Screening Rules for Lasso with Non-Convex Sparse Regularizers

Joseph Salmon

http://josephsalmon.eu Université de Montpellier

Joint work with A. Rakotomamonjy and G. Gasso









Motivation and objective

Lasso and screening

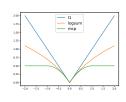
lackbox Learning sparse regression models : $\mathbf{X} \in \mathbb{R}^{n imes d}$, $\mathbf{y} \in \mathbb{R}^n$

$$\min_{\mathbf{w} = (w_1, \dots, w_d)^{\top} \in \mathbb{R}^d} \frac{1}{2} ||\mathbf{y} - \mathbf{X}\mathbf{w}||^2 + \lambda \sum_{j=1}^d |w_j|$$

► Safe screening rules (1), (2): identify vanishing coordinates of a/the solution by exploiting sparsity, convexity and duality

Extension to non-convex regularizers :

- non-convex regularizers lead to statistically better models but ...
- how to perform screening when the regularizer is non-convex?



^{(1).} L. EL GHAOUI, V. VIALLON et T. RABBANI. "Safe feature elimination in sparse supervised learning". In: Journal of Pacific Optimization (8 2012), p. 667-698.

^{(2).} Antoine BONNEFOY et al. "Dynamic screening: Accelerating first-order algorithms for the lasso and group-lasso". In: IEEE Trans. Signal Process. 63.19 (2015), p. 5121-5132.

Non-convex sparse regression

Non convex regularization : $r_{\lambda}(\cdot)$ smooth & concave on $[0,\infty[$

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \sum_{j=1}^d r_{\lambda}(|w_j|)$$

- ► Log Sum penalty (LSP) (3)
- ► Smoothly Clipped Absolute Deviation (SCAD) (4)

- $\underline{\mathsf{Examples}}: \qquad \blacktriangleright \quad \mathit{capped-}\ell_1 \ \mathit{penalty}^{(5)}$
 - ► Minimax Concave Penalty (MCP) (6)

Rem: for pros & cons of such formulations cf. Soubles et al. (7)

^{(3).} Emmanuel J CANDÈS, Michael B WAKIN et Stephen P BOYD. "Enhancing Sparsity by Reweighted l₁ Minimization". In: J. Fourier Anal. Applicat. 14.5-6 (2008), p. 877-905.

^{(4).} Jianging FAN et Runze LI, "Variable selection via nonconcave penalized likelihood and its oracle properties". In: J. Amer. Statist. Assoc. 96,456 (2001), p. 1348-1360.

