$\begin{array}{c} \textbf{Optimizational and statistical}\\ \textbf{contributions to the } \ell_{2,1} \textbf{-regularized}\\ \textbf{M/EEG inverse problem} \end{array}$

PhD defense Mathurin Massias (INRIA)

- G. Peyré (Rapporteur)
- M. Schmidt (Rapporteur)
- N. Pustelnik (Examinatrice)
- O. Fercoq (Examinateur)

- J. Mairal (Examinateur)
- J. Salmon (Directeur)
- A. Gramfort (Co-directeur)

Down by the pool



The M/EEG inverse problem

- observe magnetoelectric field outside the scalp (100 sensors)
- reconstruct cerebral activity inside the brain (10,000 locations)



 $n \ll p$: ill-posed problem!

Signals can often be represented combining few atoms/features:

Fourier decomposition for sounds



¹I. Daubechies. Ten lectures on wavelets. SIAM, 1992.

Signals can often be represented combining few atoms/features:

- Fourier decomposition for sounds
- Wavelets for images (1990's)¹



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Signals can often be represented combining few atoms/features:

- Fourier decomposition for sounds
- ▶ Wavelets for images (1990's)¹
- Dictionary learning for images (2000's)²



¹I. Daubechies. Ten lectures on wavelets. SIAM, 1992.

Signals can often be represented combining few atoms/features:

- Fourier decomposition for sounds
- ▶ Wavelets for images (1990's)¹
- Dictionary learning for images (2000's)²
- Here we assume that measurements are explained by a few active brain sources



¹I. Daubechies. Ten lectures on wavelets. SIAM, 1992.

Justification for dipolarity assumption

- short duration
- simple cognitive task
- repetitions of experiment average out other sources
- ► ICA recovers dipolar patterns,³ well modelled by focal sources:



³A. Delorme et al. "Independent EEG sources are dipolar". In: PloS one 7.2 (2012), e30135.

Mathematical model: linear regression



Lasso^{4,5}: the "modern least-squares"⁶

$$\hat{\beta} \in \underset{\beta \in \mathbb{R}^{p}}{\operatorname{arg\,min}} \underbrace{\frac{1}{2} \left\| y - X\beta \right\|^{2} + \lambda \left\| \beta \right\|_{1}}_{\mathcal{P}(\beta)}$$

- $y \in \mathbb{R}^n$: observations
- $X = [X_1| \dots |X_p] \in \mathbb{R}^{n \times p}$: design matrix
- sparsity: for λ large enough, $\|\hat{\beta}\|_0 \ll p$

⁴R. Tibshirani. "Regression Shrinkage and Selection via the Lasso". In: J. R. Stat. Soc. Ser. B Stat. Methodol. 58.1 (1996), pp. 267–288.

⁵S. S. Chen and D. L. Donoho. "Atomic decomposition by basis pursuit". In: SPIE. 1995.

⁶E. J. Candès, M. B. Wakin, and S. P. Boyd. "Enhancing Sparsity by Reweighted *l*₁ Minimization". In: J. Fourier Anal. Applicat. 14.5-6 (2008), pp. 877–905.

Sparsity inducing penalties⁷

$$\hat{\mathbf{B}} \in \underset{\mathbf{B} \in \mathbb{R}^{p \times T}}{\operatorname{arg\,min}} \left(\frac{1}{2nT} \| Y - X\mathbf{B} \|_{F}^{2} + \lambda \| \mathbf{B} \|_{1} \right)$$



Sparse support: no structure X

Lasso penalty

$$\|\mathbf{B}\|_1 \triangleq \sum_{j=1}^p \sum_{t=1}^T |\mathbf{B}_{jt}|$$

⁷G. 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.

