Safe Screening for Sparse Regression with the Kullback-Leibler Divergence

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Outline

Context and Literature

- 1. Motivation
- 2. Safe screening : a quick overview

Our contribution

- 3. Problem definition
- 4. Safe screening for the Kullback-Leibler divergence
 - Dual problem and optimality conditions
 - Screening rule and Safe region
- 5. Experimental results

Motivations

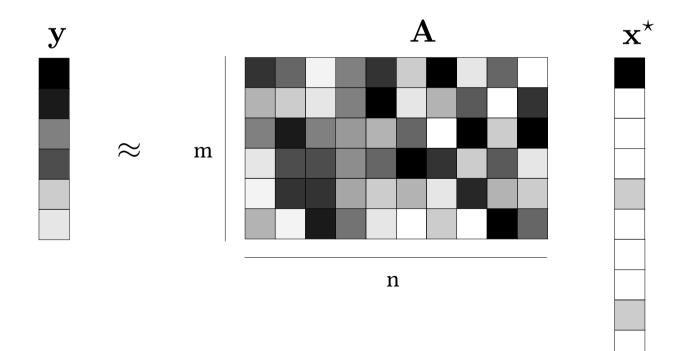
• Goal: accelerate the solution of sparse regression problems with the generalized **Kullback-Leibler** (KL) divergence \rightarrow safe screening.

$$\mathcal{D}_{\mathrm{KL}}(\mathbf{y} \mid \mathbf{z}) = \sum_{i=1}^{m} y_i \log\left(\frac{y_i}{z_i + \epsilon}\right) - y_i + (z_i + \epsilon).$$

- Maximum likelihood estimation with a **Poisson** observation model.
- Applications:
 - Sparse NMF
 - Count data
 - Text processing: word count
 - Recommendation: view / listening count
 - Medical imaging (Positron emission tomography)

• Accelerate the solution of **sparse regression problems**.

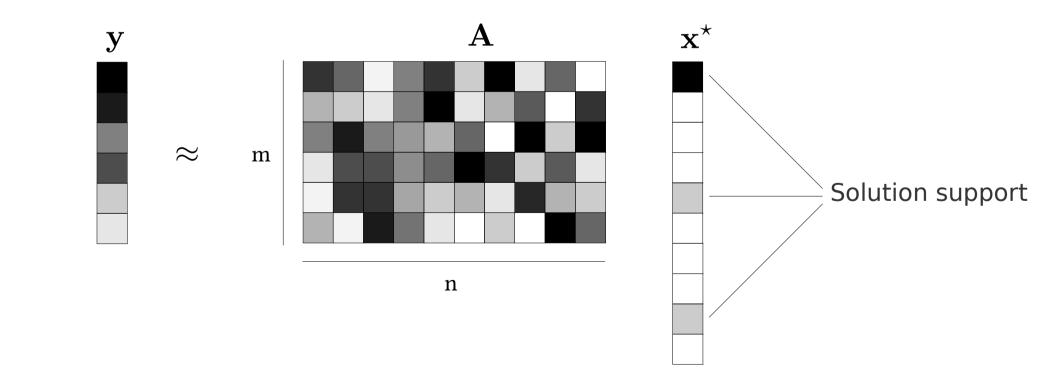
 $\mathbf{y} \approx \mathbf{A} \mathbf{x}$, with \mathbf{x} sparse



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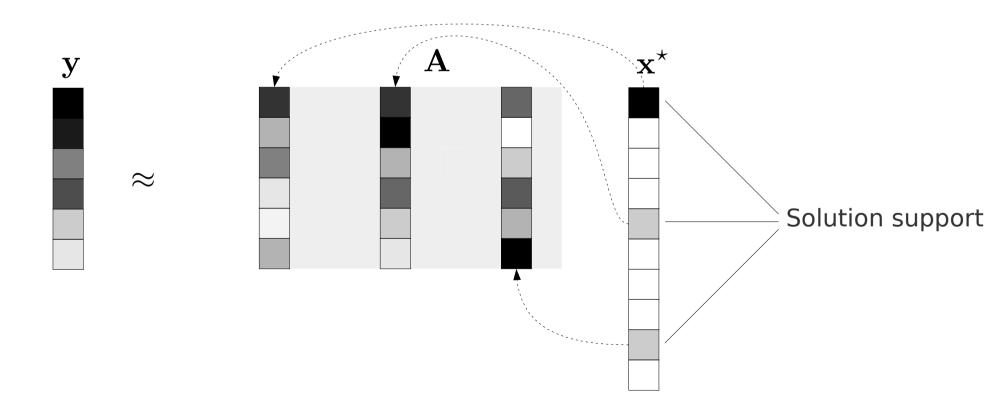
Core idea: identify and eliminate coordinates not belonging to the solution support.



