Celer[1]: a fast Lasso solver with dual extrapolation

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[1] Constraint Elimination for the Lasso with Extrapolated Residuals

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The Lasso[2,3]

$$\hat{\mathbf{w}} \in \arg\min_{\mathbf{w}\in\mathbb{R}^p} \underbrace{\frac{1}{2}\left\|\mathbf{y} - X\mathbf{w}\right\|^2 + \lambda \left\|\mathbf{w}\right\|_1}_{\mathcal{P}(\mathbf{w})}$$

- $y \in \mathbb{R}^n$: observations
- $X = [\mathbf{x}_1, \ldots, \mathbf{x}_p] \in \mathbb{R}^{n \times p}$: design matrix
- $\lambda > 0$: trade-off parameter between data-fit and regularization
- sparsity: for λ large enough, $\|\hat{\mathbf{w}}\|_0 \ll p$

Rem: uniqueness is not guaranteed, more later

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

[3] S. S. Chen and D. L. Donoho. "Atomic decomposition by basis pursuit". In: *SPIE*. 1995.

Duality for the Lasso

$$\hat{\boldsymbol{\theta}} = \underset{\theta \in \Delta_X}{\arg\max} \underbrace{\frac{1}{2}\left\|\mathbf{y}\right\|^2 - \frac{\lambda^2}{2}\left\|\mathbf{y}/\lambda - \boldsymbol{\theta}\right\|^2}_{\mathcal{D}(\boldsymbol{\theta})}$$

$\Delta_X = \left\{\boldsymbol{\theta} \in \mathbb{R}^n \,:\, \forall j \in [p],\ |\mathbf{x}_j^\top \boldsymbol{\theta}| \leq 1\right\}$: dual feasible set

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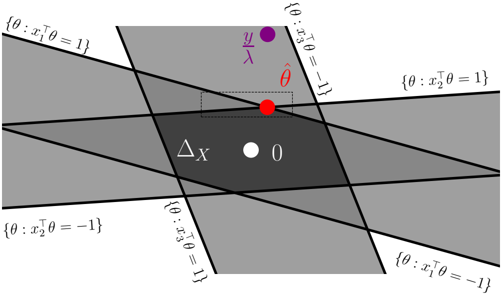

Toy visualization example: $n = 2, p = 3$

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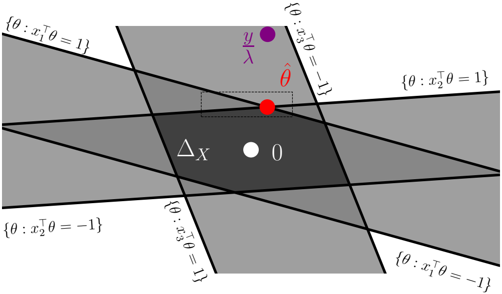

Projection problem: $\hat{\boldsymbol{\theta}} = \Pi_{\Delta_X}(\mathbf{y}/\lambda)$

Solving the Lasso

So-called *smooth* + *separable* problem

- In signal processing: use ISTA/FISTA[4]
- In ML: state-of-the-art algorithm when X is not an implicit operator: coordinate descent (CD)[5,6]

  Iterative algorithm: minimize $\mathcal{P}(\mathbf{w}) = \mathcal{P}(\mathbf{w}_1, \dots, \mathbf{w}_p)$ *w.r.t.* $\mathbf{w}_1$, then $\mathbf{w}_2$, etc.

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[4] A. Beck and M. Teboulle. "A fast iterative shrinkage-thresholding algorithm for linear inverse problems". In: *SIAM J. Imaging Sci.* 2.1 (2009), pp. 183–202.

[5] J. Friedman et al. "Pathwise coordinate optimization". In: *Ann. Appl. Stat.* 1.2 (2007), pp. 302–332.

[6] P. Tseng. "Convergence of a block coordinate descent method for nondifferentiable minimization". In: *J. Optim. Theory Appl.* 109.3 (2001), pp. 475–494.

