Implicit differentiation for hyperparameter optimization of Lasso-type models

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https://QB3.github.io

Joint work with:
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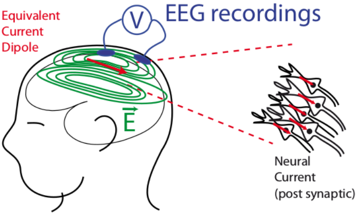
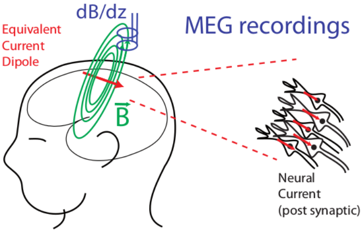
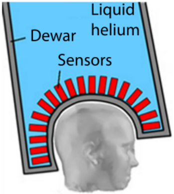
M/EEG inverse problem for brain imaging

- sensors: electric and magnetic fields during a cognitive task
- goal: which parts of the brain are responsible for the signals?
- applications: epilepsy treatment, brain aging, anesthesia risks



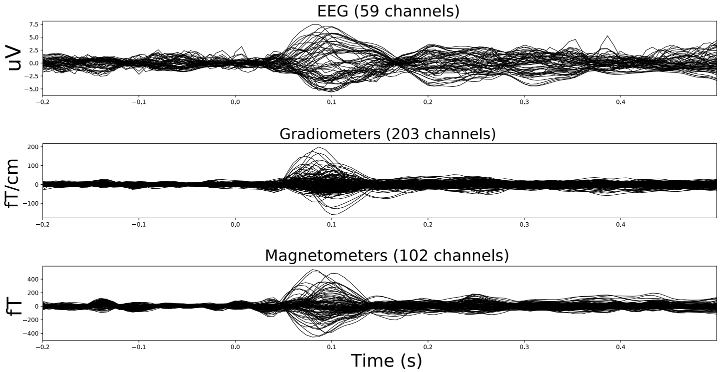


First EEG recordings in 1929 by H. Berger



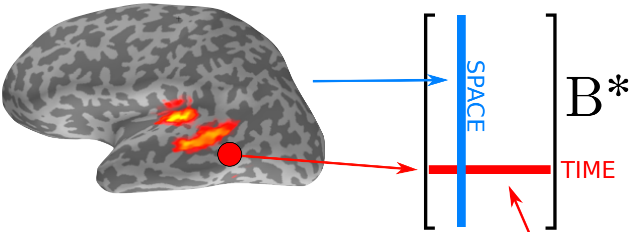
Hôpital La Timone Marseille, France

M/EEG data

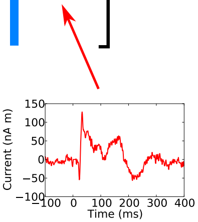


- 3 different types of sensor

Source modeling (discretization with voxels)

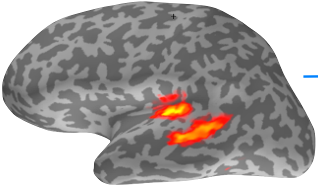


Position a few thousands candidate sources over the brain (*e.g.*, every 5mm)

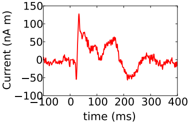


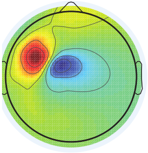
$$B^* \in \mathbb{R}^{p \times q}$$

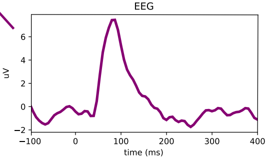
The M/EEG inverse problem: modeling



$$\underbrace{Y}_{n \approx 100,\; T \approx 100} = \underbrace{X}_{p \approx 10000} \, B^* + E$$





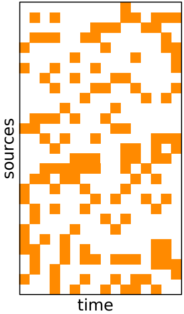


$$n << p$$

Multi-Task penalties[1]

Popular convex penalties considered:

$$\hat{\mathrm{B}} \in \underset{\mathrm{B}\in\mathbb{R}^{p\times T}}{\arg\min} \left(\frac{1}{2nT} \|Y - X\mathrm{B}\|_F^2 + \lambda\Omega(\mathrm{B}) \right)$$



Parameter $\hat{\mathrm{B}} \in \mathbb{R}^{p\times T}$

Sparse support: no structure

Penalty: **Lasso type**

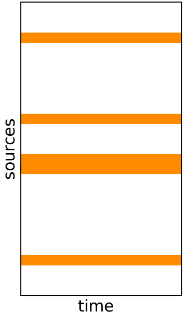
$$\Omega(\mathrm{B}) = \|\mathrm{B}\|_1 = \sum_{j=1}^{p} \sum_{k=1}^{T} |\mathrm{B}_{j,k}|$$

[1] G. 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.