Sparsity inducing penalties⁷

$$\hat{\mathbf{B}} \in \operatorname*{arg\,min}_{\mathbf{B} \in \mathbb{R}^{p \times T}} \left(\frac{1}{2nT} \left\| Y - X\mathbf{B} \right\|_{F}^{2} + \lambda \|\mathbf{B}\|_{2,1} \right)$$



Sparse support: group structure 🗸

Group-Lasso penalty

$$\|\mathbf{B}\|_{2,1} \triangleq \sum_{j=1}^{p} \|\mathbf{B}_{j:}\|_{2}$$

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

⁷G. 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.

Lasso-type problems

Lasso
$$\underset{\beta \in \mathbb{R}^p}{\operatorname{arg\,min}} \frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|_1$$

Lasso-type problems

$$\begin{array}{lll} \text{Lasso} & \displaystyle \mathop{\arg\min}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|_1 \\ \text{sparse Log. reg.} & \displaystyle \mathop{\arg\min}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n \log\left(1 + \exp(-y_i\beta^\top x_i)\right) + \lambda \|\beta\|_1 \end{array}$$

Lasso-type problems

$$\begin{array}{ll} \text{Lasso} & \displaystyle \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \frac{1}{2} \|y - X\beta\|^2 + \lambda \|\beta\|_1 \\ \text{sparse Log. reg.} & \displaystyle \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \sum_{i=1}^n \log \left(1 + \exp(-y_i \beta^\top x_i)\right) + \lambda \|\beta\|_1 \\ \text{Multi-task Lasso} & \displaystyle \operatorname*{arg\,min}_{\mathrm{B} \in \mathbb{R}^{p \times T}} \frac{1}{2} \|Y - X\mathbf{B}\|^2 + \lambda \|\mathbf{B}\|_{2,1} \end{array}$$

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Duality for the Lasso

primal
$$\hat{\beta} \in \underset{\beta \in \mathbb{R}^{p}}{\operatorname{arg\,min}} \underbrace{\frac{1}{2} \|y - X\beta\|^{2} + \lambda \|\beta\|_{1}}_{\mathcal{P}(\beta)}$$

dual $\hat{\theta} = \underset{\theta \in \Delta_{X}}{\operatorname{arg\,max}} \underbrace{\frac{1}{2} \|y\|^{2} - \frac{\lambda^{2}}{2} \|y/\lambda - \theta\|^{2}}_{\mathcal{D}(\theta)}$

 $\Delta_X = \Big\{ \theta \in \mathbb{R}^n \, : \, \forall j \in [p], \; |X_j^\top \theta| \leq 1 \Big\} : \text{ dual feasible set}$

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 $\Delta_X = \left\{ \theta \in \mathbb{R}^n \, : \, \forall j \in [p], \; |X_j^\top \theta| \le 1 \right\} : \text{ dual feasible set}$



To minimize:
$$\mathcal{P}(\beta) = \frac{1}{2} \|y - \sum_{j=1}^{p} X_j \beta_j\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

 $eta^{(0)} = \mathbf{0}_p \in \mathbb{R}^p$ for $t = 1, \dots$ do

⁸J. Friedman, T. J. Hastie, and R. Tibshirani. "Regularization paths for generalized linear models via coordinate descent". In: *J. Stat. Softw.* 33.1 (2010), p. 1.

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$$\mathcal{P}(\beta) = \frac{1}{2} \|y - \sum_{j=1}^{p} X_j \beta_j\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$\beta^{(0)} = \mathbf{0}_{p} \in \mathbb{R}^{p}$$
for $t = 1, \dots$ do
$$\beta_{1}^{(t)} \approx \underset{\beta_{1} \in \mathbb{R}}{\operatorname{arg\,min}} \mathcal{P}(\beta_{1}, \beta_{2}^{(t-1)}, \beta_{3}^{(t-1)}, \dots, \beta_{p-1}^{(t-1)}, \beta_{p}^{(t-1)})$$

⁸J. Friedman, T. J. Hastie, and R. Tibshirani. "Regularization paths for generalized linear models via coordinate descent". In: *J. Stat. Softw.* 33.1 (2010), p. 1.