Solving the Lasso: cyclic CD

To minimize : $\mathcal{P}(\mathbf{w}) = \frac{1}{2}\|\mathbf{y} - \sum_{j=1}^{p} \mathbf{x}_j \mathbf{w}_j\|^2 + \lambda \sum_{j=1}^{p} |\mathbf{w}_j|$

Algorithm: Cyclic CD

Initialization: $\mathbf{w}^0 = 0 \in \mathbb{R}^p$

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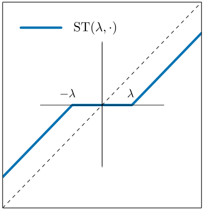
CD update: soft-thresholding

Coordinate-wise minimization is easy:

$$\mathbf{w}_j \leftarrow \mathrm{ST}\left(\frac{\lambda}{\|\mathbf{x}_j\|^2}, \mathbf{w}_j + \frac{\mathbf{x}_j^\top(\mathbf{y} - X\mathbf{w})}{\|\mathbf{x}_j\|^2}\right)$$



1 update is $\mathcal{O}(n)$

Variants: minimize *w.r.t.* $\mathbf{w}_j$ with j chosen at random, or **shuffle** order every epoch (1 epoch $= p$ updates)

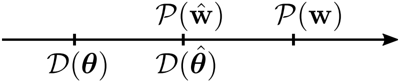
Rem: equivalent to performing Dykstra Algorithm in the dual[7]

[7] R. J. Tibshirani. "Dykstra's Algorithm, ADMM, and Coordinate Descent: Connections, Insights, and Extensions". In: *NIPS*. 2017, pp. 517–528.

Duality gap as a stopping criterion

For any primal-dual pair $(\mathbf{w}, \boldsymbol{\theta})$:

$$\mathcal{P}(\mathbf{w}) \geq \mathcal{P}(\hat{\mathbf{w}}) = \mathcal{D}(\hat{\boldsymbol{\theta}}) \geq \mathcal{D}(\boldsymbol{\theta})$$



The **duality gap** $\mathcal{P}(\mathbf{w}) - \mathcal{D}(\boldsymbol{\theta}) =: \mathrm{gap}(\mathbf{w}, \boldsymbol{\theta})$ is an upper bound of the **suboptimality gap** $\mathcal{P}(\mathbf{w}) - \mathcal{P}(\hat{\mathbf{w}})$:

$$\forall \mathbf{w}, (\exists \boldsymbol{\theta} \in \Delta_X, \mathrm{gap}(\mathbf{w}, \boldsymbol{\theta}) \leq \epsilon) \Rightarrow \mathcal{P}(\mathbf{w}) - \mathcal{P}(\hat{\mathbf{w}}) \leq \epsilon$$

i.e., $\mathbf{w}$ is an ϵ-solution

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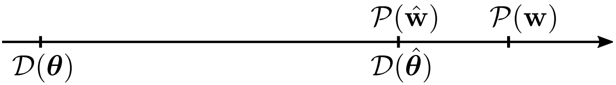

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Choice of dual point

Primal-dual link at optimum:

$$\boxed{\hat{\boldsymbol{\theta}} = (\mathbf{y} - X\hat{\mathbf{w}})/\lambda}$$

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

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Standard approach[8]: at epoch t, corresponding to iterate $\mathbf{w}^t$ and **residuals** $\mathbf{r}^t := \mathbf{y} - X\mathbf{w}^t$, take

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Beware: might not be feasible!

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residuals rescaling

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residuals rescaling

- converges to $\hat{\boldsymbol{\theta}}$ (provided $\mathbf{w}^t$ converges to $\hat{\mathbf{w}}$)
- $\mathcal{O}(np)$ to compute ($=$ 1 epoch of CD)
  $\rightarrow$ rule of thumb: compute $\boldsymbol{\theta}^t_{\mathrm{res}}$ and gap every $f = 10$ epochs

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

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Speeding up solvers

Key property leveraged: we expect sparse solutions/small supports

$$\mathcal{S}_{\hat{\mathbf{w}}} := \{j \in [p] \,:\, \hat{\mathbf{w}}_j \neq 0\}$$