Multi-Task penalties[1]

Popular convex penalties considered: Multi-Task Lasso (MTL)

$$\hat{\mathrm{B}} \in \mathop{\arg\min}_{\mathrm{B}\in\mathbb{R}^{p\times T}} \left(\frac{1}{2nT} \|Y - X\mathrm{B}\|_F^2 + \lambda \Omega(\mathrm{B}) \right)$$



Parameter $\hat{\mathrm{B}} \in \mathbb{R}^{p\times T}$

Sparse support: group structure ✓

Penalty: **Group-Lasso type**

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

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

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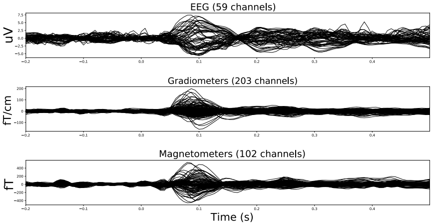
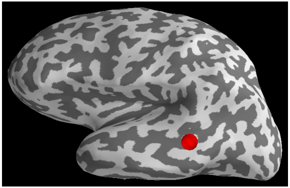
Summary



What you have: Y



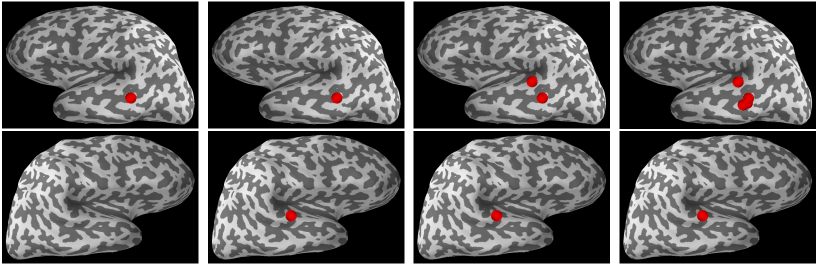
What you want B

This is typically done using optimization based estimators:

$$\hat{\mathrm{B}} \in \underset{\mathrm{B} \in \mathbb{R}^{p \times T}}{\arg\min} \left(\frac{1}{2nT} \| Y - X\mathrm{B} \|_F^2 + \lambda \Omega(\mathrm{B}) \right)$$

Which λ to pick?

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



$\lambda = 0.85\lambda_{\max}$ $\lambda = 0.82\lambda_{\max}$ $\lambda = 0.80\lambda_{\max}$ $\lambda = 0.75\lambda_{\max}$

Real MEEG data. Brain source reconstruction using multitask Lasso with multiple λ. Which λ to pick? How to *automatically* select λ?

- When $\lambda \geq \lambda_{\max}$, $\hat{\mathrm{B}} = 0$ no sources are recovered

Which λ to pick? A statistical persective[2] (i.i.d. case, Single-Task, $y = X\beta + \sigma^*\varepsilon$)

$$\hat{\beta} \in \operatorname*{arg\,min}_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$$

Theorem

- i.i.d. Gaussian noise
- $+$ X satisfying the "Restricted Eigenvalue" property
- $+$ $\lambda = 2\sigma_* \sqrt{\frac{2\log(p/\delta)}{n}}$
- $\Longrightarrow$ with probability $1-\delta$:

$$\frac{1}{n}\|X\beta^* - X\hat{\beta}^{(\lambda)}\|^2 \leq \frac{18}{\kappa_{s^*}^2} \frac{\sigma_*^2 s^*}{n} \log\left(\frac{p}{\delta}\right)$$

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

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

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Which λ to pick? A statistical persective II[3] (i.i.d. case, Single-Task)

$$\hat{\beta} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{\sqrt{n}} \|y - X\beta\|_2 + \lambda \|\beta\|_1$$

Theorem

- i.i.d. Gaussian noise
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- $\implies$ with probability $1-\delta$:

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λ does not depend on σ_* anymore!

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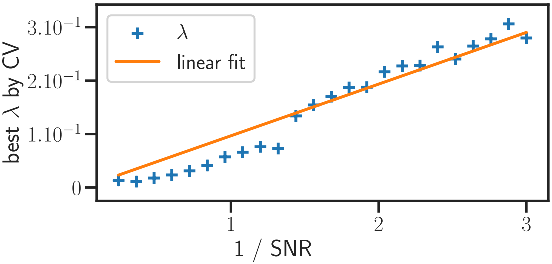
Which λ to pick? A statistical persective III

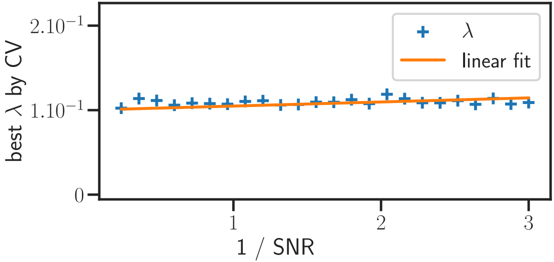
$$\boxed{\hat{\beta}_{\text{Lasso}} \in \arg\min_{\beta \in \mathbb{R}^p} \left(\frac{1}{2n} \|y - X\beta\|^2 + \lambda \|\beta\|_1 \right)}$$



Lasso

Which λ to pick? A statistical persective III

$$\boxed{\hat{\beta}_{\sqrt{\text{Lasso}}} \in \underset{\beta \in \mathbb{R}^p}{\arg\min} \left(\frac{1}{\sqrt{n}} \|y - X\beta\| + \lambda \|\beta\|_1 \right)}$$



Square-root Lasso

Which λ to pick? A statistical persective III

- $\lambda \sim \sigma^*$ and λ independent of σ^* confirmed in practice ✓
- Strong statistical assumptions, not verified in practice ✗
- Still unknown quantities in the closed-form formula for λ: still needs calibration in practice ✗

Hyperparameter optimization (HO)

Possible selection criterion:

- Good generalization[4] of $\hat{\beta}^{(\lambda)}$
- AIC/BIC,[5] SURE[6] that control model complexity

[4] L. R. A. Stone and J.C. Ramer. "Estimating WAIS IQ from Shipley Scale scores: Another cross-validation". In: *Journal of clinical psychology* 21.3 (1965), pp. 297–297.

