Implicit differentiation for fast hyperparameter selection in non-smooth convex learning

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https://QB3.github.io

Joint work with:
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Motivation

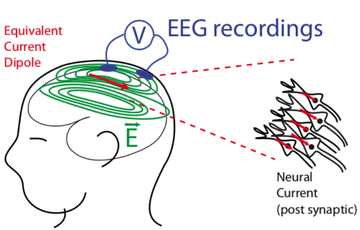
Hyperparameter optimization

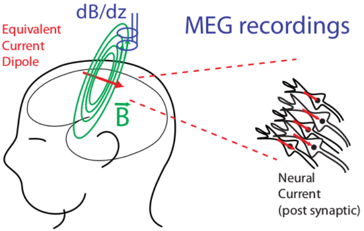
Hypergradient computation

Experiments

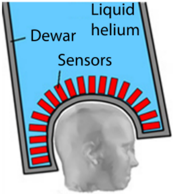
M/EEG inverse problem for brain imaging

- 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



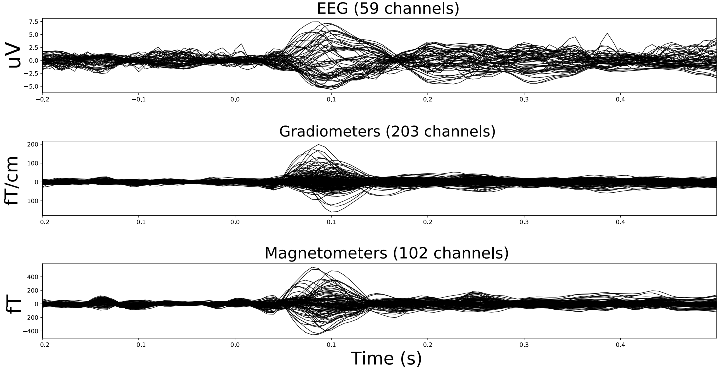


First EEG
recordings
in 1929
by H. Berger



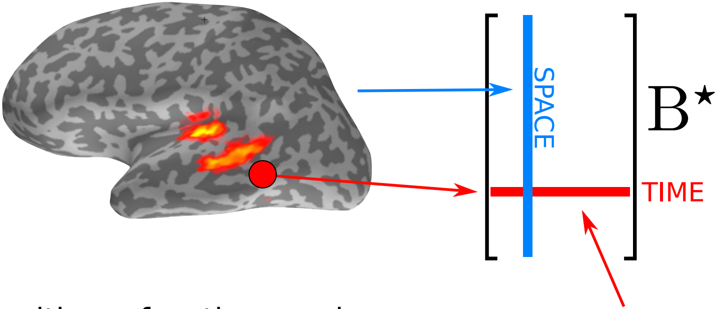
Hôpital La Timone
Marseille, France

M/EEG data

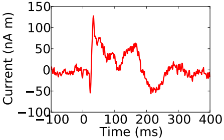


- 3 different types of sensor

Source modeling (discretization with voxels)

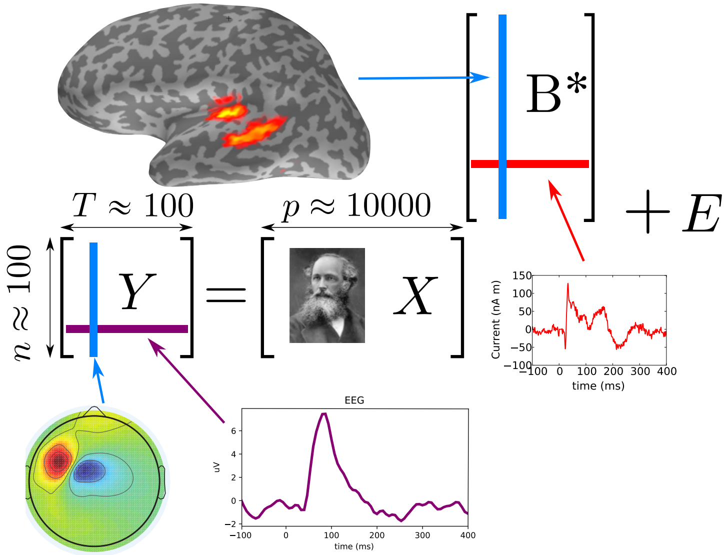


Position a few thousands candidate sources over the brain (*e.g.*, every 5mm)



