Fast solvers for sparse multi-task problems

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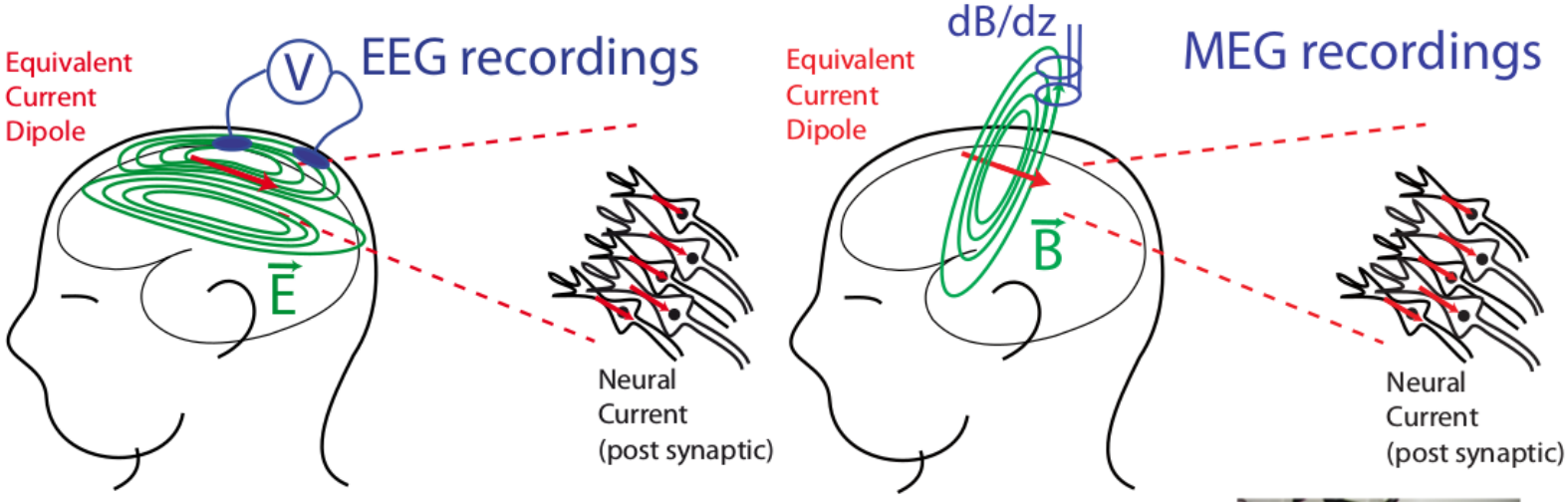
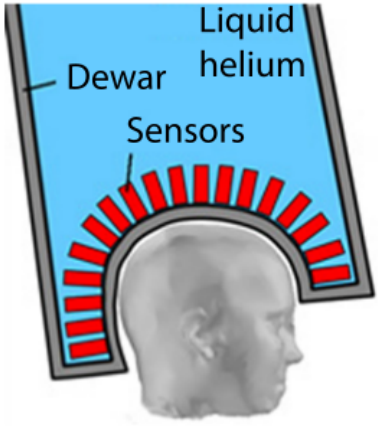
"One" motivation: M/EEG inverse problem

- sensors: magneto- and electro-encephalogram measurements during a cognitive experiment (*e.g.*, sensory or memory)
- sources: brain locations