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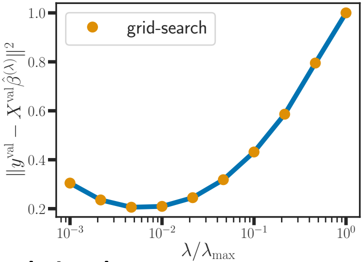

Real-sim dataset

Validation loss as a function of λ.

Example

Model: Lasso

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{\|y^{\text{train}} - X^{\text{train}}\beta\|^2}{2n} + \lambda\|\beta\|_1$$

Criterion: held-out loss

$$\arg\min_{\lambda} \|y^{\text{val}} - X^{\text{val}}\hat{\beta}^{(\lambda)}\|^2$$

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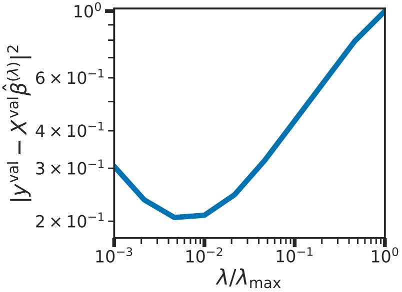
HO as a bilevel optimization problem[7][8]

$$\overbrace{\arg\min_{\lambda\in\mathbb{R}} \left\{ \mathcal{L}(\lambda) := \|y^{\text{val}} - X^{\text{val}} \hat{\beta}^{(\lambda)}\|^2 \right\}}^{\text{outer optimization problem}}$$

$$\text{s.t. } \underbrace{\hat{\beta}^{(\lambda)} \in \arg\min_{\beta\in\mathbb{R}^p} \frac{1}{2n} \|y^{\text{train}} - X^{\text{train}} \beta\|^2 + \lambda \|\beta\|_1}_{\text{inner optimization problem}}$$



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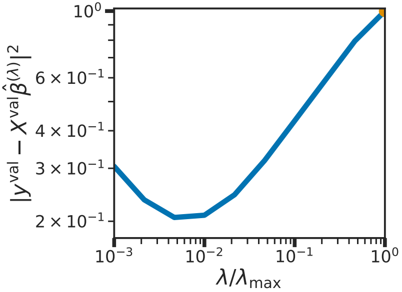

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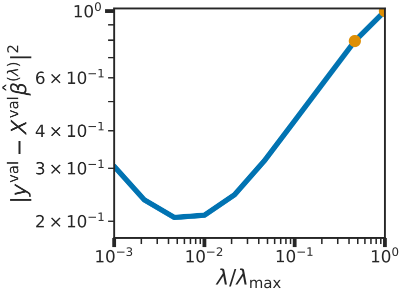

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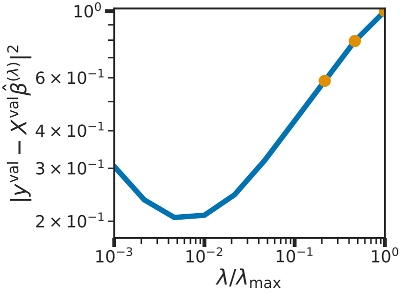

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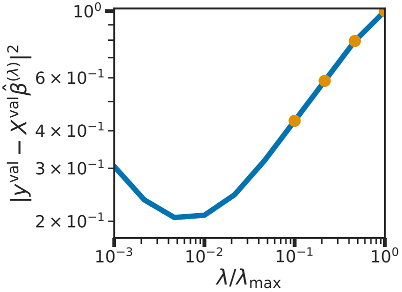

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HO as a bilevel optimization problem(7)(8)

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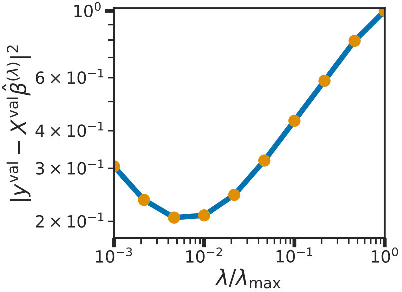

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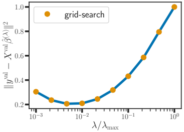
Grid-search as a 0-order optimization method



$$\arg\min_{\lambda \in \mathbb{R}} \left\{ \mathcal{L}(\lambda) := \|y^{\text{val}} - X^{\text{val}} \hat{\beta}^{(\lambda)}\|^2 \right\}$$

$$\text{s.t. } \hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \|y^{\text{train}} - X^{\text{train}} \beta\|^2 + \lambda \|\beta\|_1$$

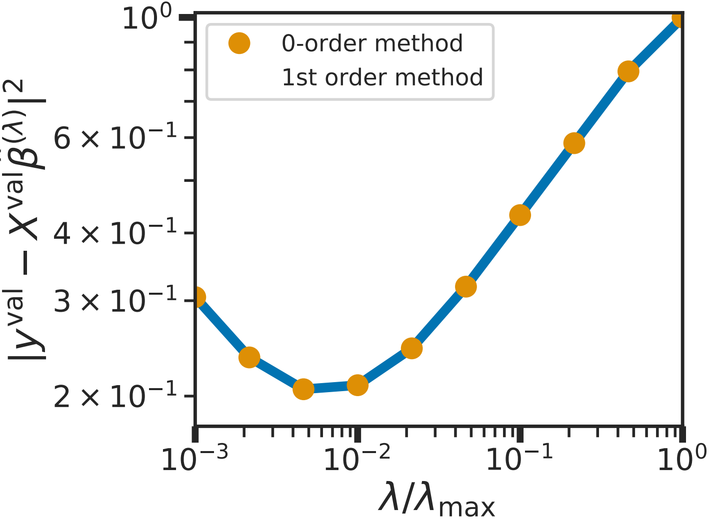
- Grid-search, random-search,[9] SMBO[10]:
  0-order methods to solve bilevel optimization problem
- **Idea:** if $\mathcal{L}$ is differentiable, use first order optimization, *i.e.*, compute $\nabla_\lambda \mathcal{L}$
- Once $\nabla_\lambda \mathcal{L}(\lambda)$ is computed, use gradient descent[11]:
  $$\lambda^{(t+1)} = \lambda^{(t)} - \rho \nabla_\lambda \mathcal{L}(\lambda^{(t)}) \quad \text{with suitable } \rho > 0$$