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

The M/EEG inverse problem: modeling

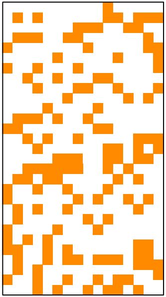


$$n \ll p$$

Multi-Task penalties[1]

Popular convex penalties considered:

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



Sparse support: no structure

Penalty: **Lasso type**

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

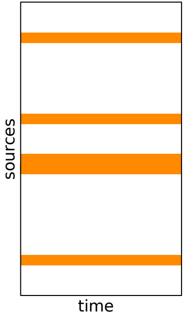
Parameter $\hat{\mathrm{B}} \in \mathbb{R}^{p \times T}$

[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)

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



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

Sparse support: 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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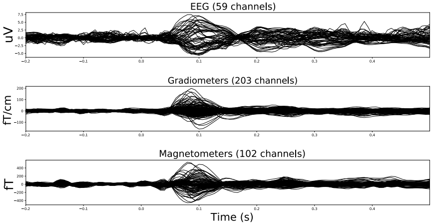
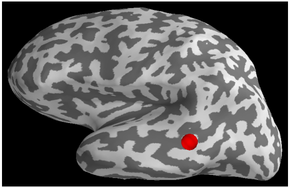
Summary



What you have: Y



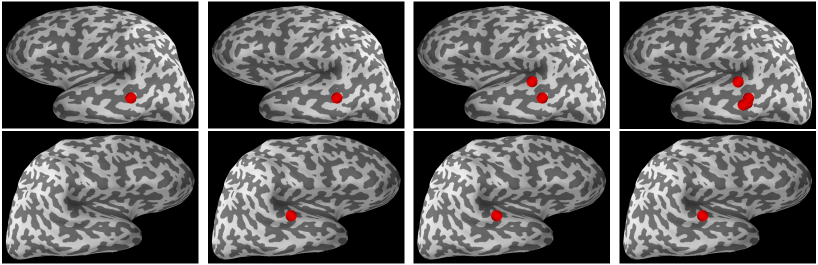
What you want B

This is typically done using optimization based estimators:

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

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, $y = X\beta + \sigma^* \varepsilon$)

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

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 unknown 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)

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

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λ does not depend on σ_* anymore!

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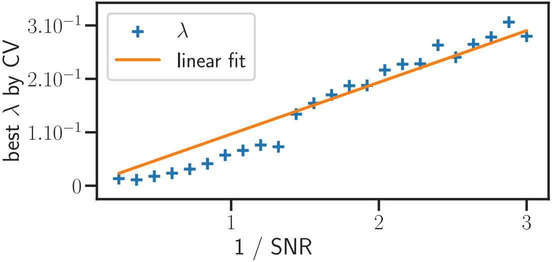
Which λ to pick? A statistical persective III

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



Lasso

Which λ to pick? A statistical persective III

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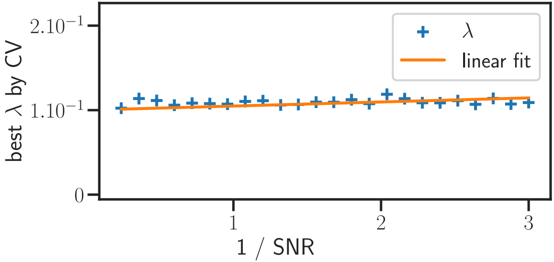