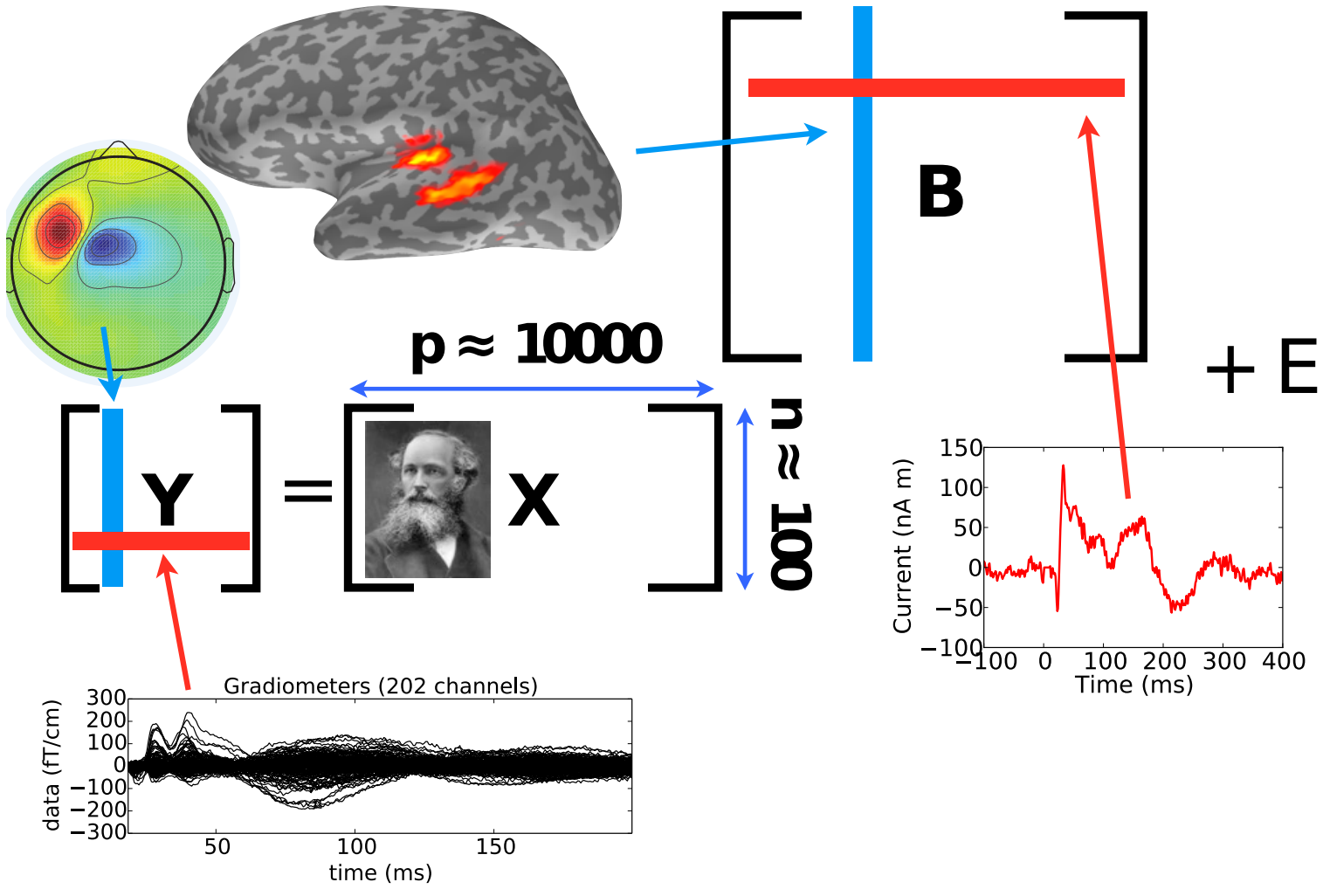


First EEG recordings in 1929 by H. Berger



Hôpital La Timone
Marseille, France

The M/EEG inverse problem



The M/EEG inverse problem: modelisation

- n: number of sensors (≈ 300)
- q: number of time instants (≈ 200)
- p: number of vertices in mesh discretization ($\approx 10,000$)
- $Y \in \mathbb{R}^{n \times q}$: matrix of measurements
- $X \in \mathbb{R}^{n \times p}$: matrix describing the physics of the problem

Model:

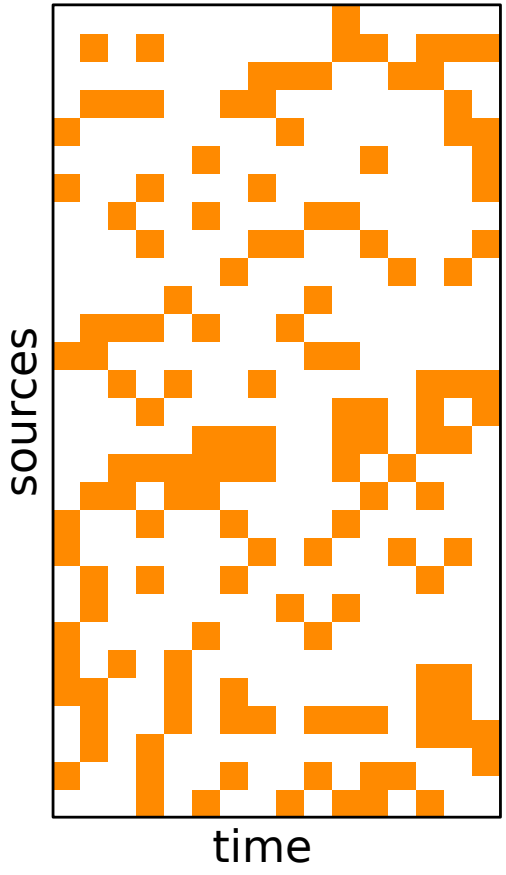
$$\boxed{Y = X\mathrm{B} + E}$$

$\mathrm{B} \in \mathbb{R}^{p \times q}$:source activity matrix ; $E \in \mathbb{R}^{n \times q}$: additive white noise

Method: need to regularize, biological prior = few active sources

$$\hat{\mathrm{B}} \in \underset{\mathrm{B} \in \mathbb{R}^{p \times q}}{\arg\min} \frac{1}{2} \|Y - X\mathrm{B}\|_F^2 + \underbrace{\lambda \Omega(\mathrm{B})}_{\text{sparsity}}$$

Choice of Ω



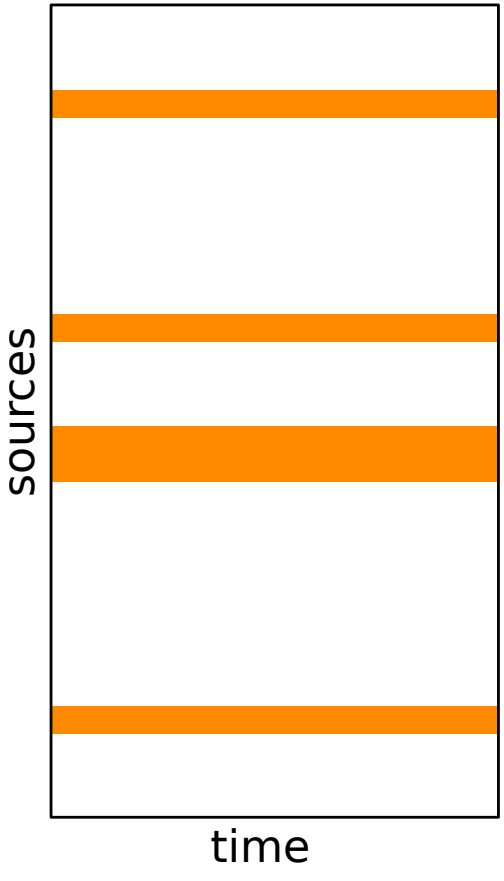
Source activity
$\hat{\mathrm{B}} \in \mathbb{R}^{p \times q}$

Penalty: Lasso (ℓ_1, Tibshirani (1996))

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

$\rightarrow$ not good: activity scattered between all sources over time

Choice of Ω



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

Penalty: Group-Lasso ($\ell_{2,1}$)

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

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

$$\hat{\mathrm{B}} \in \underset{\mathrm{B} \in \mathbb{R}^{p \times q}}{\arg\min} \frac{1}{2} \|Y - X\mathrm{B}\|_F^2 + \lambda \|\mathrm{B}\|_{2,1}$$

a.k.a. Multiple Measurement Vector (MMV) in signal processing or Multi-Task Lasso in ML

(cyclic) Block Coordinate Descent

Minimize (convex) function: $\mathcal{P}(\mathrm{B}) = \frac{1}{2}\left\|Y - X\mathrm{B}\right\|_F^2 + \lambda \sum_{j=1}^{p} \left\|\mathrm{B}_j\right\|_2$:

where $\mathrm{B}_j := \mathrm{B}_{j,:}$ for simplicity

Algorithm: BCD

Initialization: $\mathrm{B}^{(0)} = 0 \in \mathbb{R}^{p \times q}$

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cf. (Tseng, 2001), (Friedman *et al.* , 2007), (Wu *et al.* , 2008), Nesterov (2012), (Beck *et al.* ,2013), ...

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Possible Speed-ups for BCD solvers

Reminder: we expect that $\|\hat{\mathrm{B}}\|_{2,0}$ is small (few rows activated)

Idea: Can we ignore blocks which will be 0 at convergence, thus reducing the size of the problem?