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$$\beta_{2}^{(t)} \approx \underset{\beta_{2} \in \mathbb{R}}{\operatorname{arg\,min}} \mathcal{P}(\beta_{1}^{(t)}, \beta_{2}, \beta_{3}^{(t-1)}, \dots, \beta_{p-1}^{(t-1)}, \beta_{p}^{(t-1)})$$

⁸J. Friedman, T. J. Hastie, and R. Tibshirani. "Regularization paths for generalized linear models via coordinate descent". In: *J. Stat. Softw.* 33.1 (2010), p. 1.

To minimize:
$$\mathcal{P}(\beta) = \frac{1}{2} \|y - \sum_{j=1}^{p} X_j \beta_j\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

$$\begin{split} \beta^{(0)} &= \mathbf{0}_{p} \in \mathbb{R}^{p} \\ \text{for } t = 1, \dots \text{ do} \\ & \beta_{1}^{(t)} \approx \mathop{\arg\min}_{\substack{\beta_{1} \in \mathbb{R} \\ \beta_{2}^{(t)} \approx \arg\min_{\substack{\beta_{1} \in \mathbb{R} \\ \beta_{2} \in \mathbb{R}}}} \mathcal{P}(\beta_{1}^{(t)}, \beta_{2}^{(t-1)}, \beta_{3}^{(t-1)}, \dots, \beta_{p-1}^{(t-1)}, \beta_{p}^{(t-1)}) \\ & \vdots \\ & \vdots \\ & \beta_{p}^{(t)} \approx \mathop{\arg\min}_{\substack{\beta_{2} \in \mathbb{R} \\ \beta_{p} \in \mathbb{R}}} \mathcal{P}(\beta_{1}^{(t)}, \beta_{2}^{(t)}, \beta_{3}^{(t)}, \dots, \beta_{p-1}^{(t)}, \beta_{p})) \\ \end{split}$$
 1 epoch

⁸J. Friedman, T. J. Hastie, and R. Tibshirani. "Regularization paths for generalized linear models via coordinate descent". In: *J. Stat. Softw.* 33.1 (2010), p. 1.

⁹R.-E. Fan et al. "LIBLINEAR: A library for large linear classification". In: JMLR 9 (2008), pp. 1871–1874.

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$$\mathcal{P}(\beta) = \frac{1}{2} \|y - \sum_{j=1}^{p} X_j \beta_j\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

 \sim

$$\begin{split} \beta^{(0)} &= \mathbf{0}_{p} \in \mathbb{R}^{p} \\ \text{for } t = 1, \dots \text{ do} \\ & \beta_{1}^{(t)} \approx \mathop{\arg\min}_{\substack{\beta_{1} \in \mathbb{R} \\ \beta_{2}^{(t)} \approx \arg\min_{\substack{\beta_{1} \in \mathbb{R} \\ \beta_{2} \in \mathbb{R}}}} \mathcal{P}(\beta_{1}^{(t)}, \beta_{2}^{(t-1)}, \beta_{3}^{(t-1)}, \dots, \beta_{p-1}^{(t-1)}, \beta_{p}^{(t-1)}) \\ & \vdots \\ & \vdots \\ & \beta_{p}^{(t)} \approx \mathop{\arg\min}_{\substack{\beta_{2} \in \mathbb{R} \\ \beta_{p} \in \mathbb{R}}} \mathcal{P}(\beta_{1}^{(t)}, \beta_{2}^{(t)}, \beta_{3}^{(t)}, \dots, \beta_{p-1}^{(t)}, \beta_{p})) \\ \end{split}$$
 1 epoch

When do we stop?

⁸J. Friedman, T. J. Hastie, and R. Tibshirani. "Regularization paths for generalized linear models via coordinate descent". In: *J. Stat. Softw.* 33.1 (2010), p. 1.