Square-root Lasso

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

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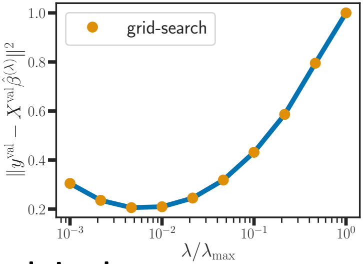

Real-sim dataset

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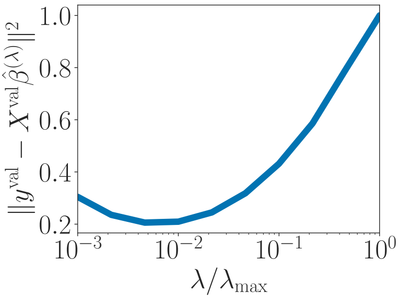
HO as a bilevel optimization problem(7)(8)

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

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



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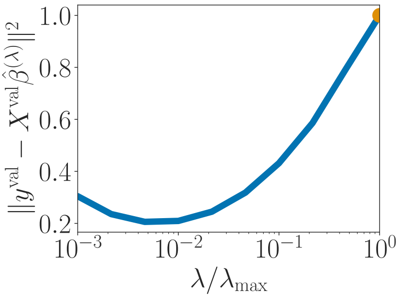

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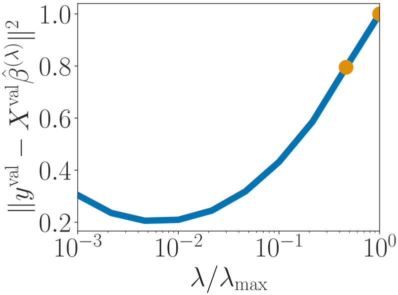

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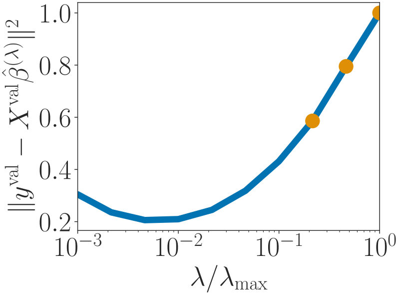

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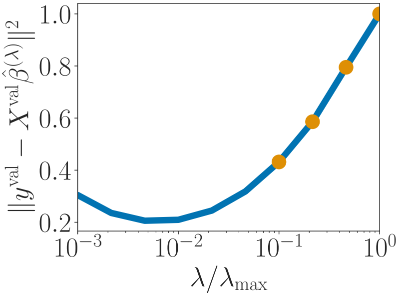

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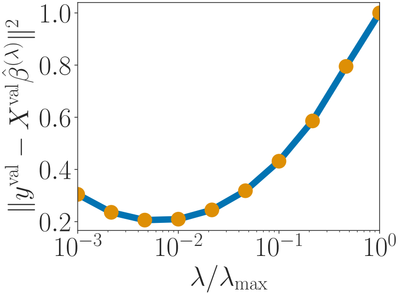

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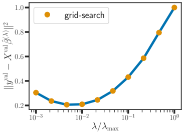
Grid-search as a 0-order optimization method



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

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- 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]:
$$\lambda^{(t+1)} = \lambda^{(t)} - \rho \nabla_\lambda \mathcal{L}(\lambda^{(t)}) \quad \text{with suitable } \rho > 0$$