"the solution restricted to its support solves the problem restricted to features in this support"

$$\hat{\mathbf{w}}_{\mathcal{S}_{\hat{\mathbf{w}}}} \in \operatorname*{arg\,min}_{w \in \mathbb{R}^{\|\hat{\mathbf{w}}\|_0}} \frac{1}{2}\|\mathbf{y} - X_{\mathcal{S}_{\hat{\mathbf{w}}}} w\|^2 + \lambda \|w\|_1$$

Usually $\|\hat{\mathbf{w}}\|_0 \ll p$; hence the second problem is much simpler

Technical details

- The primal solution/support might not be unique!
- But $\hat{\boldsymbol{\theta}}$ is unique and so is the **equicorrelation set**[9]:

$$E := \left\{ j \in [p] \, : \, |\mathbf{x}_j^\top \hat{\boldsymbol{\theta}}| = 1 \right\} = \left\{ j \in [p] \, : \, \frac{|\mathbf{x}_j^\top (\mathbf{y} - X\hat{\mathbf{w}})|}{\lambda} = 1 \right\}$$

- For any primal solution, $\mathcal{S}_{\hat{\mathbf{w}}} \subset E$

[9] R. J. Tibshirani. "The lasso problem and uniqueness". In: *Electron. J. Stat.* 7 (2013), pp. 1456–1490.

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Grail of sparse solvers: identify E, solve on E

Practical observation: generally $\#E \ll p$

[9] R. J. Tibshirani. "The lasso problem and uniqueness". In: *Electron. J. Stat.* 7 (2013), pp. 1456–1490.

Speeding-up solvers

Two approaches:

- safe screening[10,11] (**backward approach**): remove feature j when it is certified that $j \notin E$
- working set[12] (**forward approach**): focus on j's very likely to be in the equicorrelation set E

Rem: hybrid approaches possible, *e.g.*, strong rules[13]

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

[11] A. Bonnefoy et al. "A dynamic screening principle for the lasso". In: *EUSIPCO*. 2014.

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

[13] R. Tibshirani et al. "Strong rules for discarding predictors in lasso-type problems". In: *J. R. Stat. Soc. Ser. B Stat. Methodol.* 74.2 (2012), pp. 245–266.

Duality comes into play: gap screening

We want to identify $E = \left\{ j \in [p] \; : \; |\mathbf{x}_j^\top \hat{\boldsymbol{\theta}}| = 1 \right\}$ ...
... but we can't get it without $\hat{\mathbf{w}}$!

Good proxy: find a region $\mathcal{C} \subset \mathbb{R}^n$ containing $\hat{\boldsymbol{\theta}}$

$$\sup_{\boldsymbol{\theta} \in \mathcal{C}} |\mathbf{x}_j^\top \boldsymbol{\theta}| < 1 \Rightarrow |\mathbf{x}_j^\top \hat{\boldsymbol{\theta}}| < 1$$

[14] E. Ndiaye et al. "Gap Safe screening rules for sparsity enforcing penalties". In: *J. Mach. Learn. Res.* 18.128 (2017), pp. 1–33.

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Gap Safe screening rule[14]: $\mathcal{C}$ is a ball of radius $\rho = \sqrt{\frac{2}{\lambda^2} \mathrm{gap}(\mathbf{w}, \boldsymbol{\theta})}$ centered at $\boldsymbol{\theta} \in \Delta_X$

$$\boxed{\forall (\mathbf{w}, \boldsymbol{\theta}) \in \mathbb{R}^p \times \Delta_X, \quad |\mathbf{x}_j^\top \boldsymbol{\theta}| < 1 - \|\mathbf{x}_j\| \rho \Rightarrow \hat{\mathbf{w}}_j = 0}$$

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Back to dual choice

$$\boldsymbol{\theta}^t_{\mathrm{res}} = \mathbf{r}^t / \max(\lambda, \|X^\top \mathbf{r}^t\|_\infty)$$

Two drawbacks of residuals rescaling:

- ignores information from previous iterates
- workload "imbalanced": more efforts in primal than in dual