Duality gap as a stopping criterion

For any primal-dual pair $\beta \in \mathbb{R}^p, \theta \in \Delta_X$:

$$\mathcal{P}(\beta) \ge \mathcal{P}(\hat{\beta}) = \mathcal{D}(\hat{\theta}) \ge \mathcal{D}(\theta)$$



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$$\mathcal{P}(\beta) \ge \mathcal{P}(\hat{\beta}) = \mathcal{D}(\hat{\theta}) \ge \mathcal{D}(\theta)$$



 $\forall \beta, (\exists \theta \in \Delta_X, \operatorname{dgap}(\beta, \theta) \le \epsilon) \Rightarrow \mathcal{P}(\beta) - \mathcal{P}(\hat{\beta}) \le \epsilon$ $\beta \text{ is an } \epsilon \text{-solution whenever } \operatorname{dgap}(\beta, \theta) \le \epsilon$

Which dual point?

Primal-dual link at optimum:

$$\hat{\theta} = (y - X\hat{\beta})/\lambda$$

Standard approach¹⁰: at epoch t, corresponding to primal $\beta^{(t)}$ and residuals $r^{(t)} \triangleq y - X\beta^{(t)}$, take

$$\theta = \theta_{\rm res}^{(t)} \triangleq r^{(t)} / \lambda$$

¹⁰ J. Mairal. "Sparse coding for machine learning, image processing and computer vision". PhD thesis. École normale supérieure de Cachan, 2010.

Which dual point?

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"residuals rescaling"

¹⁰ J. Mairal. "Sparse coding for machine learning, image processing and computer vision". PhD thesis. École normale supérieure de Cachan, 2010.

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$$\theta = \theta_{\text{res}}^{(t)} \triangleq r^{(t)} / \max(\lambda, \|X^{\top} r^{(t)}\|_{\infty})$$

"residuals rescaling"

- converges to $\hat{\theta}$ (provided $\beta^{(t)}$ converges to $\hat{\beta}$)
- costs like 1 epoch, $\mathcal{O}(np)$

 \hookrightarrow rule of thumb: compute $\theta_{\rm res}^{(t)}$ and dgap every 10 epochs

¹⁰ J. Mairal. "Sparse coding for machine learning, image processing and computer vision". PhD thesis. École normale supérieure de Cachan, 2010.

Residuals rescaling: conservative bound

$$\theta_{\text{res}}^{(t)} = r^{(t)} / \max(\lambda, \|X^{\top} r^{(t)}\|_{\infty})$$



Leukemia dataset: p = 7129, n = 72, $\lambda = \lambda_{max}/10$

\hookrightarrow do better by exploiting previous iterates

 $\lambda_{\max} = \| X^\top y \|_\infty$ is the smallest λ leading to $\hat{\beta} = 0$

$$n = 2, p = 3, \hat{\beta} = (0, -0.6, 1.3)$$




























VAR regularity in residuals

Theorem¹¹

Under uniqueness assumption, ISTA/CD achieves sign id.: $\operatorname{sign} \beta_j^{(t)} = \operatorname{sign} \hat{\beta}_j$. Then, Lasso residuals are Vector AutoRegressive (VAR):

$$r^{(t+1)} = Ar^{(t)} + b$$

 \hookrightarrow we "only" need to fit a VAR to infer $\lim_{t\to\infty} r^{(t)} = \lambda \hat{ heta}$

We do not know when the sign is identified

Need a cheaper solution \hookrightarrow extrapolation

 $^{^{11}}$ M. Massias, A. Gramfort, and J. Salmon. "Celer: a fast solver for the Lasso with dual extrapolation". In: *ICML*. 2018, pp. 3321–3330.