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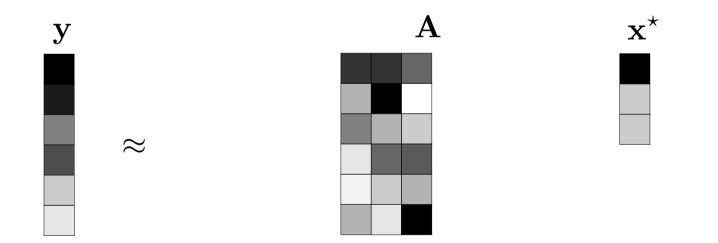
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Core idea: identify and eliminate coordinates not belonging to the solution support.



Safe Screening: state-of-the-art

• Initially proposed for the Lasso problem [El Ghaoui et al. 2012]

- Extensions:
 - Different regularizations
 - Group-lasso [El Ghaoui et al. 2012], Fused Lasso [Wang et al. 2015], Elastic Net [Fercoq et al. 2015], Sparse-Group Lasso [Wang et al. 2019] ...
 - Different data-fidelity terms
 - Sparse Logistic regression [Wang et al. 2014]
 - Different constraint sets
 - Non-negative Lasso [Wang et al. 2019]
- KL divergence case not previously addressed!

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Problem definition

• The L1-regularized Kullback-Leibler regression problem:

$$\mathbf{x}^{\star} \in \operatorname*{argmin}_{\mathbf{x} \in \mathbb{R}^{n}_{+}} P_{\lambda}(\mathbf{x}) := \mathcal{D}_{\mathrm{KL}}(\mathbf{y} \mid \mathbf{A}\mathbf{x}) + \lambda \|\mathbf{x}\|_{1} \qquad (\mathsf{KL-L1})$$

- Safe Screening for the KL-L1 problem. Technical ingredients:
 - Dual problem
 - First-order optimality conditions
 - Screening rule
 - Safe region

Dual problem

• Primal problem: $\mathbf{x}^* \in \operatorname*{argmin}_{\mathbf{x} \in \mathbb{R}^n_+} P_{\lambda}(\mathbf{x}) := \mathcal{D}_{\mathrm{KL}}(\mathbf{y} \mid \mathbf{A}\mathbf{x}) + \lambda \|\mathbf{x}\|_1$ (KL-L1)

• Dual problem:
$$\theta^* = \underset{\theta \in \mathcal{F}_{\mathbf{A}}}{\operatorname{argmax}} D_{\lambda}(\theta) := \sum_{i=1}^{m} y_i \log(1 + \lambda \theta_i) - \epsilon \lambda \theta_i,$$

with $\mathcal{F}_{\mathbf{A}} = \{ \theta \in \mathbb{R}^m \mid \lambda \theta \ge -1, \ \mathbf{A}^{\mathsf{T}} \theta \le 1 \}$

- Dual cost function D_{λ} and dual feasible set $\mathcal{F}_{\mathbf{A}}$ are obtained by taking the *Fenchel conjugate* of $\mathcal{D}_{\mathrm{KL}}$ and $\|\cdot\|_1 + \mathbb{1}_{\mathbb{R}^n_+}(\cdot)$ respectively.
- First-order optimality conditions:

1)
$$\lambda \theta^{\star} = -\nabla \mathcal{D}_{\mathrm{KL}}(\mathbf{y} \mid \mathbf{A}\mathbf{x}^{\star})$$

(primal-dual link)

2) $\mathbf{A}^{\mathsf{T}} \boldsymbol{\theta}^{\star} \in \partial \|\mathbf{x}^{\star}\|_{1} + \partial \mathbb{1}_{\mathbb{R}^{n}_{+}}(\mathbf{x}^{\star})$