- **Safe rules** (El Ghaoui *et al.* , 2012): screen out variables B_j guaranteed to be zero in $\hat{\mathrm{B}}_j$ (prior to any computation or thanks to solutions obtained for λ' close to λ)
- **Strong rules** (Tibshirani *et al.* , 2012): relaxed heuristics to start computing the $\hat{\mathrm{B}}_j$ for only a few j's
- **Working / active Set** (Joachims 1998) (Roth *et al.* , 2008), (Kim & Park, 2010), (Kowalski *et al.* , 2011), (Jonhson and Guestrin, 2015,16): solve problems with growing sizes

Dual problem detour (Kim *et al.* , 2007)

Primal function : $$\mathcal{P}(\mathrm{B}) = \frac{1}{2}\|Y - X\mathrm{B}\|^2 + \lambda\|\mathrm{B}\|_{2,1}$$

Dual problem : $$\hat{\Theta} = \underset{\Theta \in \Delta_X}{\arg\max} \underbrace{\frac{1}{2}\|Y\|^2 - \frac{\lambda^2}{2}\left\|\Theta - \frac{Y}{\lambda}\right\|^2}_{:=\mathcal{D}(\Theta)}$$

Dual feasible set : $$\Delta_X = \left\{\Theta \in \mathbb{R}^{n\times q} \ : \ \left\|X_{:,j}^\top \Theta\right\|_2 \leq 1, \forall j \in [p]\right\}$$

- $\Delta_X = \left\{\Theta \in \mathbb{R}^{n\times q} : \left\|X^\top \Theta\right\|_{2,\infty} \leq 1\right\}$ is a convex set
- The (unique) dual solution is the **projection** of Y/λ over Δ_X:

$$\hat{\Theta} = \underset{\Theta \in \Delta_X}{\arg\min} \left\|\frac{Y}{\lambda} - \Theta\right\|^2 := \Pi_{\Delta_X}\left(\frac{Y}{\lambda}\right)$$

Geometric interpretation

The dual optimal solution is the projection of Y/λ over the dual feasible set $\Delta_X = \left\{\Theta \in \mathbb{R}^{n\times q} : \left\|X^\top \Theta\right\|_{2,\infty} \leq 1\right\} : \hat{\Theta} = \Pi_{\Delta_X}\left(\frac{Y}{\lambda}\right)$

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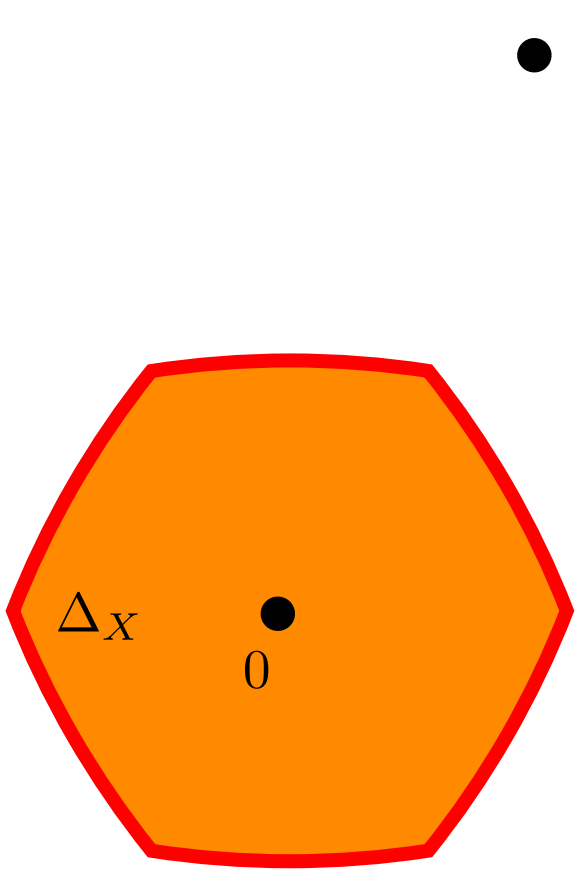

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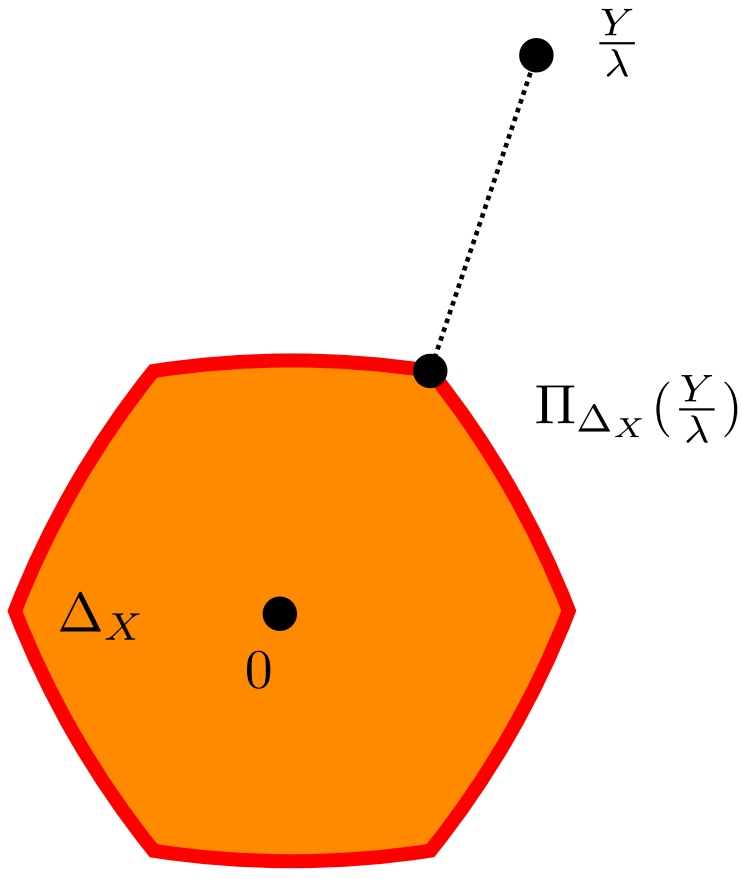


Fermat rule / KKT conditions

- **Primal solution :** $\hat{\mathrm{B}} \in \mathbb{R}^{p \times q}$
- **Dual solution :** $\hat{\Theta} \in \Delta_X \subset \mathbb{R}^{n \times q}$