[9] J. Bergstra and Y. Bengio. “Random search for hyper-parameter optimization”. In: *J. Mach. Learn. Res.* (2012).

[10] E. Brochu, V. M. Cora, and N. De Freitas. “A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning”. In: (2010).

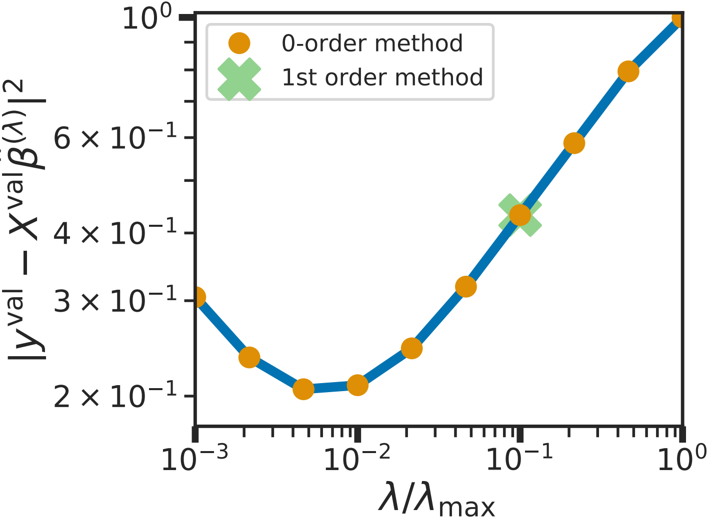
[11] F. Pedregosa. “Hyperparameter optimization with approximate gradient”. In: *ICML*. 2016.

First order optimization in λ, Lasso



Real-sim dataset. Validation loss as a function of λ.

First order optimization in λ, Lasso



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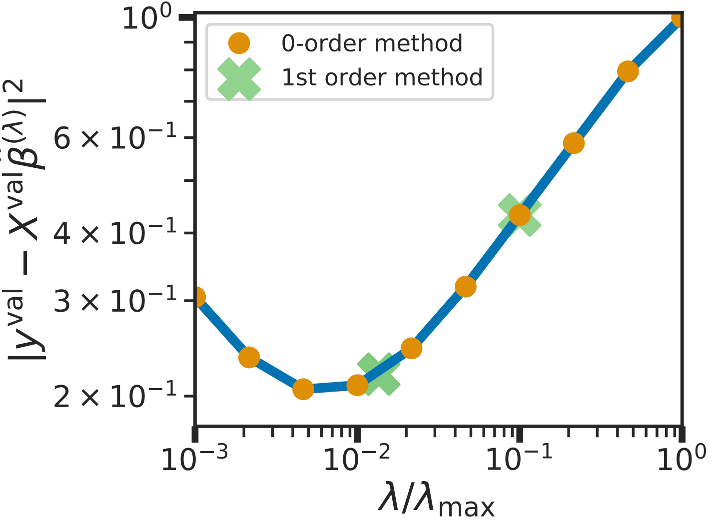

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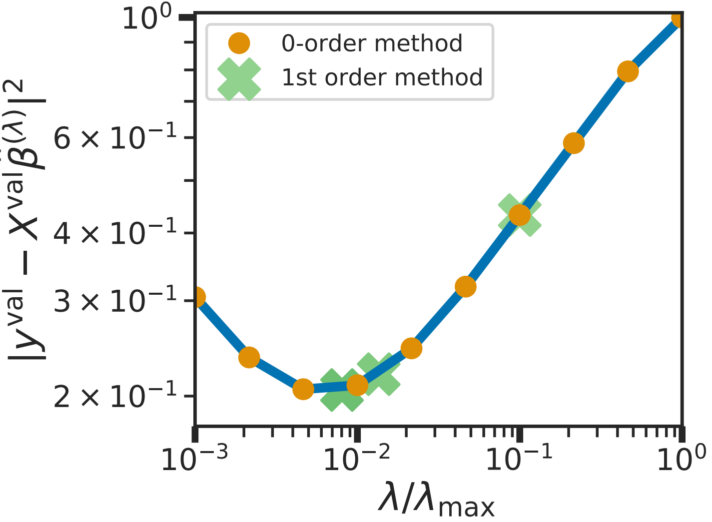