$\lambda_{\max} = \|X^\top y\|_\infty$ is the smallest λ giving $\hat{\mathbf{w}} = 0$

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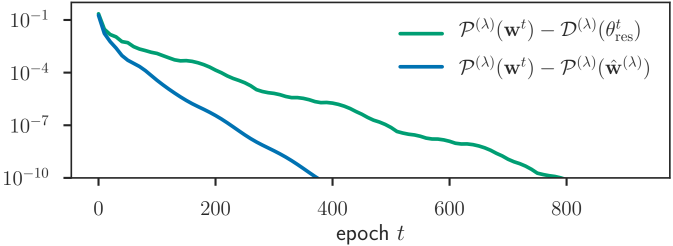

Leukemia dataset ($p = 7129, n = 72$), for $\lambda = \lambda_{\max}/20$

$\lambda_{\max} = \|X^\top y\|_\infty$ is the smallest λ giving $\hat{\mathbf{w}} = 0$

Acceleration through residuals extrapolation[15]

What is the limit of $(0, \frac{1}{2}, \frac{3}{4}, \frac{7}{8}, \frac{15}{16}, \ldots)$?

[15] D. Scieur, A. d'Aspremont, and F. Bach. "Regularized Nonlinear Acceleration". In: *NIPS*. 2016, pp. 712–720.

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What is the limit of $(0, \frac{1}{2}, \frac{3}{4}, \frac{7}{8}, \frac{15}{16}, \ldots)$?

extrapolation!

$\rightarrow$ use the same idea to infer $\lim_{t \to \infty} \mathbf{r}^t = \lambda \hat{\boldsymbol{\theta}}$

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Extrapolation justification

If $(x_t)_{t\in\mathbb{N}}$ follows a converging autoregressive process (AR):

$$x_t = a x_{t-1} - b \qquad (|a| < 1) \quad \text{with} \lim_{t\to\infty} x_t = x^*$$

we have

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

Aitken's Δ^2: 2 unknowns, so 2 equations/3 points x_t, x_{t-1}, x_{t-2} are enough to find x^*![16]

Rem: Aitken's rule replaces x_{n+1} by

$$\Delta^2 = x_n + \frac{1}{\frac{1}{x_{n+1}-x_n} - \frac{1}{x_n - x_{n-1}}}$$

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

Aitken application

$$\lim_{t\to\infty}\sum_{i=0}^{t}\frac{(-1)^i}{2i+1}=\frac{\pi}{4}=0.785398...$$

t	$\sum_{i=0}^{t}\frac{(-1)^i}{2i+1}$	Δ^2
0	1.0000	–
1	0.66667	–
2	0.86667	**0.7**9167
3	**0.7**2381	**0.78**333
4	0.83492	**0.78**631
5	**0.7**4401	**0.78**492
6	0.82093	**0.785**68
7	**0.7**5427	**0.785**22
8	0.81309	**0.785**52
9	**0.7**6046	**0.7853**1

Approximate Minimal Polynomial Extrapolation (AMPE)

Approximate Minimal Polynomial Extrapolation: generalization for vector autoregressive (VAR) process

$$\mathbf{r}_{k+1} - \mathbf{r}^* = A(\mathbf{r}_k - \mathbf{r}^*), \quad \text{where } A \text{ is a matrix}$$

This leads to:

$$\sum_{k=1}^{K} c_k(\mathbf{r}_k - \mathbf{r}^*) = \sum_{k=1}^{K} c_k A^k(\mathbf{r}_0 - \mathbf{r}^*)$$

and setting $\sum_{k=1}^{K} c_k = 1$ then one has:

$$\sum_{k=1}^{K} c_k \mathbf{r}_k - \mathbf{r}^* = (\sum_{k=1}^{K} c_k A^k)(\mathbf{r}_0 - \mathbf{r}^*)$$

Consequence: one can approximate $\mathbf{r}^*$ by a combination of the $\mathbf{r}_k$

$$\min_{c^\top \mathbf{1}=1} \left\| \sum_{k=1}^{K} c_k(\mathbf{r}_k - \mathbf{r}^*) \right\|$$