Primal/Dual link: $\boxed{Y = X\hat{\mathrm{B}} + \lambda\hat{\Theta}}$

Necessary and sufficient optimality conditions:

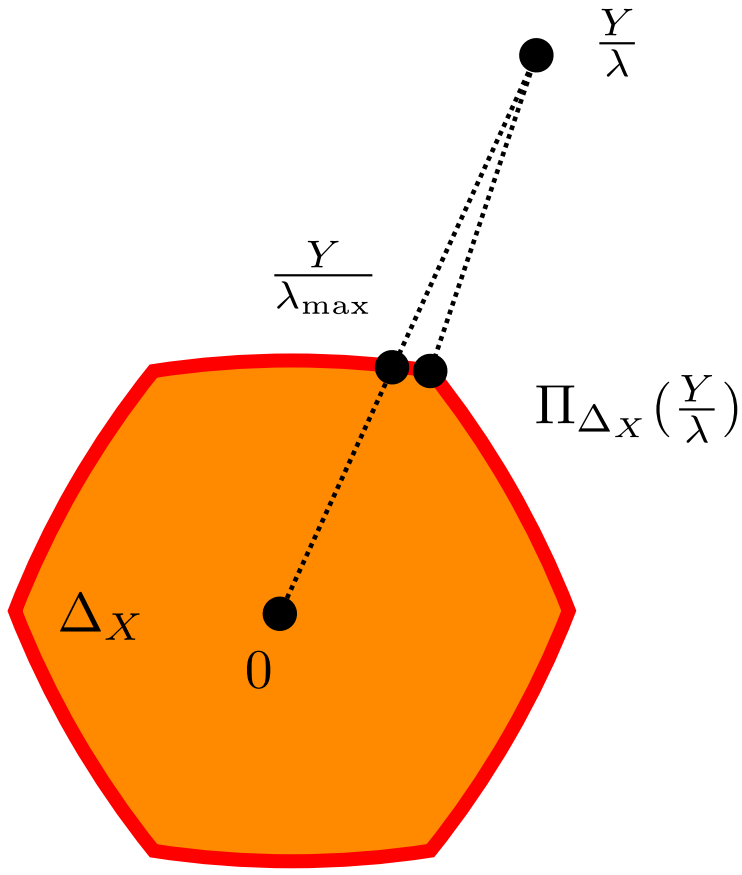
KKT/Fermat: $$\boxed{\forall j \in [p],\ X_{:,j}^\top \hat{\Theta} \in \begin{cases} \{\frac{\hat{\mathrm{B}}_j}{\|\mathrm{B}_j\|_2}\} & \text{if} \quad \hat{\mathrm{B}}_j \neq 0, \\ \mathcal{B}(0,1) & \text{if} \quad \hat{\mathrm{B}}_j = 0. \end{cases}}$$

Mother of safe rules:
Fermat's rule implies that if $\lambda \geq \lambda_{\max} = \|X^\top Y\|_{2,\infty}$, then $\hat{\mathrm{B}} = 0$ is a primal solution ($\hat{\Theta} = Y/\lambda$ is the associated dual)

Rem: $\mathcal{B}(0,1)$ is the standard Euclidean unit ball

Geometric interpretation (II)

Simple dual (feasible) point: $\frac{Y}{\lambda_{\max}} \in \Delta_X$, with $\lambda_{\max} = \|X^\top Y\|_{2,\infty}$



Rem: $(Y - X \cdot 0)/\lambda \in \Delta_X$ if $\lambda \geq \lambda_{\max}$, hence $\hat{\mathrm{B}} = Y/\lambda, \hat{\mathrm{B}} = 0$

Safe Screening rules: (El Ghaoui *et al.* , 2012)

Screening thanks to Fermat's Rule: $\boxed{\text{If } \left\| X_{:,j}^\top \hat{\Theta} \right\|_2 < 1 \text{ then, } \hat{\mathrm{B}}_j = 0}$

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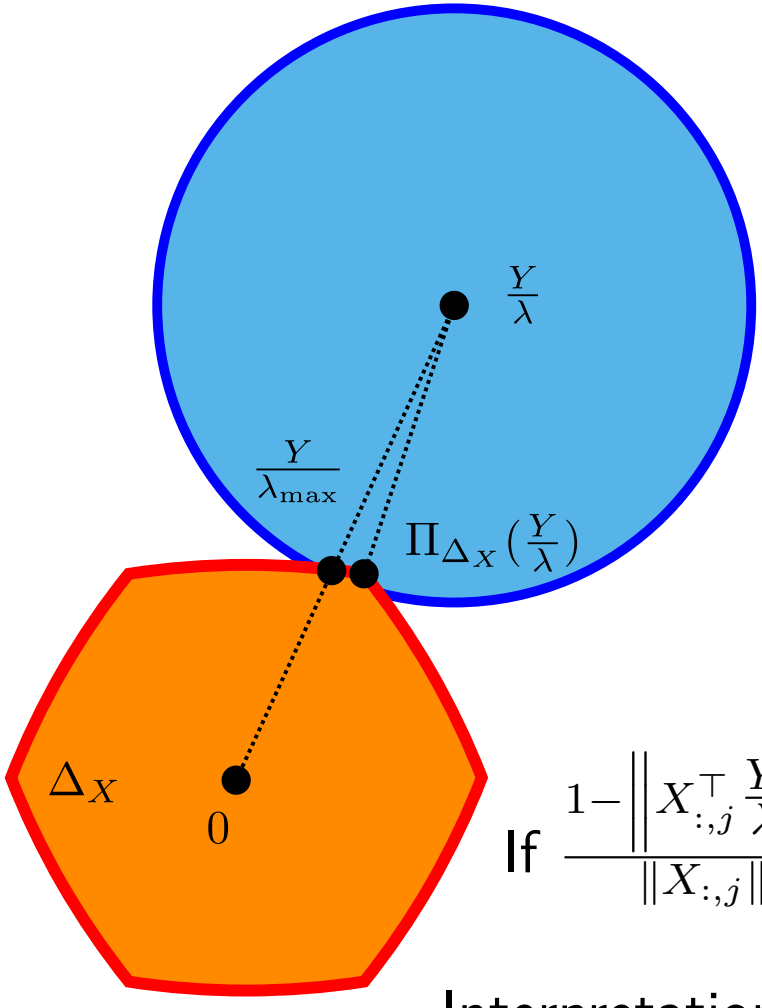
Yet, if one knows a **safe** ball $\mathcal{B}$ containing $\hat{\Theta}$, *i.e.*, a set s.t. $\hat{\Theta} \in \mathcal{B}$:

$$\textbf{safe rule}: \quad \boxed{\text{If } \sup_{\Theta \in \mathcal{B}} \left\| X_{:,j}^\top \Theta \right\|_2 < 1 \text{ then } \hat{\mathrm{B}}_j = 0} \qquad (\star)$$