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Majorization-Minimization

Algorithm: Maximization minimization

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\begin{aligned} & \text{input : max. iterations } k_{\text{max}}, \text{ stopping criterion } \epsilon, \ \alpha, \ \mathbf{w}^0 (=0) \\ & \text{for } k = 0, \dots, k_{\text{max}} - 1 \ \text{do} \\ & \text{Break if stopping criterion smaller than } \epsilon \\ & \lambda_j^k \leftarrow r_\lambda'(|w_j^k|) & \text{// Majorization} \\ & \mathbf{w}^k \leftarrow \arg\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{2} \|\mathbf{y} - \mathbf{X} \mathbf{w}\|^2 & \text{// Minimization} \\ & + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j^k |w_j| \end{aligned}
```

return \mathbf{w}^k

Majorization :
$$r_{\lambda}(|w_j|) \le r_{\lambda}(|w_j^k|) + r'_{\lambda}(|w_j^k|)(|w_j| - |w_j^k|)$$

Minimization: weighted-Lasso formulation

 $\underline{\text{Rem}}: \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2$ acts as a regularization for MM ⁽⁸⁾ (other majorization alternatives possible, *e.g.*, with gradient information)

^{(8).} Yangyang Kang, Zhihua Zhang et Wu-Jun Li. "On the global convergence of majorization minimization algorithms for nonconvex optimization problems". In : arXiv preprint arXiv:1504.07791 (2015).

Safe Screening / Two-level screening

Safe Screening: for Lasso problems, vanishing coefficients at optimality can be certified without knowing the solution

- prior computation starting from a similar set of tuning parameter (sequential ⁽⁹⁾ / dual-warm start)
- ▶ along the optimization algorithm (dynamic (10))

State-of-the-art safe screening rules : rely on duality gap (11)

Two-level screening for non-convex cases

- Inner level screening: within each (weighted) Lasso
- Outer level screening : propagate information between Lassos

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^{(11).} E. NDIAYE et al. "Gap Safe screening rules for sparsity enforcing penalties". In: Journal of Machine Learning Research 18.128 (2017), p. 1-33.

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Notation

Notation:
$$X = [\mathbf{x}_1, \dots, \mathbf{x}_d], \Lambda = (\lambda_1, \dots, \lambda_d)^{\top}$$

Inner (convex) problems:

(Primal)
$$P_{\Lambda}(\mathbf{w}) \triangleq \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j |w_j|$$

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$$X = [\mathbf{x}_1, \dots, \mathbf{x}_d], \ \Lambda = (\lambda_1, \dots, \lambda_d)^\top, \ \mathbf{s} \in \mathbb{R}^n, \ \mathbf{v} \in \mathbb{R}^d$$

Inner (convex) problems:

$$(\mathsf{Primal}) \qquad P_{\Lambda}(\mathbf{w}) \triangleq \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j |w_j|$$

$$(\mathsf{Dual}) \qquad D_{\Lambda}(\mathbf{s}, \mathbf{v}) \triangleq -\frac{1}{2} \|\mathbf{s}\|^2 - \frac{\alpha}{2} \|\mathbf{v}\|^2 + \mathbf{s}^{\top} \mathbf{y} - \mathbf{v}^{\top} \mathbf{w}^k$$

$$\mathbf{s.t.} \quad |\mathbf{X}^{\top} \mathbf{s} - \mathbf{v}| \leq \Lambda$$

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Inner (convex) problems:

$$\begin{aligned} \text{(Primal)} \qquad \qquad P_{\Lambda}(\mathbf{w}) &\triangleq \tfrac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \tfrac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j |w_j| \\ \text{(Dual)} \qquad \qquad D_{\Lambda}(\mathbf{s}, \mathbf{v}) &\triangleq -\tfrac{1}{2} \|\mathbf{s}\|^2 - \tfrac{\alpha}{2} \|\mathbf{v}\|^2 + \mathbf{s}^\top \mathbf{y} - \mathbf{v}^\top \mathbf{w}^k \\ \text{s.t.} \quad |\mathbf{X}^\top \mathbf{s} - \mathbf{v}| &\preccurlyeq \Lambda \end{aligned}$$

(Dual-Gap)
$$G_{\Lambda}(\mathbf{w}, \mathbf{s}, \mathbf{v}) \triangleq P_{\Lambda}(\mathbf{w}) - D(\mathbf{s}, \mathbf{v})$$

Screening weighted Lasso

ightharpoonup Primal optimization problem $P_{\Lambda}(\mathbf{w})$:

$$\tilde{\mathbf{w}} \leftarrow \arg\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j |w_j|$$

Screening test :
$$|\mathbf{x}_j^{\top} \tilde{\mathbf{s}} - \tilde{v}_j| < \lambda_j \implies \tilde{w}_j = 0$$
 (impractical) with $\tilde{\mathbf{s}} \triangleq \mathbf{y} - \mathbf{X}\tilde{\mathbf{w}}$ $\tilde{\mathbf{y}} \triangleq \tilde{\mathbf{w}} - \mathbf{w}^k$ (for a scalar $a(\Lambda)$ well chosen)

with $\tilde{\mathbf{s}} \triangleq \frac{\mathbf{y} - \mathbf{X}\tilde{\mathbf{w}}}{\rho(\Lambda)}$, $\tilde{\mathbf{v}} \triangleq \frac{\tilde{\mathbf{w}} - \mathbf{w}^k}{\alpha\rho(\Lambda)}$ (for a scalar $\rho(\Lambda)$ well chosen)