Simple example: extrapolation in 1D

1D autoregressive process:

$$x^{(t)} = ax^{(t-1)} + b \underset{t \to \infty}{\to} x^*$$

we have

$$x^{(t)} - x^* = a(x^{(t-1)} - x^*)$$
$$x^{(t-1)} - x^* = a(x^{(t-2)} - x^*)$$

"Aitken's Δ^2 ": 2 unknowns, so 2 eqs or 3 points $x^{(t)}, x^{(t-1)}, x^{(t-2)}$ are enough to find $x^*!^{12}$

¹²A. Aitken. "On Bernoulli's numerical solution of algebraic equations". In: Proceedings of the Royal Society of Edinburgh 46 (1926), pp. 289–305.

Generalization¹³ to VAR $r^{(t)} \in \mathbb{R}^n$

• fix
$$K = 5$$
 (small)

• keep track of K past residuals $r^{(t)}, \ldots, r^{(t+1-K)}$

►
$$U^{(t)} = [r^{(t+1-K)} - r^{(t-K)}, \dots, r^{(t)} - r^{(t-1)}] \in \mathbb{R}^{n \times K}$$

• solve
$$(U^{(t)})^{\top}U^{(t)}z = \mathbf{1}_K$$

$$\triangleright \ c = z/z^{\top} \mathbf{1}_K$$

$$r_{\text{accel}}^{(t)} \triangleq \sum_{k=1}^{K} c_k r^{(t+1-k)}$$

$$\theta_{\text{accel}}^{(t)} \triangleq r_{\text{accel}}^{(t)} / \max(\lambda, \|X^{\top} r_{\text{accel}}^{(t)}\|_{\infty})$$

Cost: $\mathcal{O}(K^3 + K^2n + np)$

¹³D. Scieur, A. d'Aspremont, and F. Bach. "Regularized Nonlinear Acceleration". In: *NeurIPS*. 2016, pp. 712–720.

Dual extrapolation for the Lasso



Leukemia dataset: p = 7129, n = 72, $\lambda = \lambda_{\max}/10$

Applicability to other models

We showed asymptotic VAR structure, also exploitable¹⁴



¹⁴M. Massias et al. "Dual extrapolation for sparse Generalized Linear Models". In: submission to JMLR (2019).

Additional speed-ups

Two approaches:

- ► safe screening^{15,16} (backward approach): remove feature j when it is certified that $\hat{\beta}_j = 0$
- ▶ working set¹⁷ (forward approach): focus on j's for which it is very likely that $\hat{\beta}_j \neq 0$

¹⁵L. El Ghaoui, V. Viallon, and T. Rabbani. "Safe feature elimination in sparse supervised learning". In: J. Pacific Optim. 8.4 (2012), pp. 667–698.

¹⁶A. Bonnefoy et al. "A dynamic screening principle for the lasso". In: EUSIPCO. 2014.

¹⁷T. B. Johnson and C. Guestrin. "Blitz: A Principled Meta-Algorithm for Scaling Sparse Optimization". In: ICML. 2015, pp. 1171–1179.

Duality strikes again: gap safe screening

Gap safe screening rule¹⁸:

$$\forall (\beta, \theta) \in \mathbb{R}^p \times \Delta_X, \quad |X_j^\top \theta| < 1 - \|X_j\| \sqrt{\frac{2}{\lambda^2} \mathsf{dgap}(\beta, \theta)} \Rightarrow \hat{\beta}_j = 0$$

better dual point \Rightarrow better gap safe screening



¹⁸E. Ndiaye et al. "Gap Safe screening rules for sparsity enforcing penalties". In: JMLR 18.128 (2017), pp. 1–33.

Celer: working sets with extrapolation & aggressive screening

Screening can be used aggressively to define WS¹⁹, a **better dual point also helps**



rcv1 dataset, fine and coarse Lasso path (wrt Gap Safe Rules) *news20* dataset, fine and coarse Logreg path (wrt Gap Safe Rules)

¹⁹M. Massias, A. Gramfort, and J. Salmon. "From safe screening rules to working sets for faster Lasso-type solvers". In: NIPS-OPT workshop. 2017.