Rem: simple bound available for the $\sup$ if $\mathcal{B}$ is a ball

Rem: if $(\star)$ is satisfied, you can remove $X_{:,j}$ from X and solving the smaller associated problem provide solution for the original one

Static safe rules: (El Ghaoui *et al.* , 2012)



Choose as a safe ball:

$$\mathcal{B} = \mathcal{B}\left(\frac{Y}{\lambda}, \left\|\frac{Y}{\lambda_{\max}} - \frac{Y}{\lambda}\right\|_2\right)$$

(static) **Safe rule** to remove $X_{:,j}$:

$$\text{If } \frac{1 - \left\|X_{:,j}^\top \frac{Y}{\lambda}\right\|_2}{\|X_{:,j}\|} > \|Y\|_2 \left|\frac{1}{\lambda} - \frac{1}{\lambda_{\max}}\right| \text{ then } \hat{\mathrm{B}}_j = 0$$

Interpretation: remove weakly correlated features
(*i.e.*, correlation screening)

Sequential safe rules - Strong rules

Often need $\hat{\mathrm{B}}^{(\lambda)}$ for $\lambda = \lambda_1, \lambda_2, \ldots,$ *e.g.*, for CV. Advice: use warm start ($=$ start solver with closest $\hat{\mathrm{B}}^{(\lambda')}$ available)

Sequential safe rules[1] (Wang *et al.* , 2013): perform safe screening rule with the safe ball $\mathcal{B} = \mathcal{B}\left(\hat{\Theta}^{(\lambda')}, \left\|\hat{\Theta}^{(\lambda')}\right\|_2 \frac{|\lambda' - \lambda|}{\lambda'}\right)$:

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Notation: For $\lambda' > \lambda$ (close) : $\begin{cases} \hat{\mathrm{B}}^{(\lambda')} : \text{ primal optimal for } \lambda' \\ \hat{\Theta}^{(\lambda')} : \text{ dual optimal for } \lambda' \end{cases}$

[1] impossible when $\Theta^{(\lambda')}$ only approximated, Fercoq *et al.* (2015), Remark 8

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Strong rules (Tibshirani *et al.* , 2012) heuristic: relax test to

$$\text{If } \frac{1 - \left\|X_{:,j}^\top \hat{\Theta}^{(\lambda')}\right\|_2}{\|X_{:,j}\|_2} > \frac{2}{\|X_{:,j}\|_2} \frac{|\lambda' - \lambda|}{\lambda'} \text{ then } \hat{\mathrm{B}}_j = 0$$

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Dynamic / Gap safe rules

Dynamic safe screening Bonnefoy *et al.* (2014, 15): perform screening at k^{th} step of a solver: periodically, screen-out variables based on Θ^k, current estimate of $\hat{\Theta}$

Gap Safe screening (Fercoq *et al.* , 2015), (Ndiaye *et al.* , 2015): same approach but rely on duality gap criterion (converging rule)

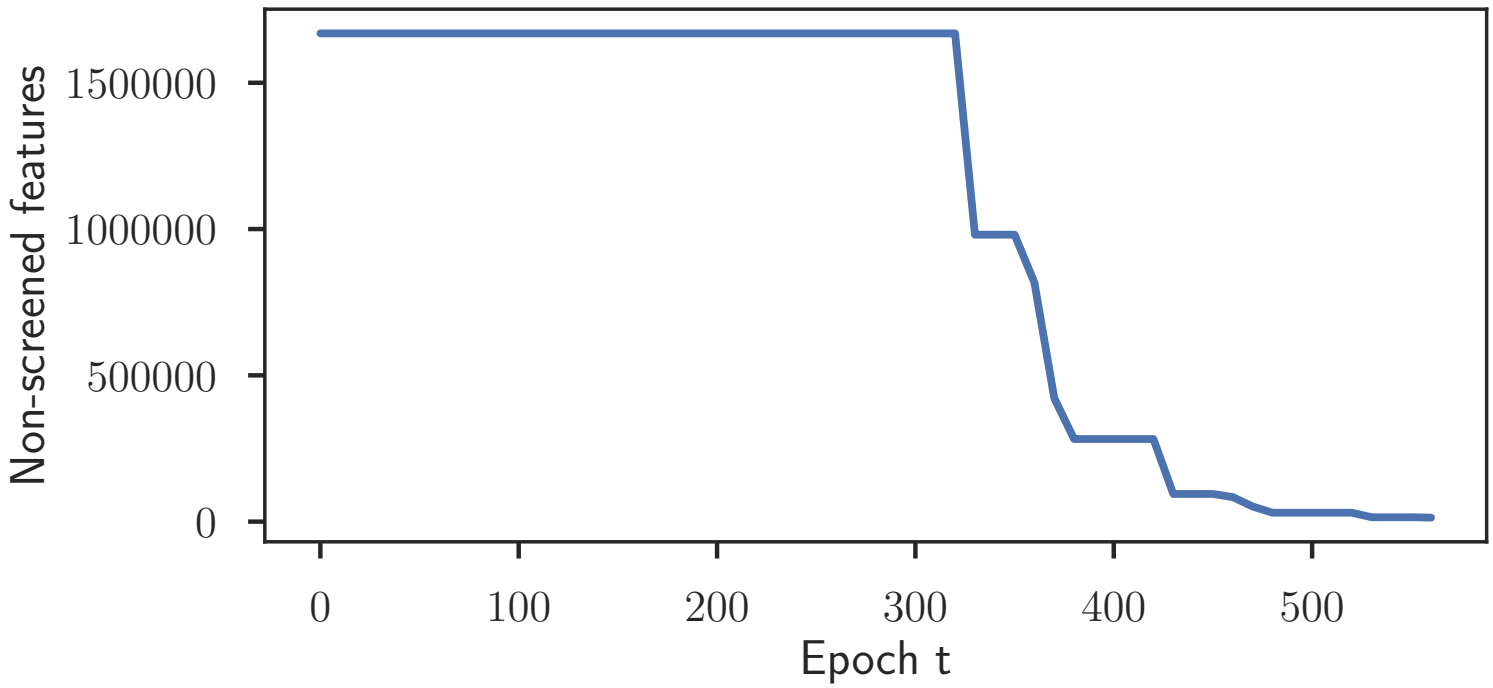
Theorem

$$d_j(\Theta^k) := \frac{1 - \left\| X_{:,j}^\top \Theta^k \right\|_2}{\|X_{:,j}\|_2} > \sqrt{\frac{2}{\lambda^2} \mathcal{G}(\mathrm{B}^k, \Theta^k)} \Rightarrow \hat{\mathrm{B}}_j = 0$$

for any primal point B^k and dual feasible point Θ^k where $\mathcal{G}(\mathrm{B}^k, \Theta^k) = \mathcal{P}(\mathrm{B}^k) - \mathcal{D}(\Theta^k)$ is the duality gap