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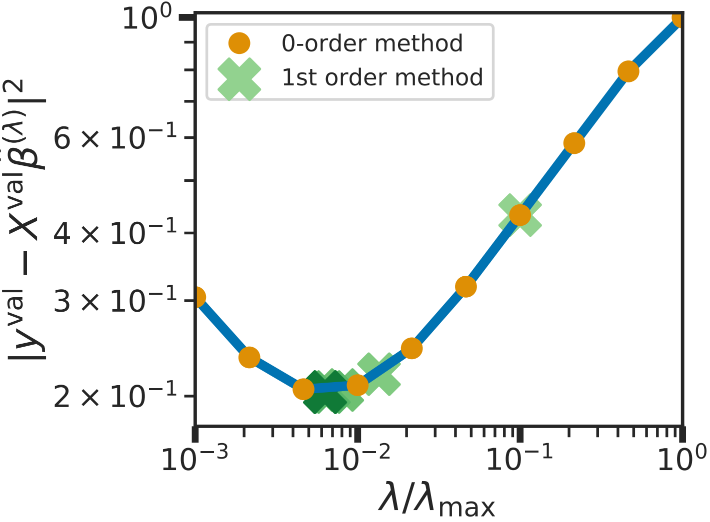

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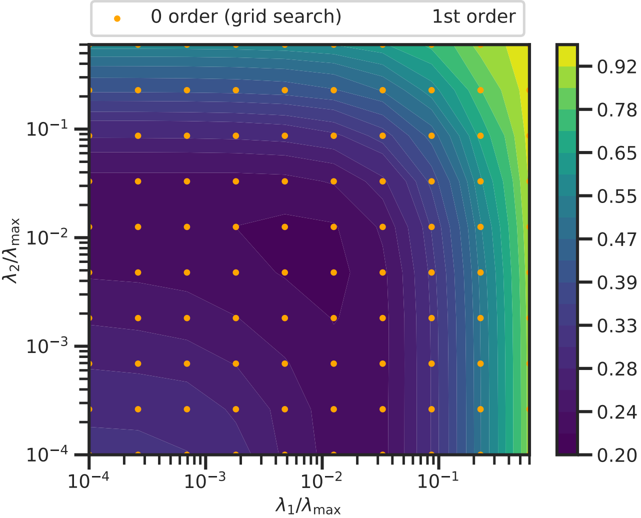
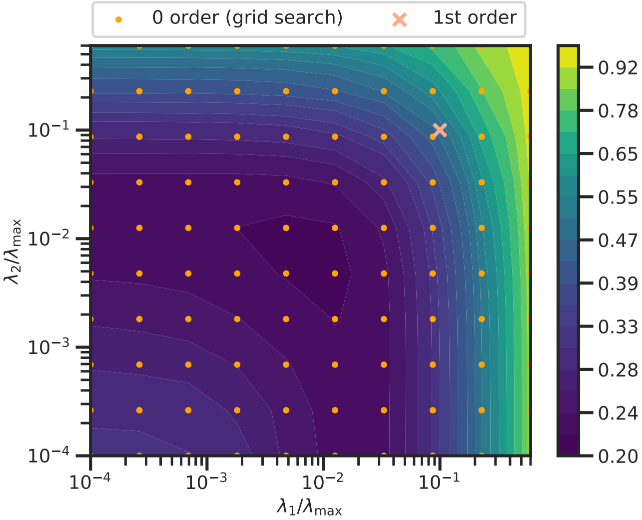
First order optimization in λ, Enet



Real-sim dataset, level sets of the validation loss (held out)

$$\arg\min_\beta \frac{1}{2n}\|y^{\text{train}} - X^{\text{train}}\beta\|^2 + \lambda_1\|\beta\|_1 + \frac{\lambda_2}{2}\|\beta\|^2$$

First order optimization in λ, Enet



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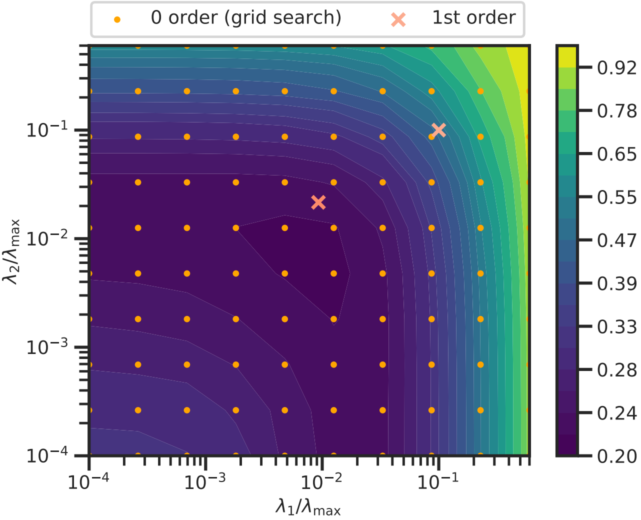

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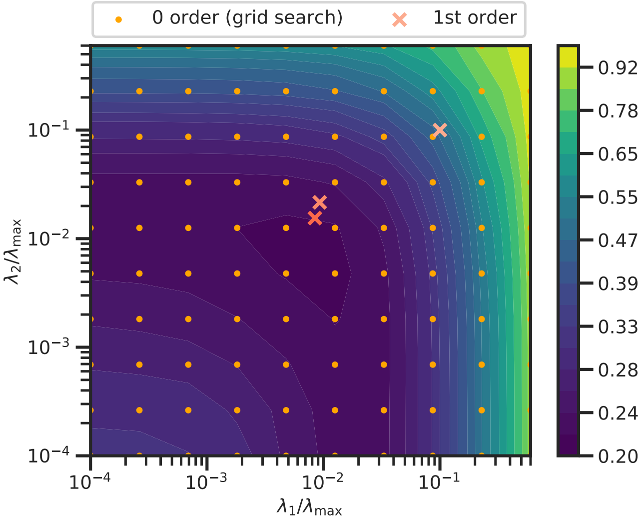

