \succeq \underline{\sigma}} \frac{1}{2} \|Z\|_{S^{-1}}^2 + \frac{1}{2} \operatorname{Tr}(S)\end{aligned}$$

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# Smoothing of the nuclear/trace norm

**Smoothed Generalized Concomitant Lasso (SGCL)<sup>(17)</sup>:**

$$(\hat{B}^{\text{SGCL}}, \hat{S}^{\text{SGCL}}) \in \arg \min_{\substack{B \in \mathbb{R}^{p \times q} \\ S \in \mathbb{S}_{++}^n, S \succeq \sigma}} \frac{\|\bar{Y} - XB\|_{S^{-1}}^2}{2nq} + \frac{\text{Tr}(S)}{2n} + \lambda \|B\|_{2,1}$$

**Concomitant Lasso with Repetitions (CLaR)<sup>(18)</sup>:**

$$(\hat{B}^{\text{CLaR}}, \hat{S}^{\text{CLaR}}) \in \arg \min_{\substack{B \in \mathbb{R}^{p \times q} \\ S \in \mathbb{S}_{++}^n, S \succeq \sigma}} \frac{\sum_{l=1}^r \|Y^{(l)} - XB\|_{S^{-1}}^2}{2nqr} + \frac{\text{Tr}(S)}{2n} + \lambda \|B\|_{2,1}$$

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<sup>(17)</sup> M. Massias et al. "Generalized Concomitant Multi-Task Lasso for Sparse Multimodal Regression". In: AISTATS. vol. 84. 2018, pp. 998–1007.

<sup>(18)</sup> Q. Bertrand et al. *Concomitant Lasso with Repetitions (CLaR): beyond averaging multiple realizations of heteroscedastic noise*. Tech. rep. 2019. arXiv: 1902.02509.

# Efficient solvers for SGCL and CLaR

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

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<sup>(19)</sup>S. van de Geer. *Estimation and testing under sparsity*. Vol. 2159. Lecture Notes in Mathematics. Lecture notes from the 45th Probability Summer School held in Saint-Flour, 2015, École d'Été de Probabilités de Saint-Flour. Springer, 2016, pp. xiii+274.

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- ▶ jointly convex formulation (=nuclear norm smoothing<sup>(19)</sup>)
- ▶ 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<sup>(20), (21)</sup>
- ▶ Strong rules<sup>(22)</sup>
- ▶ Active sets methods<sup>(23)</sup> etc.

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For SGCL and CLaR the problem can be reformulated as

$$\hat{S} = \arg \min_{S \in \mathbb{S}_{++}^n, S \succeq \underline{\sigma} \text{ Id}_n} \left( \frac{1}{2n} \text{Tr}[Z^\top S^{-1} Z] + \frac{1}{2n} \text{Tr}(S) \right)$$

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

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

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

Rem: as in the classical concomitant Lasso, at each step CLaR and SGCL estimate alternatively B and  $S$

## Main drawbacks

- ▶ Statistically<sup>(24)</sup>:  $\mathcal{O}(n^2)$  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)  
Rem: fine for MEG/EEG problems ( $n \approx 300$ )

More structure can easily be incorporated to estimate  $S$ ,  
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## Simulated scenarios

Simulated design:

- ▶  $n = 150$
- ▶  $p = 500$
- ▶  $q = 100$
- ▶  $X$  Toeplitz-correlated:  $\text{Cov}(X_i, X_j) = \rho^{|i-j|}$ ,  $\rho_X \in ]0, 1[$
- ▶  $S$  Toeplitz matrix:  $S_{i,j} = \rho^{|i-j|}$ ,  $\rho_S \in ]0, 1[$
- ▶  $\text{SNR} = \|XB^*\| / \|Y - XB^*\|$  Signal to Noise Ratio

# Computational comparison between estimators

- ▶ CLaR: Concomitant Lasso with Repetitions
- ▶ SGCL: Smoothed Generalized Concomitant Lasso
- ▶ MTLR: Multi-Task Lasso with Repetitions
- ▶ MTL: Multi-Task Lasso