Contributions

- ► Improved the numerical efficiency of Lasso-type solvers. Duality used in stopping criterion & safe feature identification (asymptotic) VAR structure of Xβ^(t) → better dual
- https://github.com/mathurinm/celer:

fast implementation, standard API, documented, easy to install and reproducible benchmarks:



Run LassoCV for crossvalidation on Leukemia

Lasso path computation on Leukemia dataset

Lasso path computation on Finance/log1p

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MEG sensors: magnetometers and gradiometers







Device

Sensors

Detail of a sensor

3 sensor types \Longrightarrow 3 noise structures



Low SNR: averaging repetitions of experiment



Our complete stats model for M/EEG

- n observations (number of sensors)
- ► T tasks (temporal information)
- p features (spatial description)
- ► r repetitions of the same experiment
- $Y^{(1)}, \ldots, Y^{(r)} \in \mathbb{R}^{n \times T}$ observation matrices; $\overline{Y} = \frac{1}{r} \sum_{l} Y^{(l)}$
- $X \in \mathbb{R}^{n \times p}$ forward matrix

$$Y^{(l)} = X\mathbf{B}^* + \mathbf{S}_*\mathbf{E}^{(l)}$$

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

Data-fitting term

M/EEG standard: use whitened, averaged signal

$$\hat{\mathbf{B}} \in \operatorname*{arg\,min}_{\mathbf{B} \in \mathbb{R}^{p \times T}} \left(\frac{1}{2nT} \left\| \overline{\mathbf{Y}} - X\mathbf{B} \right\|_{F}^{2} + \lambda \|\mathbf{B}\|_{2,1} \right)$$

- Double goal: take advantage of the number of repetitions, address correlated noise
- need to go beyond squared Frobenius norm:

$$\hat{\mathbf{B}}^{\mathsf{repet}} \in \operatorname*{arg\,min}_{\mathbf{B} \in \mathbb{R}^{p \times T}} \left(\frac{1}{2nTr} \sum_{l=1}^{r} \left\| Y^{(l)} - X\mathbf{B} \right\|_{F}^{2} + \lambda \|\mathbf{B}\|_{2,1} \right)$$

 \hookrightarrow yields the same \hat{B}

Lasso and optimal $\lambda^{20,21}$

For $y = X\beta^* + \sigma_*\varepsilon$, and X satisfying the "Restricted Eigenvalue" property, if $\lambda = 2\sigma_*\sqrt{\frac{2\log(p/\delta)}{n}}$, then $\frac{1}{n} \left\| X\beta^* - X\hat{\beta} \right\|^2 \le \frac{18}{\kappa_{s^*}^2} \frac{\sigma_*^2 s^*}{n} \log\left(\frac{p}{\delta}\right)$

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

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

BUT σ_* is <u>unknown</u> in practice !

²⁰P. J. Bickel, Y. Ritov, and A. B. Tsybakov. "Simultaneous analysis of Lasso and Dantzig selector". In: Ann. Statist. 37.4 (2009), pp. 1705–1732.

²¹A. S. Dalalyan, M. Hebiri, and J. Lederer. "On the Prediction Performance of the Lasso". In: *Bernoulli* 23.1 (2017), pp. 552–581.

Pivotality: the $\sqrt{\text{Lasso}^{23}}$

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

has an optimal λ independent of σ_*

hard to optimize \hookrightarrow use *Concomitant* Lasso²² formulation (introduced earlier!):

$$(\hat{\beta}_{\text{conco}}, \hat{\sigma}_{\text{conco}}) \in \operatorname*{arg\,min}_{\beta \in \mathbb{R}^{p}, \sigma \geq 0} \frac{\left\|y - X\beta\right\|^{2}}{2n\sigma} + \frac{\sigma}{2} + \lambda \left\|\beta\right\|_{1}$$

same solutions when
$$\|y - X \hat{\beta}_{\sqrt{\text{Lasso}}}\| \neq 0$$

²²A. B. Owen. "A robust hybrid of lasso and ridge regression". In: *Cont. Math.* 443 (2007), pp. 59–72.
²³A. 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.