(subdifferential inclusion)

m

First-order optimality conditions:
1) $\lambda \theta^* = -\nabla \mathcal{D}_{\mathrm{KL}}(\mathbf{y} \mid \mathbf{A}\mathbf{x}^*) \implies \lambda \theta^* = \frac{\mathbf{y}}{\mathbf{A}\mathbf{x}^* + \epsilon} - \mathbf{1}$ 2) $\mathbf{A}^{\mathsf{T}} \theta^* \in \partial \|\mathbf{x}^*\|_1 + \partial \mathbb{1}_{\mathbb{R}^n_+}(\mathbf{x}^*) \implies \forall j, \begin{cases} \mathbf{a}_j^{\mathsf{T}} \theta^* \leq 1, & \text{if } x_j^* = 0 \\ \mathbf{a}_i^{\mathsf{T}} \theta^* = 1 & \text{if } x_j^* \neq 0 \end{cases}$

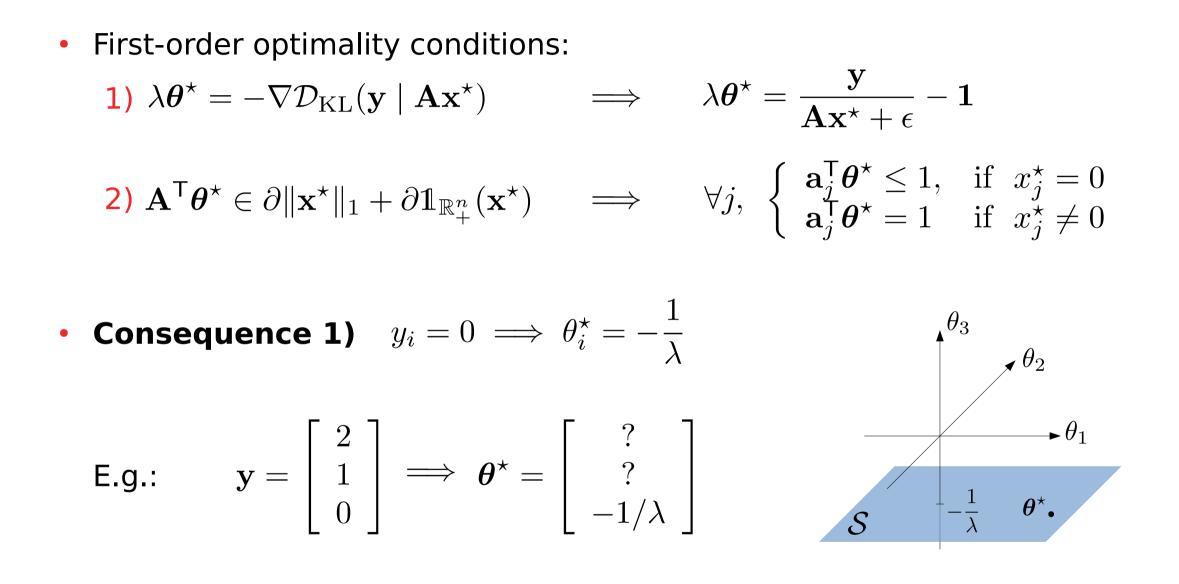
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E.g.:
$$\mathbf{y} = \begin{bmatrix} 2\\1\\0 \end{bmatrix} \implies \boldsymbol{\theta}^{\star} = \begin{bmatrix} ?\\?\\-1/\lambda \end{bmatrix}$$



 $\boldsymbol{\theta}^{\star}$ belongs to the hyperplane $\mathcal{S} = \{ \boldsymbol{\theta} \in \mathbb{R}^m \mid \theta_i = -1/\lambda, \forall i \text{ s.t. } y_i = 0 \}$

2)
$$\forall j, \begin{cases} \mathbf{a}_j^\mathsf{T} \boldsymbol{\theta}^\star \leq 1, & \text{if } x_j^\star = 0\\ \mathbf{a}_j^\mathsf{T} \boldsymbol{\theta}^\star = 1 & \text{if } x_j^\star \neq 0 \end{cases}$$

• Consequence 2) $\mathbf{a}_j^\mathsf{T} \boldsymbol{\theta}^\star < 1 \implies x_j^\star = 0$

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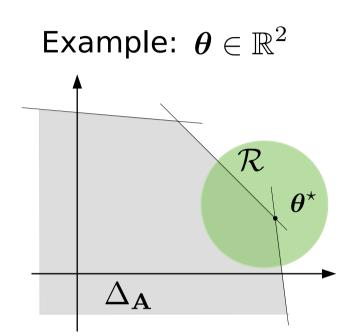
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O Define a safe region \mathcal{R} which contains θ^* .