AMPE Continued

The previous optimization problem, can not be solved due to $\mathbf{r}^*$:

$$\min_{c^\top \mathbf{1}=1} \left\| \sum_{k=1}^{K} c_k (\mathbf{r}_k - \mathbf{r}^*) \right\|$$

But note that

$$\mathbf{r}_k - \mathbf{r}_{k-1} = (\mathbf{r}_k - \mathbf{r}^*) - (\mathbf{r}_{k-1} - \mathbf{r}^*) = (A - \mathrm{Id}) A^{k-1} (\mathbf{r}_0 - \mathbf{r}^*)$$

Hence, if $\mathrm{Id} - A$ is non singular and $\sum_{k=1}^{K} c_k A^{k-1} = 0$, one must have $\sum_{k=1}^{K} c_k (\mathbf{r}_k - \mathbf{r}_{k-1}) = 0$ and the new program is simply:

$$\min_{c^\top \mathbf{1}=1} \left\| \sum_{k=1}^{K} c_k (\mathbf{r}_k - \mathbf{r}_{k-1}) \right\|$$

Extrapolated dual point[17]

- keep track of K past residuals $\mathbf{r}^t, \ldots, \mathbf{r}^{t+1-K}$
- form $U^t = [\mathbf{r}^{t+1-K} - \mathbf{r}^{t-K}, \ldots, \mathbf{r}^t - \mathbf{r}^{t-1}] \in \mathbb{R}^{n \times K}$
- solve $(U^t)^\top U^t z = \mathbf{1}_K$
- $c = \dfrac{z}{z^\top \mathbf{1}_K} \in \mathbb{R}^K$

$$\mathbf{r}^t_{\text{accel}} = \begin{cases} \mathbf{r}^t, & \text{if } t \leq K \\ \sum_{k=1}^{K} c_k \mathbf{r}^{t+1-k}, & \text{if } t > K \end{cases}$$

[17] M. Massias, A. Gramfort, and J. Salmon. "Celer: a Fast Solver for the Lasso with Dual Extrapolation". In: *ICML*. 2018.

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$K = 5$ is enough !

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Guarantees?

- convergence of $\boldsymbol{\theta}^t_{\text{accel}}$?
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$\boldsymbol{\theta}_{\mathrm{accel}}$ is $\mathcal{O}(np + K^2 n + K^3)$ to compute, so compute $\boldsymbol{\theta}_{\mathrm{res}}$ as well and pick the best

$$\text{use } \boldsymbol{\theta}^t = \mathop{\arg\max}_{\boldsymbol{\theta} \in \{\boldsymbol{\theta}^t_{\mathrm{res}}, \boldsymbol{\theta}^t_{\mathrm{accel}}, \boldsymbol{\theta}^{t-1}\}} \mathcal{D}(\boldsymbol{\theta})$$

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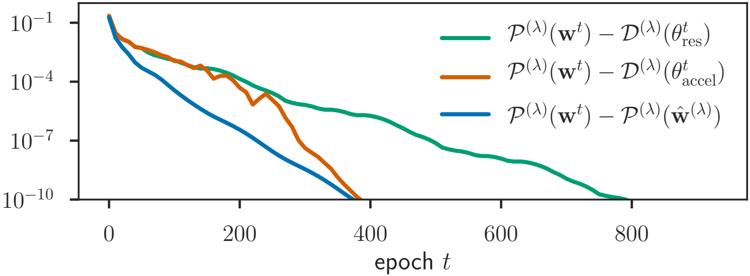
Final cost for: $f = 10$ CD epochs + gap computation $\approx$ 12 np vs. 11 np in classical approach

Does it work?



Leukemia dataset ($p = 7129, n = 72$), for $\lambda = \lambda_{\max}/20$
(consistent finding across datasets)

- $\boldsymbol{\theta}_{\mathrm{res}}$ is bad
- $\boldsymbol{\theta}_{\mathrm{accel}}$ gives a tighter bound
- $\boldsymbol{\theta}_{\mathrm{accel}}$ does not behave erratically

Which algorithm to produce $\mathbf{w}^t$?