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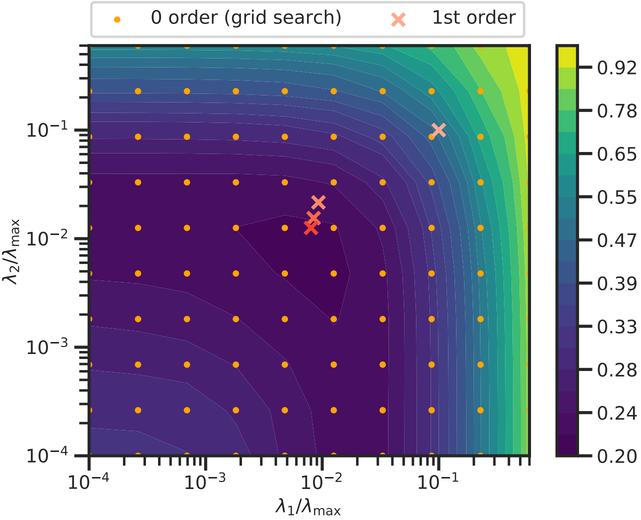

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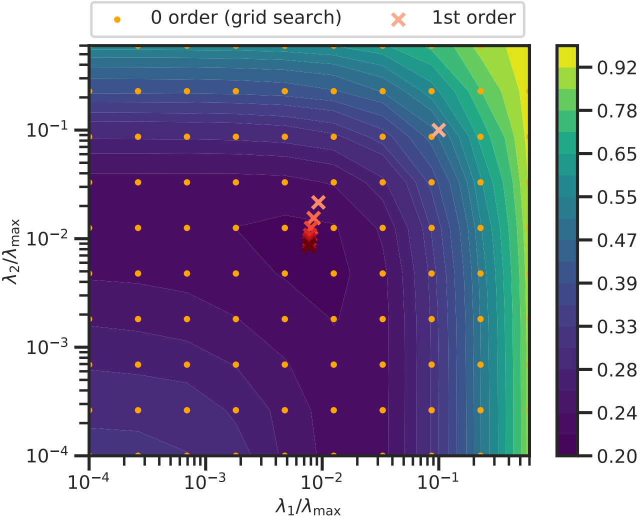

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What's hard? Computing $\nabla_\lambda \mathcal{L}(\lambda)$

$$\arg\min_{\lambda \in \mathbb{R}} \left\{ \mathcal{L}(\lambda) := C(\hat{\beta}^{(\lambda)}) := \|y^{\mathsf{val}} - X^{\mathsf{val}} \hat{\beta}^{(\lambda)}\|^2 \right\}$$
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Once $\nabla_\lambda \mathcal{L}(\lambda)$ is computed life is "easy":

- Line-search[12]
- LBFGS[13]
- Gradient descent

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How to compute $\nabla_\lambda \mathcal{L}(\lambda)$?

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Chain rule and Jacobian:

$$\nabla_\lambda \mathcal{L}(\lambda) = \underbrace{\hat{\mathcal{J}}_{(\lambda)}^\top}_{\substack{:=(\nabla_\lambda \hat\beta_1^{(\lambda)}, \dots, \nabla_\lambda \hat\beta_p^{(\lambda)}) \\ \to \text{main challenge}}} \nabla_\beta C(\hat\beta^{(\lambda)})$$

- Boils down to:

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$$\underbrace{\hat{\beta}^{(\lambda)} \in \mathop{\arg\min}_{\beta \in \mathbb{R}^p} \frac{1}{2n} \| y^{\text{train}} - X^{\text{train}} \beta \|^2 + \lambda \|\beta\|^2}_{\text{inner optimization problem}}$$

"Smooth" inner optimization problems, **well studied**:

- *Implicit differentiation* (**closed-form** formula)(14): need to solve a $p \times p$ linear system ($p = \#$features)
- *Automatic differentiation*, *forward*(15) or *backward*(16)

(14) J. Larsen et al. “Design and regularization of neural networks: the optimal use of a validation set”. In: *Neural Networks for Signal Processing VI. Proceedings of the 1996 IEEE Signal Processing Society Workshop*. 1996; Y. Bengio. “Gradient-based optimization of hyperparameters”. In: *Neural computation* 12.8 (2000), pp. 1889–1900.

(15) L. Franceschi et al. “Forward and reverse gradient-based hyperparameter optimization”. In: *ICML*. 2017, pp. 1165–1173.

(16) J. Domke. “Generic methods for optimization-based modeling”. In: *AISTATS*. vol. 22. 2012, pp. 318–326.

How to compute $\hat{\mathcal{J}}_{(\lambda)} := (\nabla_\lambda \hat{\beta}_1^{(\lambda)}, \dots, \nabla_\lambda \hat{\beta}_p^{(\lambda)})$?

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"Nonsmooth" inner optimization problems, **scarce literature**:

- *Smooth the nonsmooth term*(17)
- Use algorithms with differentiable updates(18) (19) (Bregman)

Our contributions:

- Iterative differentiation can be applied on classical proximal algorithms!
- Key point on the Jacobian: $\hat{\mathcal{J}}_{(\lambda)} := (\nabla_\lambda \hat{\beta}_1^{(\lambda)}, \dots, \nabla_\lambda \hat{\beta}_p^{(\lambda)})$ shares $\hat{\beta}^{(\lambda)}$'s **sparsity pattern**

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(17) G. Peyré and J. M. Fadili. "Learning analysis sparsity priors". In: *Sampta*. 2011.