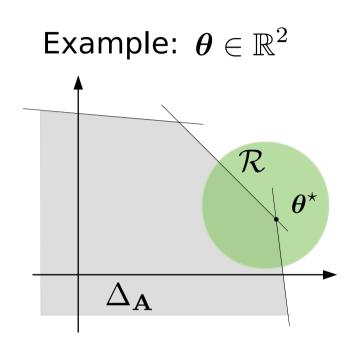
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Safe screening rule [El Ghaoui et al. 2012]

Let \mathcal{R} be a safe region, then:

$$\max_{\boldsymbol{\xi}\in\mathcal{R}} \mathbf{a}_j^{\mathsf{T}}\boldsymbol{\xi} < 1 \implies \mathbf{a}_j^{\mathsf{T}}\boldsymbol{\theta}^{\star} < 1 \implies x_j^{\star} = 0$$

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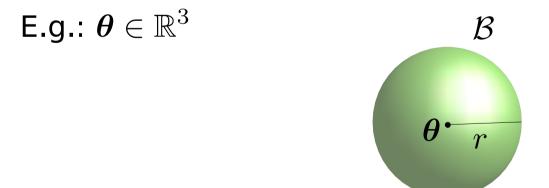
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• \mathcal{R} is a sphere $\mathcal{B}(\theta, r)$ with center θ and radius r

Safe screening rule [El Ghaoui et al. 2012]

Let $\mathcal{B}(\boldsymbol{\theta}, r)$ be a safe region, then:

$$\max_{\boldsymbol{\xi}\in\mathcal{B}(\boldsymbol{\theta},r)}\mathbf{a}_{j}^{\mathsf{T}}\boldsymbol{\xi}=\mathbf{a}_{j}^{\mathsf{T}}\boldsymbol{\theta}+r\|\mathbf{a}_{j}\|_{2}<1 \implies x_{j}^{\star}=0$$

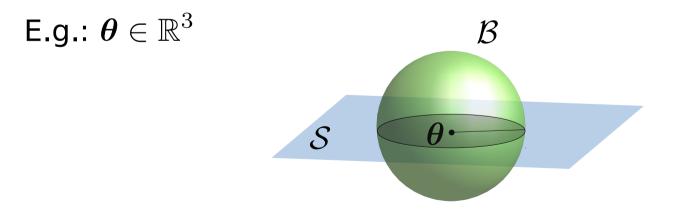


Safe Screening rule for KL

• Improved screening rule for the KL divergence

KL-L1 Safe screening rule [D.S.F. 2021]

Let $\mathcal{B}(\theta, r)$ be a safe region and $\mathcal{S} = \{\theta \in \mathbb{R}^m \mid \theta_{\mathcal{I}} = -1/\lambda\}$ with $\mathcal{I} = \{i \in [m] : y_i = 0\}$ and $\theta \in \mathcal{S}$, then: $\max_{\xi \in \mathcal{B}(\theta, r) \cap \mathcal{S}} \mathbf{a}_j^\mathsf{T} \xi = \mathbf{a}_j^\mathsf{T} \theta + r \| [\mathbf{a}_j]_{\mathcal{I}^c} \|_2 < 1 \implies x_j^\star = 0$



GAP Safe sphere [Ndiaye et al. 2017]

For any feasible primal-dual pair $(\mathbf{x}, \boldsymbol{\theta}) \in \mathbb{R}^n_+ imes \mathcal{F}_{\mathbf{A}}$

$$\boldsymbol{\theta}^{\star} \in \mathcal{B}(\boldsymbol{\theta}, r), \text{ with } r = \sqrt{\frac{2\operatorname{Gap}_{\lambda}(\mathbf{x}, \boldsymbol{\theta})}{\alpha}}$$

where α is the strong concavity constant of D_{λ} .

where $\operatorname{Gap}_{\lambda}(\mathbf{x}, \boldsymbol{\theta}) := P_{\lambda}(\mathbf{x}) - D_{\lambda}(\boldsymbol{\theta})$ denotes the duality gap.