Easy to solve

$$(\hat{\beta}, \hat{\sigma}) \in \underset{\beta \in \mathbb{R}^{p}, \sigma > 0}{\arg\min} \frac{\|y - X\beta\|^{2}}{2n\sigma} + \frac{\sigma}{2} + \lambda \|\beta\|_{1}$$

Jointly convex formulation, smooth + separable: optimized by alternate minimization w.r.t. β and σ



Easy to solve

$$(\hat{\beta}, \hat{\sigma}) \in \underset{\beta \in \mathbb{R}^{p}, \sigma \geq \underline{\sigma}}{\operatorname{arg\,min}} \frac{\|y - X\beta\|^{2}}{2n\sigma} + \frac{\sigma}{2} + \lambda \, \|\beta\|_{1}$$

Jointly convex formulation, smooth + separable: optimized by alternate minimization w.r.t. β and σ Smooth Concomitant: gradient is Lipschitz!



Concomitant origin: smoothing the $\sqrt{\rm Lasso}^{26}$

"Huberization", replace $\|\cdot\|$ by a smooth approximation:

$$\begin{split} \mathsf{huber}_{\underline{\sigma}}(\|z\|) &= \begin{cases} \frac{\|z\|^2}{2\underline{\sigma}} + \frac{\sigma}{2} & \text{if } \|z\| \leq \underline{\sigma} \\ \|z\| & \text{if } \|z\| > \underline{\sigma} \\ &= \min_{\underline{\sigma} \geq \underline{\sigma}} \left(\frac{\|z\|^2}{2\sigma} + \frac{\sigma}{2} \right) = \|\cdot\| \,\Box(\frac{1}{2\underline{\sigma}}\|\cdot\|^2 + \frac{\sigma}{2}) \end{split}$$

Leads to the Smoothed^{24,25} Concomitant Lasso formulation:

$$(\hat{\beta}, \hat{\sigma}) \in \operatorname*{arg\,min}_{\beta \in \mathbb{R}^{p}, \sigma \geq \underline{\sigma}} \left(\frac{\|y - X\beta\|^{2}}{2n\sigma} + \frac{\sigma}{2} + \lambda \, \|\beta\|_{1} \right)$$

²⁴A. Beck and M. Teboulle. "Smoothing and first order methods: A unified framework". In: SIAM J. Optim. 22.2 (2012), pp. 557–580.

²⁵Y. Nesterov. "Smooth minimization of non-smooth functions". In: Math. Program. 103.1 (2005), pp. 127–152.

²⁶E. Ndiaye et al. "Efficient Smoothed Concomitant Lasso Estimation for High Dimensional Regression". In: Journal of Physics: Conference Series 904.1 (2017), p. 012006.

Multitask generalization

To address correlated noise, we had introduced a Smooth Generalized Concomitant Lasso (SGCL): 27

$$\underset{\substack{\mathbf{B} \in \mathbb{R}^{p \times T} \\ S \succ \underline{\sigma} \operatorname{Id}_n}}{\operatorname{arg\,min}} \frac{1}{2nT} \|Y - X\mathbf{B}\|_{S^{-1}}^2 + \frac{1}{2n} \operatorname{Tr}(S) + \lambda \, \|\mathbf{B}\|_{2,1}$$

S. van de Geer introduced the pivotal multivariate \sqrt{Lasso}^{28} :

$$\underset{\mathbf{B}\in\mathbb{R}^{p\times T}}{\arg\min}\,\frac{1}{\sqrt{nT}}\,\|Y-X\mathbf{B}\|_{\mathscr{S},1}+\lambda\,\|\mathbf{B}\|_{2,1}$$

SGCL turns out to be a smoothed multivariate square-root Lasso!

Smoothing makes optimization and statistical analysis easy!