	CD epoch	gap computation
CLaR	$\mathcal{O}\left(\frac{n^3+qn^2}{f} + pn^2 + pnq\right)$	$\mathcal{O}(rnq + p)$
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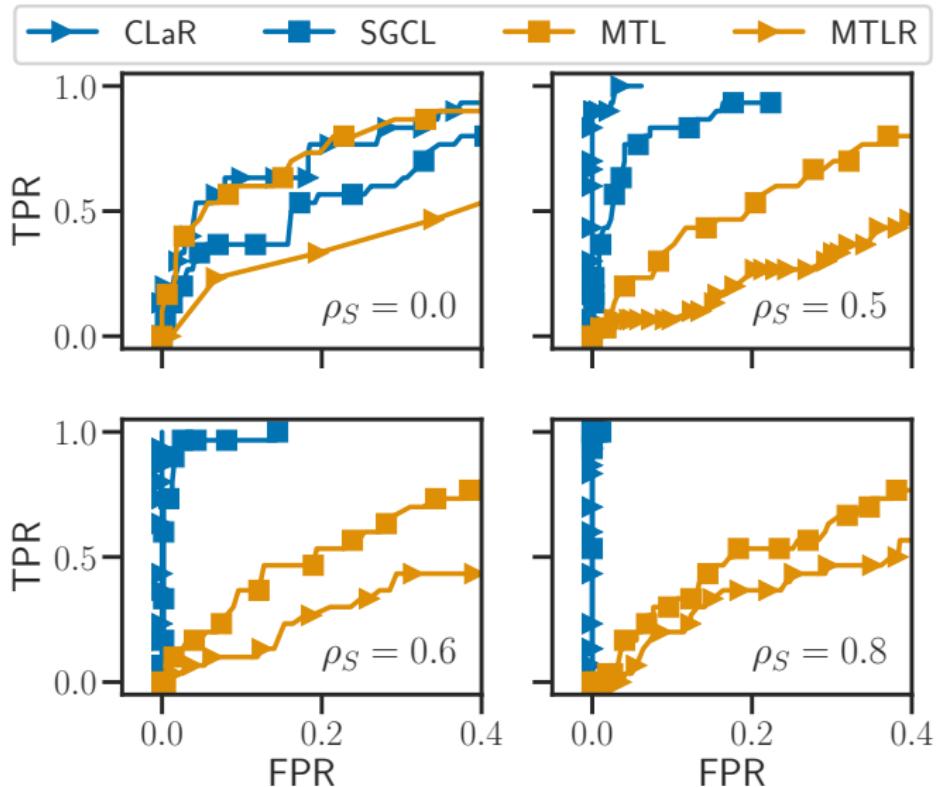
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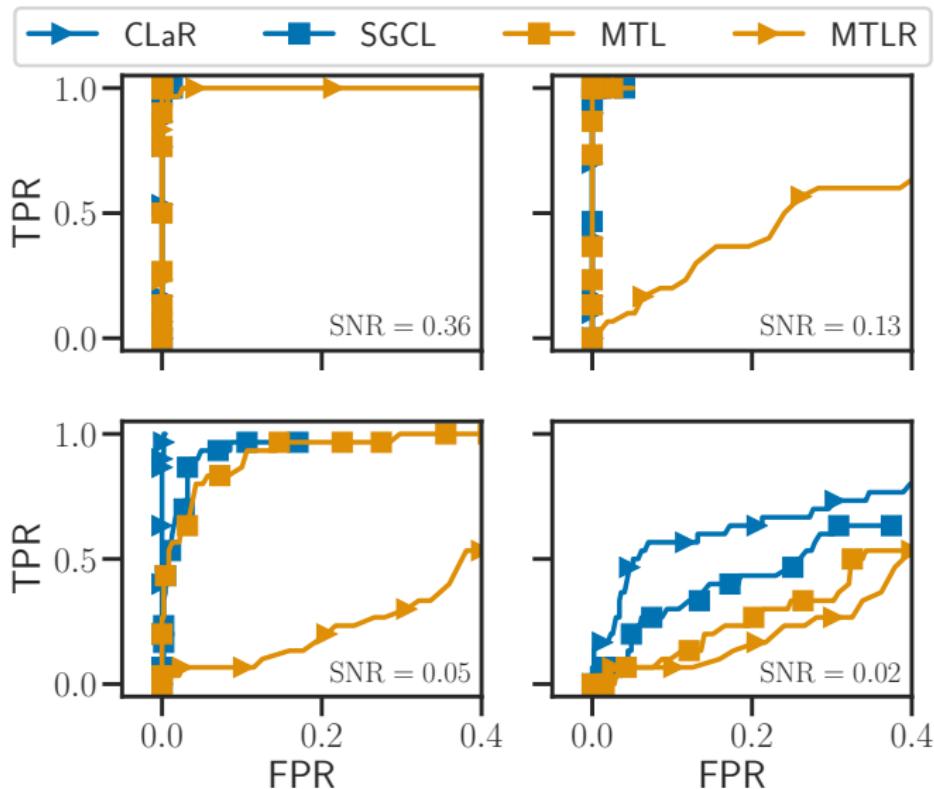
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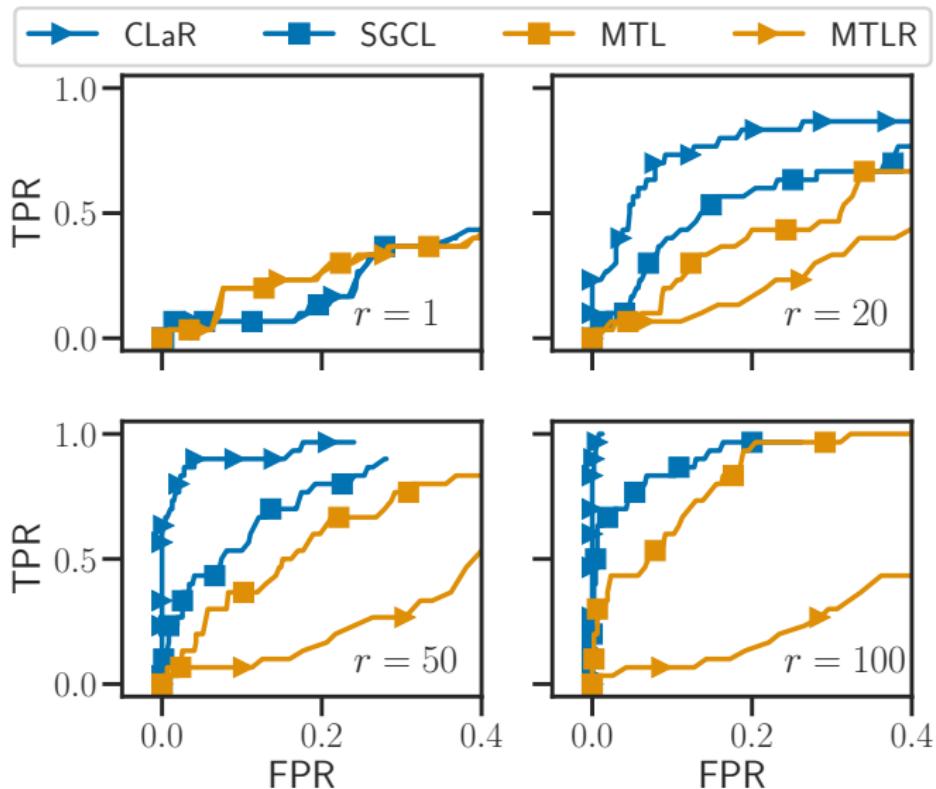
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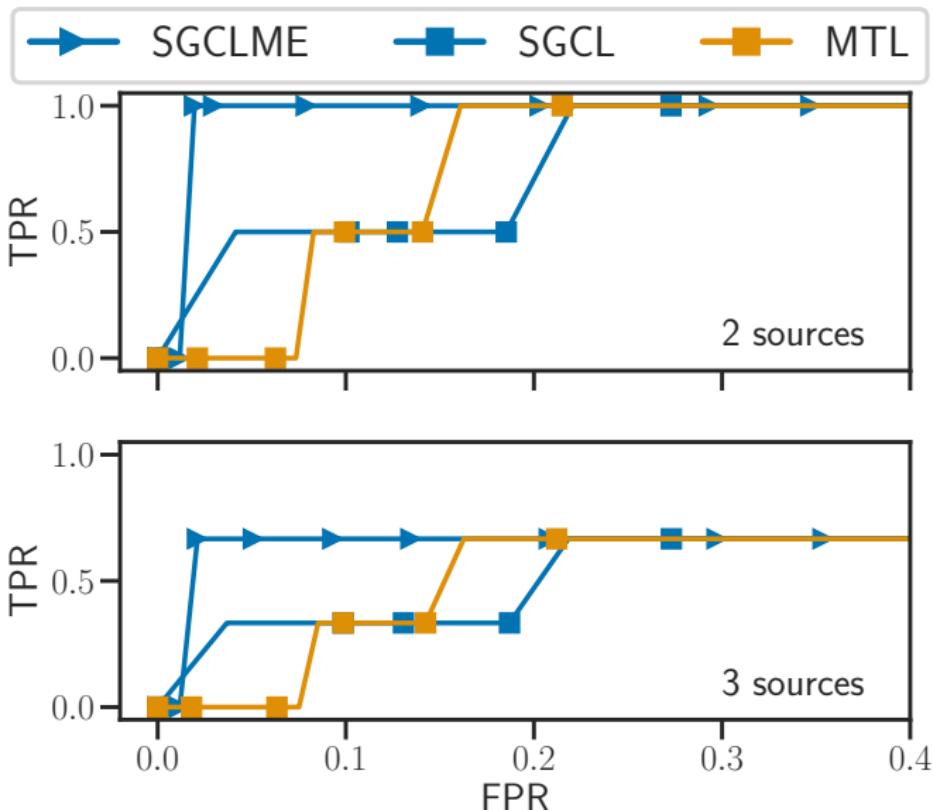


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## Semi-real data: real $X$ and $S$



## 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 / personnal webpage<sup>(25), (26)</sup>
- ▶ Python code online for CLaR <https://github.com/QB3/CLaR>
- ▶ Python code online for SHCL <https://github.com/mathurinm/SHCL>



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<sup>(25)</sup> M. Massias et al. “Generalized Concomitant Multi-Task Lasso for Sparse Multimodal Regression”. In: *AISTATS*. vol. 84. 2018, pp. 998–1007.

<sup>(26)</sup> Q. Bertrand et al. *Concomitant Lasso with Repetitions (CLaR): beyond averaging multiple realizations of heteroscedastic noise*. Tech. rep. 2019. arXiv: [1902.02509](https://arxiv.org/abs/1902.02509).

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