E. Ndiaye, O. Fercoq, A. Gramfort, J. Salmon. Gap Safe Screening Rules for Sparsity Enforcing Penalties. JMLR, 2017.

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- Requires **global** strong concavity of D_{λ}
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- IDEA: Use **local** strong concavity.

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Safe Region for KL

KL-L1 GAP Safe sphere [D.S.F. 2021]

For any feasible primal-dual pair $(\mathbf{x}, \boldsymbol{\theta}) \in \mathbb{R}^n_+ \times (\mathcal{F}_{\mathbf{A}} \cap \mathcal{S})$

$$\boldsymbol{\theta}^{\star} \in \mathcal{B}(\boldsymbol{\theta}, r), \text{ with } r = \sqrt{\frac{2\operatorname{Gap}_{\lambda}(\mathbf{x}, \boldsymbol{\theta})}{\bar{\alpha}}}$$

and
$$\bar{\alpha} = \lambda^2 \min_{i \in \mathcal{I}^{\mathsf{G}}} \frac{y_i}{(1 + \max(\|\mathbf{A}\|_1, \lambda) \|\mathbf{a}_i^{\dagger}\|_1)^2}$$

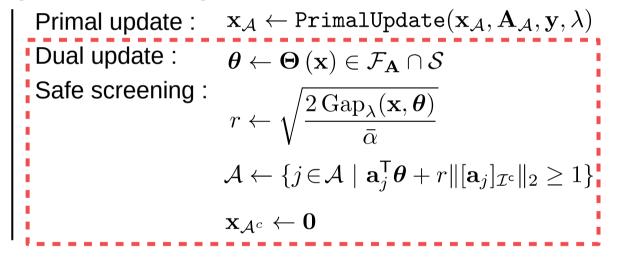
- D_{λ} is $\bar{\alpha}$ -strongly concave on $\mathcal{F}_{\mathbf{A}} \cap \mathcal{S}$
- Note that D_{λ} is not strongly concave on $\mathcal{F}_{\mathbf{A}}$ only.

Proposed Algorithm

Algorithm 1 : KL-L1 Dynamic GAP Safe Screening [D.S.F. 2021]

Initialize $\mathbf{x} \in \mathbb{R}^n$, $\mathcal{A} = \{1, \dots, n\}$, $\bar{\alpha}$ strong concavity bound on $\mathcal{F}_{\mathbf{A}} \cap \mathcal{S}$

Repeat until convergence



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Repeat until convergence

Primal update :	$\mathbf{x}_\mathcal{A} \leftarrow \texttt{PrimalUpdate}(\mathbf{x}_\mathcal{A}, \mathbf{A}_\mathcal{A}, \mathbf{y}, \lambda)$
Dual update :	$oldsymbol{ heta} \leftarrow oldsymbol{\Theta}\left(\mathbf{x} ight) \in \mathcal{F}_{\mathbf{A}} \cap \mathcal{S}$
Safe screening :	$r \leftarrow \sqrt{\frac{2 \operatorname{Gap}_{\lambda}(\mathbf{x}, \boldsymbol{\theta})}{\bar{\alpha}}}$ $\mathcal{A} \leftarrow \{j \in \mathcal{A} \mid \mathbf{a}_{j}^{T} \boldsymbol{\theta} + r \ [\mathbf{a}_{j}]_{\mathcal{I}^{c}} \ _{2} \geq 1\}$
	$\mathbf{x}_{\mathcal{A}^c} \leftarrow 0$

Considered solvers:

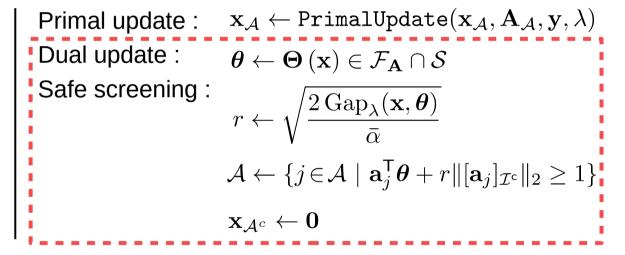
- Proximal gradient [Harmany et al. 2012]
- Coordinate descent [Hsieh, Dhillon, 2011]
- Majorize-minimize (Multiplicative Update) [Févotte, Idier 2011]

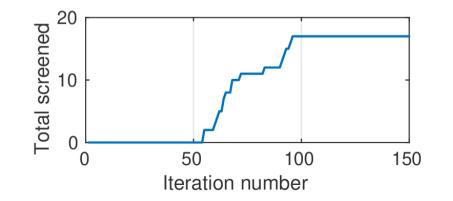
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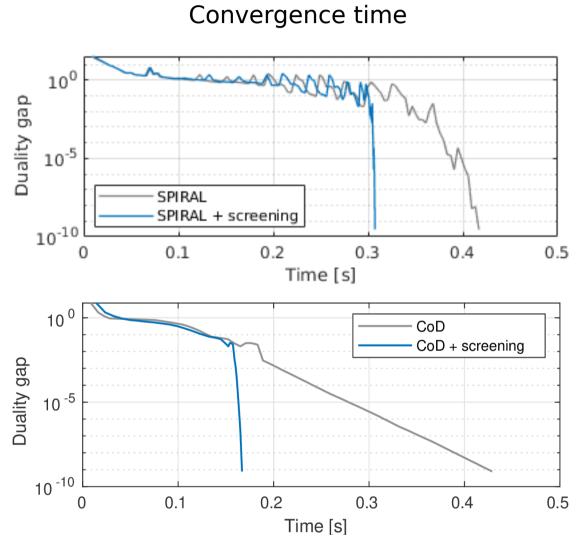


Figure: Convergence vs. Time. 20-Newsgroup data, $\lambda = 10^{-2} \lambda_{max}$.

Experiments

- Solvers: Prox. grad. (SPIRAL), Multiplicative update (MU), Coord. descent (CoD).
- Real count datasets: 20-Newsgroups, NIPS papers (word counts) TasteProfile (song listening counts).
- Input vector \mathbf{y} is a random column of the dataset. Remaining data forms \mathbf{A} .

	$\lambda/\lambda_{ m max}$	10^{-1}		10^{-3}	
	$arepsilon_{ ext{gap}}$	10^{-5}	10^{-7}	10^{-5}	10^{-7}
20 Newsgr.	SPIRAL	1.44	1.59	1.60	1.78
	CoD	2.44	3.42	2.46	3.22
	MU	4.80	7.72	4.49	7.28
NIPS papers	SPIRAL	2.77	3.21	2.26	2.53
	CoD	4.19	5.35	4.12	5.06
	MU	6.71	8.88	5.74	7.31
TasteProfile	SPIRAL	2.54	3.00	2.82	3.21
	CoD	1.75	2.20	2.44	4.22
	MU	2.81	4.11	2.94	4.35

 Table 1: Average speedups (time without/with screening).

 $\lambda_{\max} = \max \left(\mathbf{A}^{\mathsf{T}}(\mathbf{y} - \epsilon) \right) / \epsilon$ is the bound above which $\mathbf{x}^{\star} = \mathbf{0}$.

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Concluding remarks

- Main contribution : safe screening technique for the KL-L1 problem.
 - Improved screening rule for the particular KL case.
 - Adaptation of GAP Safe sphere exploiting **local properties** of the cost function.
- Significant improvements in terms of convergence time.
- Extensions: check our **follow-up paper** (below)!
 - Other group-decomposable regularizations.
 - Other β -divergences as data fidelity.
 - Tighter local strong concavity bound.

C. F. Dantas, E. Soubies, C. Févotte. Expanding Boundaries of GAP Safe Screening. 2021.

Available at: hal.archives-ouvertes.fr/hal-03147502

Matlab code: github.com/cassiofragadantas

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Contact me: cassio.fraga-dantas@irit.fr

Safe Screening

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KL-L1 Solvers

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