²⁷M. Massias et al. "Generalized concomitant multi-task Lasso for sparse multimodal regression". In: AISTATS. 2018, pp. 998–1007.

²⁸S. van de Geer. Estimation and testing under sparsity. Lecture Notes in Mathematics. Springer, 2016.

Leveraging repetitions

Smoothed Generalized Concomitant Lasso (SGCL)²⁹

$$(\hat{\mathbf{B}}^{\mathrm{SGCL}}, \hat{S}^{\mathrm{SGCL}}) \! \in \! \mathop{\mathrm{arg\,min}}_{\substack{\mathbf{B} \in \mathbb{R}^{p \times T} \\ S \succeq \underline{\sigma} \, \mathrm{Id}_n}} \frac{\|\bar{Y} - X\mathbf{B}\|_{S^{-1}}^2}{2nT} + \frac{\mathrm{Tr}(S)}{2n} + \lambda \, \|\mathbf{B}\|_{2,1}$$

Concomitant Lasso with Repetitions (CLaR)³⁰

$$(\hat{\mathbf{B}}^{\text{CLaR}}, \hat{S}^{\text{CLaR}}) \in \underset{\substack{\mathbf{B} \in \mathbb{R}^{p \times T} \\ S \succeq \underline{\sigma} \text{ Id}_n}}{\operatorname{arg min}} \frac{\sum\limits_{l=1}^{r} \|\boldsymbol{Y}^{(l)} - X\mathbf{B}\|_{S^{-1}}^2}{2nTr} + \frac{\operatorname{Tr}(S)}{2n} + \lambda \|\mathbf{B}\|_{2,1}$$

³⁰Q. Bertrand et al. "Handling correlated and repeated measurements with the smoothed multivariate square-root Lasso". In: *NeurIPS*. 2019.

²⁹M. Massias et al. "Generalized concomitant multi-task Lasso for sparse multimodal regression". In: AISTATS. 2018, pp. 998–1007.

SGCL and CLaR computations: ${\rm B}$ update

Alternate minimization converges

 \underline{B} update (*S* fixed): standard MTL optimization, off-the-shelf techniques and refinements of 1st part

S update (B fixed):

$$\operatorname*{arg\,min}_{S\succeq\underline{\sigma}} \, \left(\frac{1}{2n} \mathrm{Tr}[Z^\top S^{-1}Z] + \frac{1}{2n} \, \mathrm{Tr}(S) \right)$$

closed-form solution involving clipped EVD of:

$$\frac{1}{T}(\bar{Y} - XB)(\bar{Y} - XB)^{\top} \text{ or } \frac{1}{rT} \sum_{l=1}^{r} (Y^{(l)} - XB)(Y^{(l)} - XB)^{\top})$$

Leveraging repetitions

 \blacktriangleright Statistically: $\mathcal{O}(n^2)$ parameters to estimate for S

- SGCL: only nT observations (need T large w.r.t. n)
- CLaR: *nTr* observations
- Computationally: SVD for S costs $\mathcal{O}(n^3)$, high in general but fine for MEG/EEG problems ($n \approx 300$)

<u>Rem</u>: more structure can easily be incorporated to estimate S, *e.g.*, block diagonal, etc.

Dissemination

MLE: $\underset{\substack{\mathbf{B}\in\mathbb{R}^{p\times T}\\\Sigma\succ 0}}{\arg\min} \frac{1}{2} \|\bar{Y} - X\mathbf{B}\|_{\Sigma^{-1}}^2 - \log\det(\Sigma^{-1}) + \lambda \|\mathbf{B}\|_{2,1}$



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

Figure: Real data, sources found after right auditory stimulations.

SGCL & CLaR, https://github.com/mathurinm/sgcl Also implemented non convex time frequency solvers as a preliminary step to my algorithms in MNE

Thank you

Joseph, Alexandre, Olivier, Samuel, Quentin, Pierre A, Thomas



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