Practical) Dynamic Gap safe screening test (12), (13): $|\mathbf{x}_{j}^{\top}\mathbf{s} - v_{j}| + \sqrt{2G_{\Lambda}(\mathbf{w}, \mathbf{s}, \mathbf{v})} \left(||\mathbf{x}_{j}|| + \frac{1}{\alpha} \right) < \lambda_{j}$

 $T_j^{(\Lambda)}(\mathbf{w}, \mathbf{s}, \mathbf{v})$

given a primal-dual approximate solution triplet $(\mathbf{w}, \mathbf{s}, \mathbf{v})$

^{(12).} O. FERCOQ, A. GRAMFORT et J. SALMON. "Mind the duality gap: safer rules for the lasso". In: ICML. 2015, p. 333-342.

^{(13).} E. NDIAYE et al. "Gap Safe screening rules for sparsity enforcing penalties". In: Journal of Machine Learning Research 18.128 (2017), p. 1-33.

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ightharpoonup Primal optimization problem $P_{\Lambda}(\mathbf{w})$:

$$\tilde{\mathbf{w}} \leftarrow \underset{\mathbf{w} \in \mathbb{R}^d}{\min} \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^d \lambda_j |w_j|$$

Screening test :
$$\mathbf{x}_{j}^{\top}\tilde{\mathbf{s}} - \tilde{v}_{j} | < \lambda_{j} \implies \tilde{w}_{j} = 0$$
 (impractical)

with $\tilde{\mathbf{s}} \triangleq \frac{\mathbf{y} - \mathbf{X}\tilde{\mathbf{w}}}{\rho(\Lambda)}$, $\tilde{\mathbf{v}} \triangleq \frac{\tilde{\mathbf{w}} - \mathbf{w}^k}{\alpha\rho(\Lambda)}$ (for a scalar $\rho(\Lambda)$ well chosen)

► (Practical) Dynamic Gap safe screening test (12), (13):

$$\underbrace{|\mathbf{x}_{j}^{\top}\mathbf{s} - v_{j}| + \sqrt{2G_{\Lambda}(\mathbf{w}, \mathbf{s}, \mathbf{v})} \left(\|\mathbf{x}_{j}\| + \frac{1}{\alpha}\right)}_{T_{j}^{(\Lambda)}(\mathbf{w}, \mathbf{s}, \mathbf{v})} < \lambda_{j}$$

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Inner level screening and speed-ups

After iteration k, one receives approximate solutions \mathbf{w}^k , \mathbf{s}^k and \mathbf{v}^k for weighted Lasso with weights Λ^k

Set of screened variables:

$$\mathcal{S} \triangleq \left\{ j \in [\![1,d]\!] : T_j^{(\Lambda^k)}(\mathbf{w}^k,\mathbf{s}^k,\mathbf{v}^k) < \lambda_j^k \right\}$$

▶ Speed-ups : reduced weighted Lasso problem size substituting

$$X \leftarrow X_{S^c}$$

Rem : most beneficiary with coordinate descent type solvers

Outer screening level / screening propagation

Before iteration k+1

- lacktriangle change of weights $\Lambda^{k+1}=\{\lambda_j^{k+1}\}_{j=1,\dots,d}$
- $\qquad \text{update } (\mathbf{w}^{k+1}, \mathbf{s}^{k+1}, \mathbf{v}^{k+1}) \leftarrow \left(\mathbf{w}^k, \frac{\mathbf{y} \mathbf{X} \mathbf{w}^k}{\rho(\Lambda^{k+1})}, \frac{\mathbf{w}^{k+1} \mathbf{w}^k}{\rho(\Lambda^{k+1})}\right)$

Screening propagation test

$$T_j^{(\Lambda^k)}(\hat{\mathbf{w}}, \hat{\mathbf{s}}, \hat{\mathbf{v}}) + \|\mathbf{x}_j\|(a + \sqrt{2b}) + c + \frac{1}{\alpha}\sqrt{2b} < \lambda_j^{k+1}$$

with

$$\|\mathbf{s}^{k+1} - \mathbf{s}^k\| \le a$$

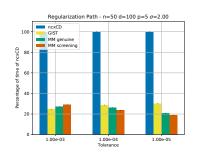
$$|G_{\Lambda}(\mathbf{w}^k, \mathbf{s}^k, \mathbf{v}^k) - G_{\Lambda^{k+1}}(\mathbf{w}^{k+1}, \mathbf{s}^{k+1}, \mathbf{v}^{k+1})| \le b$$

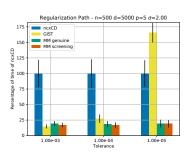
$$|v_j^{k+1} - v_j^k| \le c$$

Rem: same flavor as sequential screening (14)

^{(14).} L. EL GHAOUI, V. VIALLON et T. RABBANI. "Safe feature elimination in sparse supervised learning". In: Journal of Pacific Optimization (8 2012), p. 667-698.

Experiments (log-sum penalty)





- ncxCD : coordinate descent
- ► GIST : majorization + iterative-soft thresholding
- ▶ MM-genuine : screening inside proximal weighted Lasso steps
- ▶ MM-screening : adding screening propagation to the later

Conclusion

- ► First approach for screening with non-convex regularizers
- Convexification and propagation
- Limits (they exist!) : $\lambda_j > 0$ (cannot handle MCP easily)
- ► Variants : active set extension (15) following Massias et al. (16)
- More technical details (17) and code online https://github.com/arakotom/screening_ncvx_penalty

^{(15).} A. RAKOTOMAMONJY et al. Provably Convergent Working Set Algorithm for Non-Convex Regularized Regression. Rapp. tech. 2020.

^{(16).} M. MASSIAS, A. GRAMFORT et J. SALMON. "Celer: a Fast Solver for the Lasso with Dual Extrapolation". In: ICML. 2018.

^{(17).} A. RAKOTOMAMONJY, G. GASSO et J. SALMON. "Screening Rules for Lasso with Non-Convex Sparse Regularizers". In: ICML. T. 97. 2019, p. 5341-5350.

BenchOpt : https://benchopt.github.io/

BenchOpt: package to simplify, make more transparent and more reproducible (18) the comparisons of optimization algorithms

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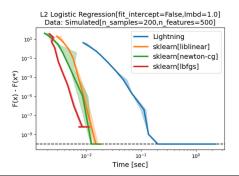
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```
$ git clone https://github.com/benchopt/benchmark_logreg_12
$ benchopt run ./benchmark_logreg_12
```