(18) P. Ochs et al. "Bilevel optimization with nonsmooth lower level problems". In: *International Conference on Scale Space and Variational Methods in Computer Vision*. 2015, pp. 654–665.

(19) J. Frecon, S. Salzo, and M. Pontil. "Bilevel learning of the group lasso structure". In: *Advances in Neural Information Processing Systems*. 2018, pp. 8301–8311.

Iterative forward differentiation on PGD

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \overbrace{f}^{\text{smooth}}(\beta) + \lambda \overbrace{g}^{\text{non-smooth}}(\beta) \quad (1)$$

Algorithm: Proximal gradient descent (PGD)

init : $\beta = 0_p, \quad , L$

for $\text{iter} = 1, \dots,$ **do**

$z \leftarrow \beta - \frac{1}{L} \nabla f(\beta)$ `// gradient step`

$\beta \leftarrow \text{prox}_{\lambda g / L}(z)$ `// proximal step`

return β

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Algorithm: Iterative forward diff. (for PGD)

---

init : $\beta = 0_p, \quad , L$

for $\text{iter} = 1, \dots,$ **do**

$\quad z \leftarrow \beta - \frac{1}{L} \nabla f(\beta)$ `// gradient step`

$\quad dz \leftarrow \left(\mathrm{Id}_p - \frac{1}{L} \nabla^2 f(\beta)\right) \mathcal{J}$ `// diff w.r.t. λ: chain rule`

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init : $\beta = 0_p$, $\mathcal{J} = 0_p$, L

for iter $= 1, \ldots,$ **do**

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$\beta \leftarrow \mathrm{prox}_{\lambda g / L}(z)$ `// proximal step`

$\mathcal{J} \leftarrow \partial_z \, \mathrm{prox}_{\lambda g / L}(z) dz$ `// diff w.r.t. λ: chain rule`

return β, $\mathcal{J}$

Iterative forward differentiation on PGD

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \overbrace{f}^{\text{smooth}}(\beta) + \lambda \overbrace{g}^{\text{non-smooth}}(\beta) \tag{1}$$

Algorithm: Forward iterative differentiation (for PGD)

init : $\beta = 0_p$, $\mathcal{J} = 0_p$, L

for $\text{iter} = 1, \ldots,$ **do**

- $z \leftarrow \beta - \frac{1}{L}\nabla f(\beta)$ `// gradient step`
- $dz \leftarrow \left(\mathrm{Id}_p - \frac{1}{L}\nabla^2 f(\beta)\right)\mathcal{J}$ `// diff w.r.t. λ: chain rule`
- $\beta \leftarrow \mathrm{prox}_{\lambda g/L}(z)$ `// proximal step`
- $\mathcal{J} \leftarrow \partial_z \, \mathrm{prox}_{\lambda g/L}(z) dz$ `// diff w.r.t. λ: chain rule`
  $\quad + \partial_\lambda \, \mathrm{prox}_{\lambda g/L}(z)$ `// do not forget this term!`

return β, $\mathcal{J}$

Forward iterative differentiation on BCD

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \| y^{\mathsf{train}} - X^{\mathsf{train}} \beta \|^2 + \lambda \|\beta\|_1 \tag{2}$$

- Iterative forward can generalize to **coordinate descent** (BCD, state of art algorithm for the Lasso)
- **Convergence** of the Jacobian sequence $\mathcal{J}$?

Forward iterative differentiation on BCD

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} \| y^{\text{train}} - X^{\text{train}} \beta \|^2 + \lambda \|\beta\|_1 \tag{2}$$

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Contribution

- Prove Jacobian sequence convergence

Forward iterative differentiation on BCD

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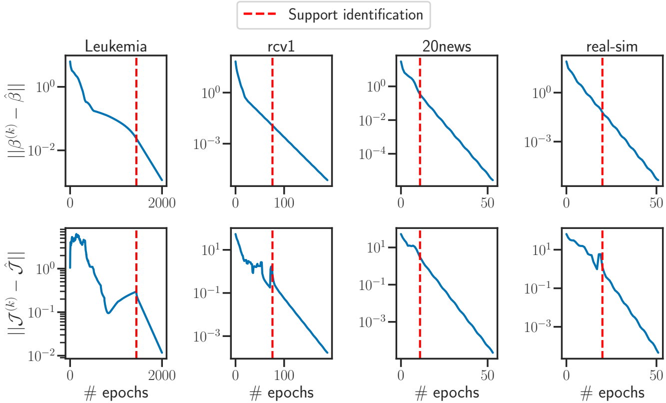
Contribution

- Prove Jacobian sequence convergence

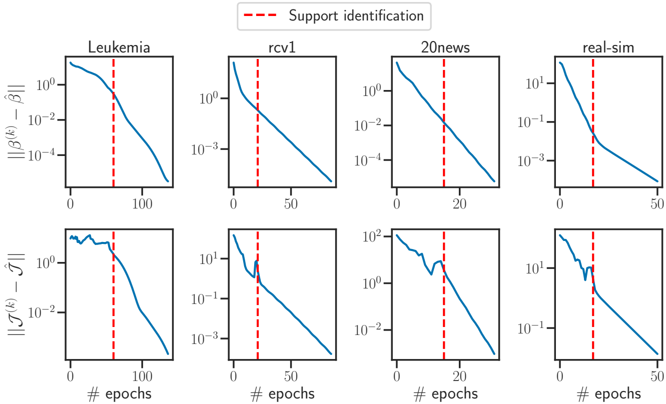
Local linear convergence of the Jacobian (I)

Proposition: forward diff. convergence (Lasso)

Assuming that the Lasso inner optimization has a unique minimizer, then the Jacobian sequence based on forward diff. of BCD converges to the true Jacobian. Once the support (*i.e.*, non-zeros coefs.) has been identified, convergence is linear.