Key assumption for extrapolation[18]: $\mathbf{r}^t$ follows a VAR.

- True for ISTA and the Lasso, once support is identified[19] (but ISTA/FISTA slow on our statistical scenarios)

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Rem: Shuffle CD breaks the regularity

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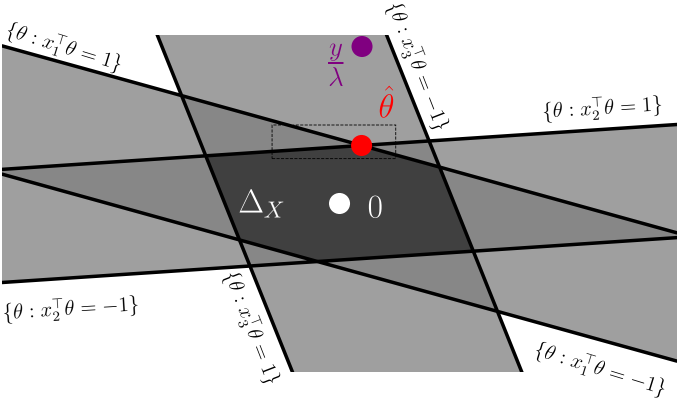
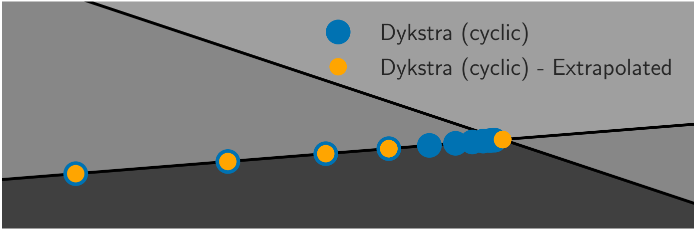
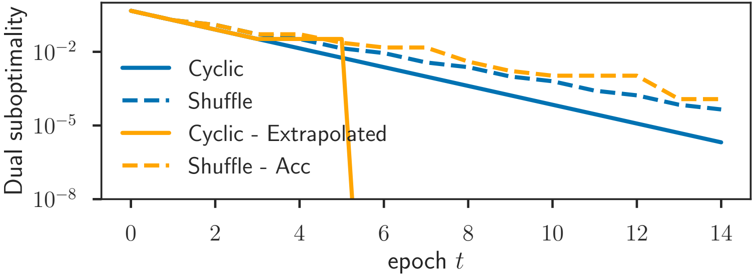
Back to toy example

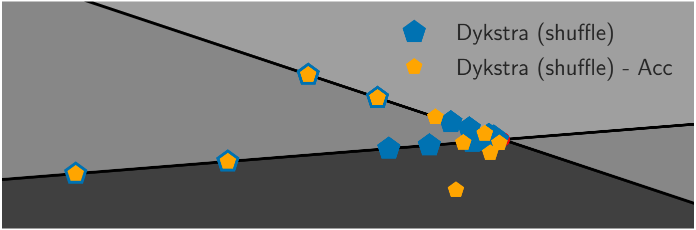


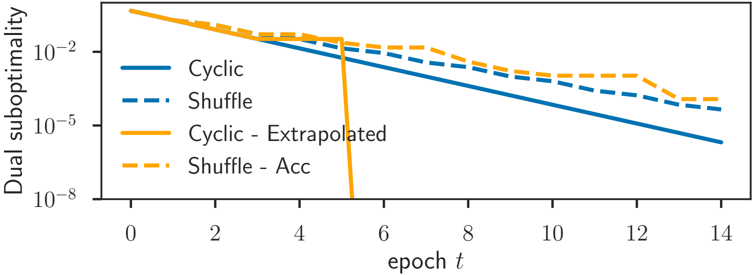
Toy dual zoom: cyclic





Toy dual zoom: shuffle





Better safe screening

Recall Gap Safe screening rule:

$$\forall \boldsymbol{\theta} \in \Delta_X, |\mathbf{x}_j^\top \boldsymbol{\theta}| < 1 - \|\mathbf{x}_j\| \sqrt{\frac{2}{\lambda^2} \mathsf{gap}(\mathbf{w}, \boldsymbol{\theta})} \Rightarrow \hat{\mathbf{w}}_j = 0$$

better dual point $\Rightarrow$ better safe screening

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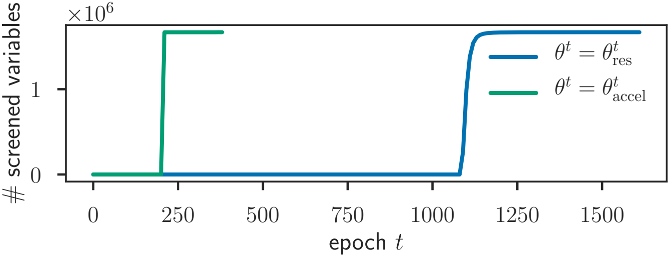
better dual point ⇒ better safe screening



Finance dataset: $(p = 1.5 \times 10^6, n = 1.5 \times 10^4)$, $\lambda = \lambda_{\max}/5$

Screening vs Working sets

$$|\mathbf{x}_j^\top \boldsymbol{\theta}| < 1 - \|\mathbf{x}_j\| \sqrt{\frac{2}{\lambda^2} \mathsf{gap}(\mathbf{w}, \boldsymbol{\theta})} \Rightarrow \hat{\mathbf{w}}_j = 0$$

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$$\Leftrightarrow$$

$$d_j(\boldsymbol{\theta}) > \sqrt{\frac{2}{\lambda^2} \mathsf{gap}(\mathbf{w}, \boldsymbol{\theta})} \Rightarrow \hat{\mathbf{w}}_j = 0$$

$$\text{with } d_j(\boldsymbol{\theta}) := \frac{1 - |\mathbf{x}_j^\top \boldsymbol{\theta}|}{\|\mathbf{x}_j\|}$$

$d_j(\boldsymbol{\theta})$ larger than threshold $\rightarrow$ exclude feature j

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Alternative: Solve subproblem with small $d_j(\boldsymbol{\theta})$ only (WS)

Working/active set

Algorithm: Generic WS algorithm

Initialization: $\mathbf{w}^0 = 0 \in \mathbb{R}^p$

for $it = 1, \dots, it_{\max}$ **do**

  define working set $\mathcal{W}_{it} \subset [p]$

  approximately solve Lasso restricted to features in $\mathcal{W}_{it}$

  update $\mathbf{w}_{\mathcal{W}_{it}}$

3 questions for working sets

- how to prioritize features?

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Guarantees convergence

Rem: : pruning variant also tested where working set can decrease in size & features can leave the working set

Similarities[20,21]

$$\boxed{d_j(\boldsymbol{\theta}) := \frac{1 - |\mathbf{x}_j^\top \boldsymbol{\theta}|}{\|\mathbf{x}_j\|}}$$

[20] J. Fan and J. Lv. "Sure independence screening for ultrahigh dimensional feature space". In: *J. R. Stat. Soc. Ser. B Stat. Methodol.* 70.5 (2008), pp. 849–911.

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Lasso case with $\boldsymbol{\theta} = \boldsymbol{\theta}_{\mathrm{res}}$ and normalized $\mathbf{x}_j$'s:

$$1 - d_j(\boldsymbol{\theta}) \propto |\mathbf{x}_j^\top \mathbf{r}^t|$$

small $d_j(\boldsymbol{\theta}) =$ high correlation with residuals/high norm of partial gradient of data-fitting term...