Running these commands will fetch the benchmark files and give you a benchmark plot on I2-regularized logistic regression:



Disclaimer on BenchOpt

<u>Use-cases</u>: research, review, fast speed check on a machine

"For now we handle convex batch methods, but we can do much more with your help (stochastic, non-convex, etc.)" T. Moreau

"We are family! Come work with us:)" A. Gramfort

Give it a try: https://benchopt.github.io/

Papers and code



Github: @josephsalmon

Joseph Salmon

joseph.salmon@umontpellier.fr



Twitter: @salmonjsph



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Appendix

Computation of ρ , needed for feasibility :

$$j^{\dagger} = \underset{j:\lambda_{j}>0}{\arg\max} \underbrace{\frac{1}{\lambda_{j}} \left| \mathbf{x}_{j}^{\top} (\mathbf{y} - \mathbf{X} \mathbf{w}) - \frac{1}{\alpha} (\hat{w}_{j} - \hat{w}_{j}) \right|}_{\rho^{\Lambda}(j)} . \tag{1}$$

with \mathbf{w}^k coming from the previous problem, *i.e.*, solving :

$$P_{\Lambda}(\mathbf{w}) \triangleq \frac{1}{2} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2 + \frac{1}{2\alpha} \|\mathbf{w} - \mathbf{w}^k\|^2 + \sum_{j=1}^{n} \lambda_j |w_j|$$