Local linear convergence of the Jacobian (II)



Exemple: sparse logistic regression

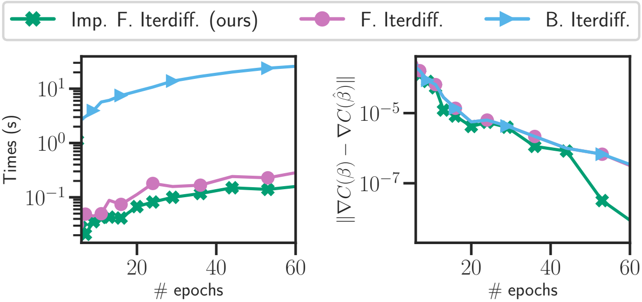
$$\arg\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_i \frac{1}{1 + \exp(-y_i X_{i,:} \beta)} + \lambda \|\beta\|_1$$

Proposed algorithm: Implicit forward diff.

- Jacobian $\hat{\mathcal{J}}^{(\lambda)}$ shares $\hat{\beta}^{(\lambda)}$ sparsity pattern
- Leverage sparsity to **speed up computation**

2-step algorithm:

1. Solve the inner Lasso problem to get $\hat{\beta}^{(\lambda)}$ and its support $\hat{S}^{(\lambda)}$
2. Compute Jacobian only on the support $\hat{S}^{(\lambda)}$ using the forward iterations of coordinate descent



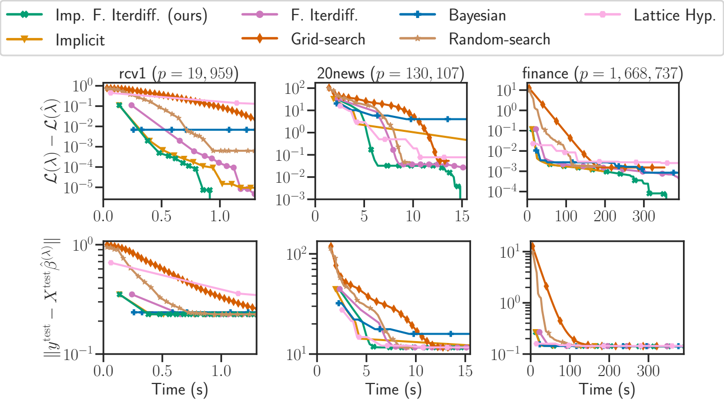
Convergence on synthetic data

Experiments I - Real datasets

- **Outer criterion:** held-out loss. **Inner problems:** the Lasso

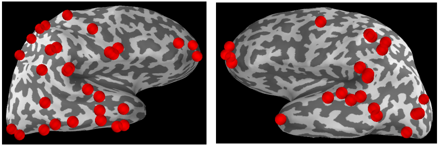
$$\arg\min_{\lambda \in \mathbb{R}} \mathcal{L}(\lambda) := ||y^{\text{val}} - X^{\text{val}} \hat{\beta}^{(\lambda)}||^2$$

$$\text{s.t } \hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2n} ||y^{\text{train}} - X^{\text{train}} \beta||_2^2 + \lambda ||\beta||_1$$



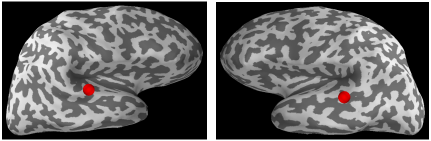
Experiments III - Real MEEG data

- **Outer criterion:** SURE
- **Inner problems:** the Lasso and weighted Lasso



Vanilla Lasso (1 parameter)

$$\underset{\beta \in \mathbb{R}^p}{\arg\min} \frac{1}{2n} ||y - X\beta||_2^2 + \lambda \|\beta\|_1$$



Weighted Lasso (p parameters)

$$\underset{\beta \in \mathbb{R}^p}{\arg\min} \frac{1}{2n} ||y - X\beta||_2^2 + \sum_{j=1}^{p} \lambda_j |\beta_j|$$

Limitations

- May require specific parametrization e^λ
- Need a **differentiable criterion**: cannot use 0/1-loss
- Need a **continuous estimator** *w.r.t.* data and hyperparameters: does not apply yet to **non-convex** penalties[20] nor reweighted Lasso[21]
- Optimized function often **non-convex**: possibly multiple local minima
- Rely on **line-search**: hidden hyperparameters control the convergence speed

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(20) P. Breheny and J. Huang. "Coordinate descent algorithms for nonconvex penalized regression, with applications to biological feature selection". In: *Ann. Appl. Stat.* 5.1 (2011), p. 232.

(21) E. 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.

Conclusion

Hyperparameter optimization cast as a **bilevel optimization problem**, on which we applied 1st order optimization:

- Proved **locally linear convergence** of the Jacobian
- **Leverage sparsity** to speed up Jacobian computation

Future work:

- Extension to other **sparse models** (group Lasso, sparse multiclass logistic regression)
- Extend work on **inexact gradient** to non-smooth inner pb

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- Paper https://proceedings.icml.cc/paper/2020/file/e0ab531ec312161511493b002f9be2ee-Paper.pdf
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