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BUT our strength is that we can use any $\boldsymbol{\theta}$, in particular $\boldsymbol{\theta}_{\mathrm{accel}}$

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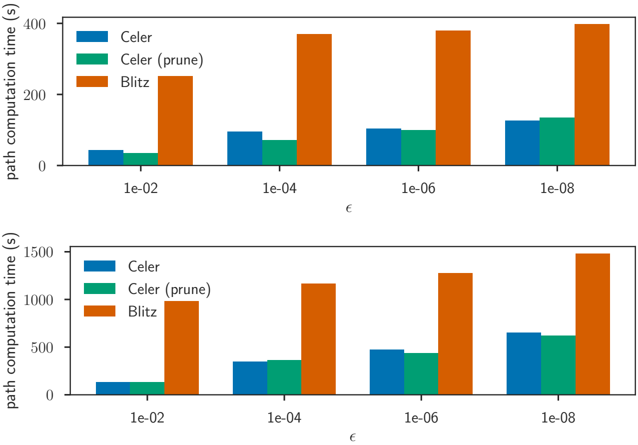
Comparison

State-of-the-art WS solver for sparse problems: Blitz[22]

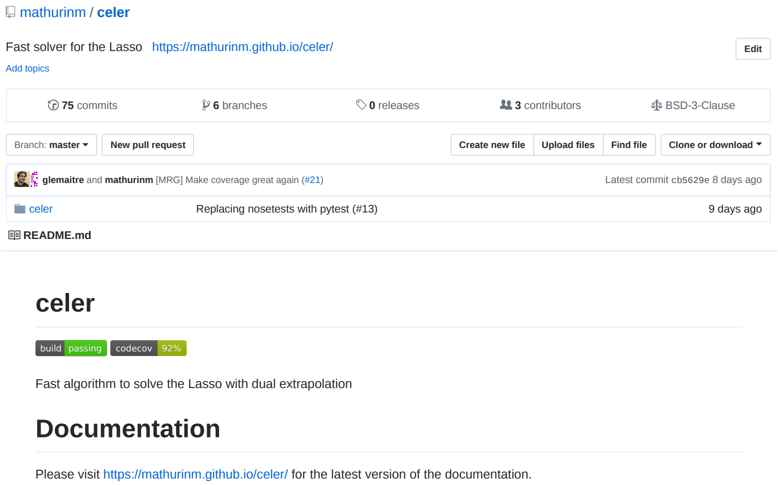


Finance dataset, Lasso path of 10 (top) or 100 (bottom) λ's from $\lambda_{\max}$ to $\lambda_{\max}/100$

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

Reusable science

https://github.com/mathurinm/celer: code with continuous integration, code coverage, bug tracker

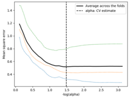


Examples gallery

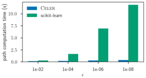
https://mathurinm.github.io/celer: documentation (examples, API)

Fork me on GitHub

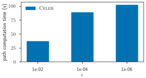
Examples Gallery¶



Run LassoCV for cross-validation on Leukemia



Lasso path computation on Leukemia dataset



Lasso path computation on Finance/log1p

Drop-in sklearn replacement

```python
from sklearn.linear_model import Lasso, LassoCV
from celer import Lasso, LassoCV
```

Fork me on GitHub

celer.Lasso

class `celer.` **Lasso** (*alpha=1.0, max_iter=100, gap_freq=10, max_epochs=50000, p0=10, verbose=*
tol=1e-06, prune=0, fit_intercept=True)

Lasso scikit-learn estimator based on Celer solver

The optimization objective for Lasso is:

```
(1 / (2 * n_samples)) * ||y - X beta||^2_2 + alpha * ||beta||_1
```

Parameters:

alpha : float, optional

> Constant that multiplies the L1 term. Defaults to 1.0. `alpha = 0` is equivalent to an ordinary least square. For numerical reasons, using `alpha = 0` with the `Lasso` object is not advised.

max_iter : int, optional

> The maximum number of iterations (subproblem definitions)

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From 10,000 s to 50 s for cross-validation on Finance

Fork me on GitHub

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Conclusion

Duality matters at several levels for the Lasso:

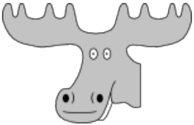
- stopping criterion
- feature identification (screening or working set)

Key improvement: residuals rescaling $\rightarrow$ residuals extrapolation

Future works:

- Can it work for sparse logreg, group Lasso?
- Can we prove convergence of $\boldsymbol{\theta}_{\mathrm{accel}}$ and give rates?

Feedback welcome on the online code!



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