Rem: harmonize dynamic and sequential safe screening
Rem: get Θ^k by residual scaling, *i.e.*, rescale $Y - X\mathrm{B}^k$ to be in Δ_X

Can we speed up solvers more?



(E2006-log1p: $n = 16,087, p = 1,668,737, q = 1$, Lasso case)

$\rightarrow$ useless features are still included in the beginning !

Aggressive screening and working sets (WS)

Idea: to reduce the number of features, **drop the safety**.

Gap Safe: exclude source j if $d_j(\Theta^k) > \sqrt{\frac{2}{\lambda^2}\mathcal{G}(\mathrm{B}^k, \Theta^k)}$

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for some $r \in [0, 1]$ to be chosen (Johnson and Guestrin, 2015,16)

- outer loop: only include few features with the smallest $d_j(\Theta)$

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- outer loop: only include few features with the smallest $d_j(\Theta)$
- inner loop: solve subproblem keeping only these features (fast)

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- outer loop: only include few features with the smallest $d_j(\Theta)$
- inner loop: solve subproblem keeping only these features (fast)
- repeat

Aggressive screening and working sets (WS)

Idea: to reduce the number of features, **drop the safety**.

Gap Safe: exclude source j if $d_j(\Theta^k) > \sqrt{\frac{2}{\lambda^2}\mathcal{G}(\mathrm{B}^k, \Theta^k)}$

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Previous working/active set techniques for Lasso-type problems:
(Roth *et al.* , 2008), (Kim & Park, 2010), (Kowalski *et al.* , 2011),

AGGressive Gap Greedy with Gram (A5G)

Algorithm: $\mathrm{A5G}$

input : X, Y, λ

param: $\mathrm{B}_0 = 0_{p,q}, \bar{\epsilon} = 10^{-6}, r \in]0, 1[$

// Outer loop:

for $k = 1, \ldots, K$ **do**

Compute dual point Θ^k and dual gap g^k

if $g^k \leq \bar{\epsilon}$ **then**

Break

for $j = 1, \ldots, p$ **do**

Compute $d_j^k = (1 - \|X_{:,j}^\top \Theta^k\|)/\|X_{:,j}\|$

$\mathcal{W}^k = \{j \in [p] : d_j^k < r\sqrt{2g^k}/\lambda \cup \{j : \mathrm{B}_j^{k-1} \neq 0\}$

// Inner loop:

Solve problem restricted to $\mathcal{W}^k$ approximately and get B^k

return B^k

Rem: easy to add gap safe screening once g^k and d_j^k computed

AGGressive Gap Greedy with Gram (A5G)

Algorithm: A5G

input : X, Y, λ

param: $\mathrm{B}_0 = 0_{p,q}, \bar{\epsilon} = 10^{-6}, r \in]0, 1[, p^0 = 100$ (or other guess)

// Outer loop:

for $k = 1, \ldots, K$ **do**

  Compute dual point Θ^k and dual gap g^k

  if $g^k \leq \bar{\epsilon}$ **then**

    Break

  for $j = 1, \ldots, p$ **do**

    Compute $d_j^k = (1 - \|X_{:,j}^\top \Theta^k\|)/\|X_{:,j}\|$

  $p^k = \max(p_0, \min(2 \left\|\mathrm{B}^{k-1}\right\|_{2,0}, p))$ // clipping

  $\mathcal{W}^k = \{j \in [p] : d_j^k$ among $p^k/2$ smallest ones$\} \cup \{j : \mathrm{B}_j^{k-1} \neq 0\}$

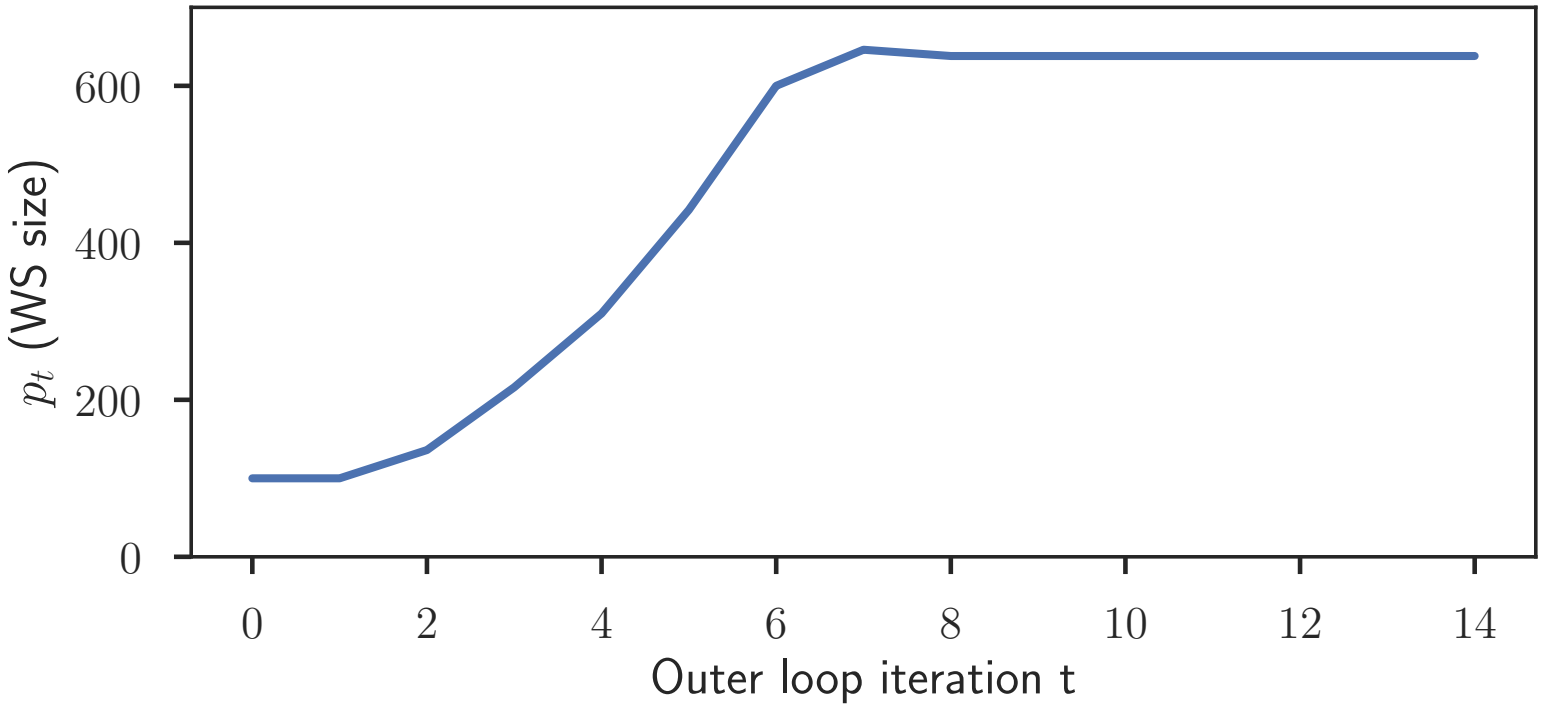
  // Inner loop:

  Solve problem restricted to $\mathcal{W}^k$ approximately and get B^k

return B^k

Rem: easy to add gap safe screening once g^k and d_j^k computed

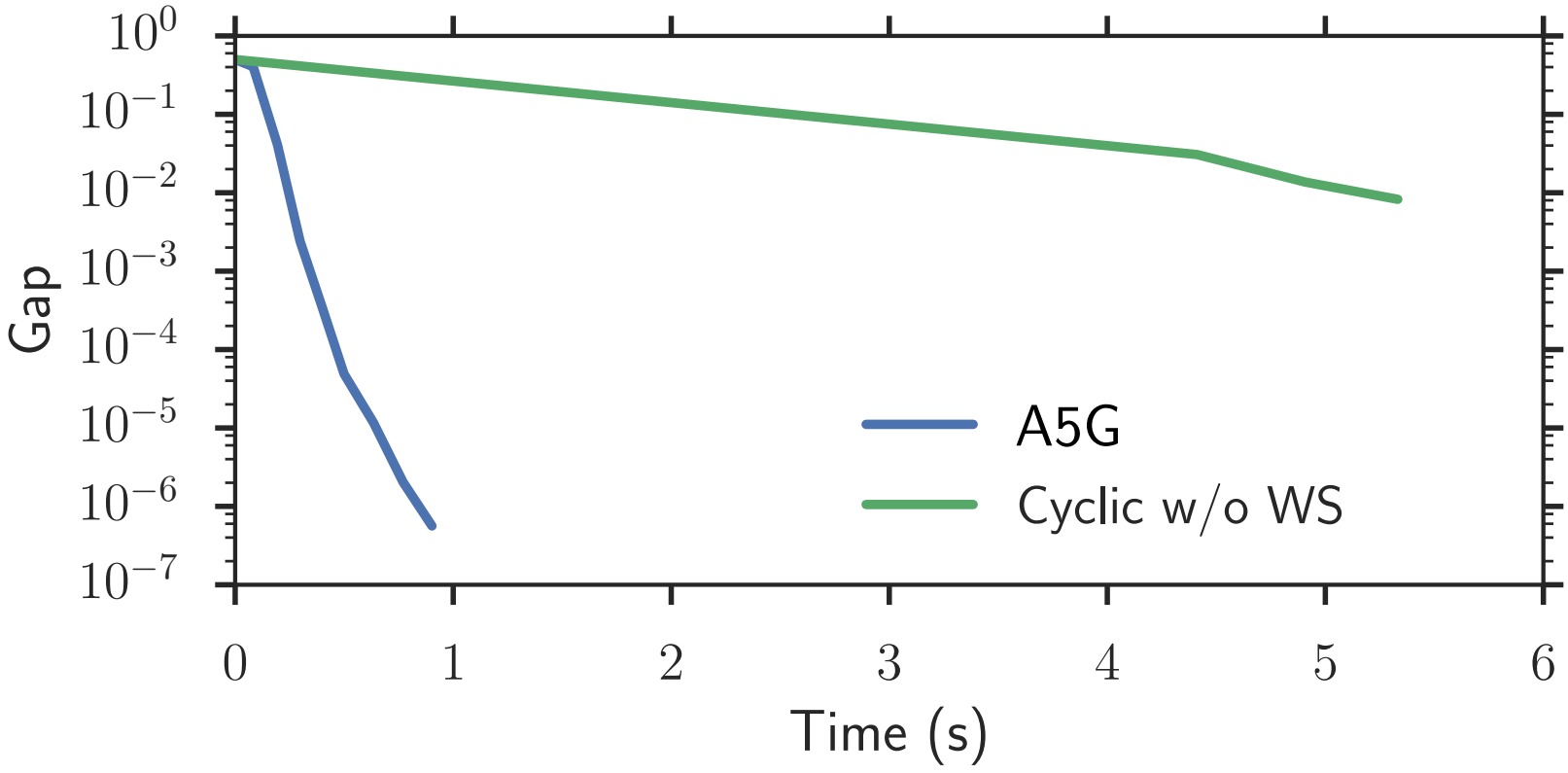
Further speed improvement



(E2006-log1p: $n = 16,087, p = 1,668,737, q = 1$, Lasso case)

Smaller subproblems solved $\rightarrow$ Gram matrix $X_{\mathcal{W}^k}^\top X_{\mathcal{W}^k}$ fits in, and one can use greedy BCD method

Results on MEG data



(MEG: $n = 302, p = 7498, q = 181$)

about $10\times$ speed-up w.r.t. state-of-the-art multi-task Lasso solver from `scikit-learn` (Pedregosa *et al.* , 2011)

Take home message

- Safe screening rules can help (**sequential**, **dynamic**, . . .)
- Relaxing safety / aggressive screening : provide **growth strategy** for working set (WS)

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More info : Papers / Code

Papers:

- Gap Safe Rules: ICML 2015 (Lasso case), NIPS 2015 (General loss + multi-task), long version ArXiV 1611.05780

A5G:

- ArXiV 1703.07285

Codes:

- Python Code on-line: `https://github.com/EugeneNdiaye`
- pull requests (#5075) (#7853) on `sklearn`
- A5G code: `https://github.com/mathurinm/A5G`

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Block updates

One does not need the exact solution of $\underset{z \in \mathbb{R}^q}{\arg\min}\, \mathcal{P}(\mathrm{B}_1, \dots, \mathrm{B}_{j-1}, z, \mathrm{B}_{j+1}, \dots, \mathrm{B}_p)$, "descent" step enough

The update rule is (Kowalski, 2009) or (Parikh & Boyd, 2013)

$$\mathrm{B}_j \leftarrow \mathrm{BST}\left(\mathrm{B}_j - \frac{\nabla_j f(\mathrm{B})}{\|X_{:,j}\|^2}, \frac{\lambda}{\|X_{:,j}\|^2}\right) \ ,$$

where $\nabla_j f(\mathrm{B})$ is the gradient of the data fitting term *w.r.t.* B_j:

$$\nabla_j f(\mathrm{B}) = X_{:,j}^\top (X\mathrm{B} - Y) \ ,$$

and BST is the **block soft-thresholding** operator:

$$\mathrm{BST}(z, \mu) := \left(1 - \frac{\mu}{\|z\|}\right)_+ z \ .$$

Rem: $(\cdot)_+ = \max(0, \cdot)$ makes the iterates block-sparse

Fast update with pre-computed Gram

When one can pre-compute and store the Gram matrix

$$Q = X^\top X = [Q_1, \dots, Q_p] \in \mathbb{R}^{p \times p}$$

maintain the gradients

$$H^k = X^\top (X \mathrm{B}^k - Y) \in \mathbb{R}^{p \times q}$$

rather than the residuals, and use

$$\textbf{BCD update} : \begin{cases} \delta \mathrm{B}_j & \leftarrow \mathrm{BST}\left(\mathrm{B}_j^{k-1} - \frac{H_j^{k-1}}{\|X_{:,j}\|^2}, \frac{\lambda}{\|X_{:,j}\|^2}\right) - \mathrm{B}_j^{k-1} \\ \mathrm{B}_j^k & \leftarrow \mathrm{B}_j^{k-1} + \delta \mathrm{B}_j \quad \text{if} \quad \delta \mathrm{B}_j \neq 0 \\ H^k & \leftarrow H^{k-1} + Q_j \delta \mathrm{B}_j \quad \text{if} \quad \delta \mathrm{B}_j \neq 0 \end{cases}$$

Rem: For "non 0-updates", the main cost is a $p \times q$ matrix rank one update (the third line); "0-updates" almost free

Gauss-Southwell (GS) selection rule

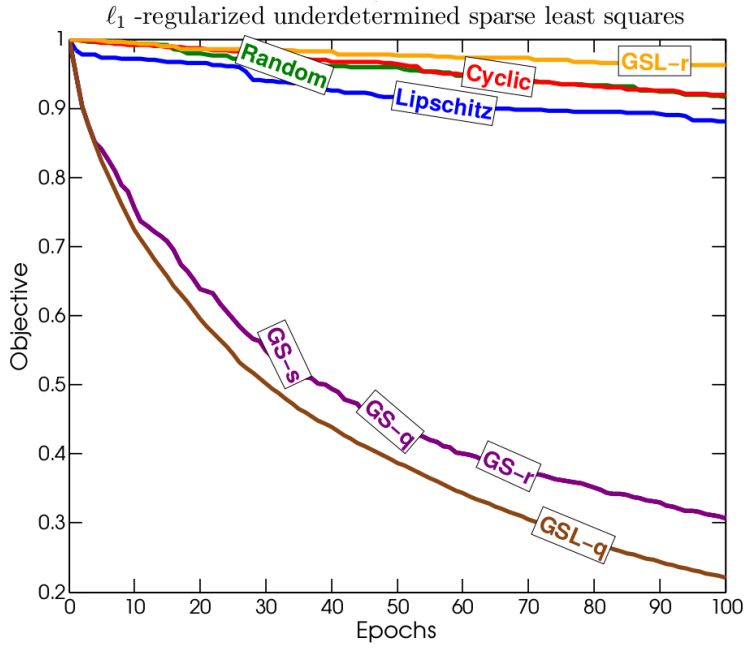

Figure: courtesy of Nutini *et al.* (2015), various BCD strategies

Greedy selection rules for BCD (Soutwhell, 1941), (Tseng & Yun, 2009) instead of cyclic:

- larger decrease in objective for each update
- but costly to compute

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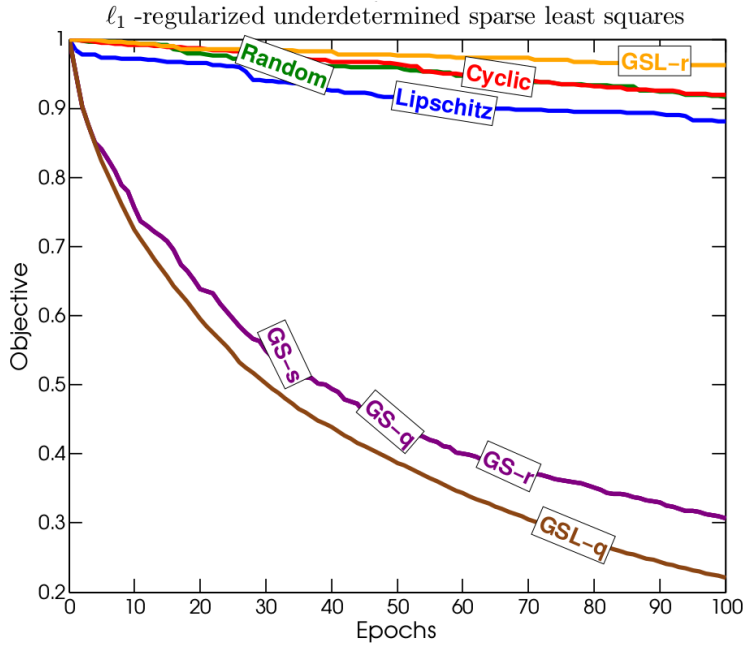

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Greedy selection rules for BCD (Soutwhell, 1941), (Tseng & Yun, 2009) instead of cyclic:

- larger decrease in objective for each update
- but costly to compute
- way **cheaper when the Gram matrix is available !**