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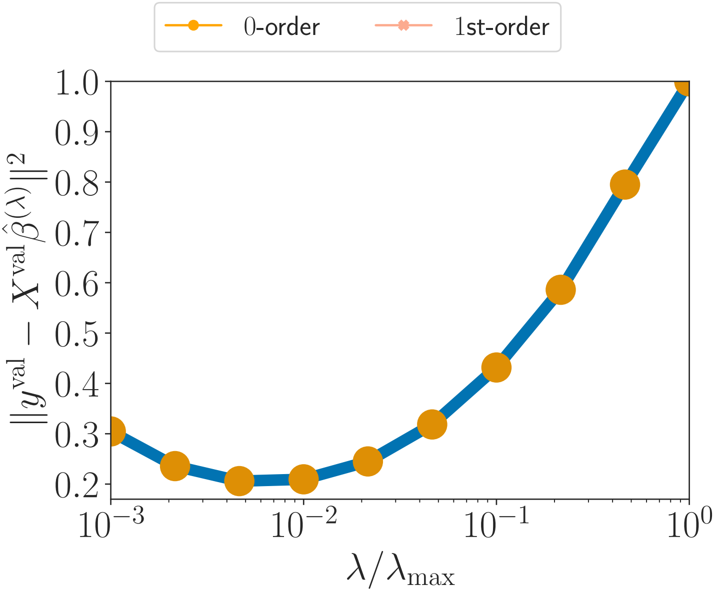
[9] J. Bergstra and Y. Bengio. "Random search for hyper-parameter optimization". In: *Journal of Machine Learning Research* 13.2 (2012).

[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).

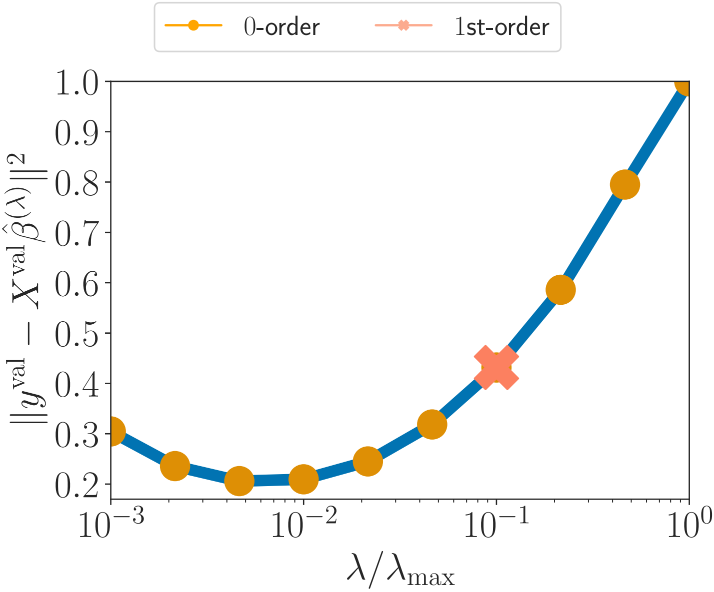
[11] F. Pedregosa. "Hyperparameter optimization with approximate gradient". In: *ICML*. vol. 48. 2016, pp. 737–746.

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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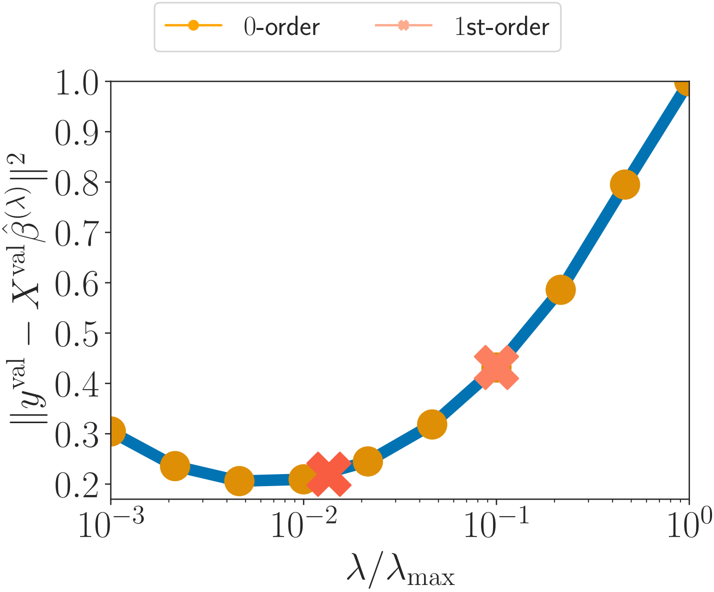

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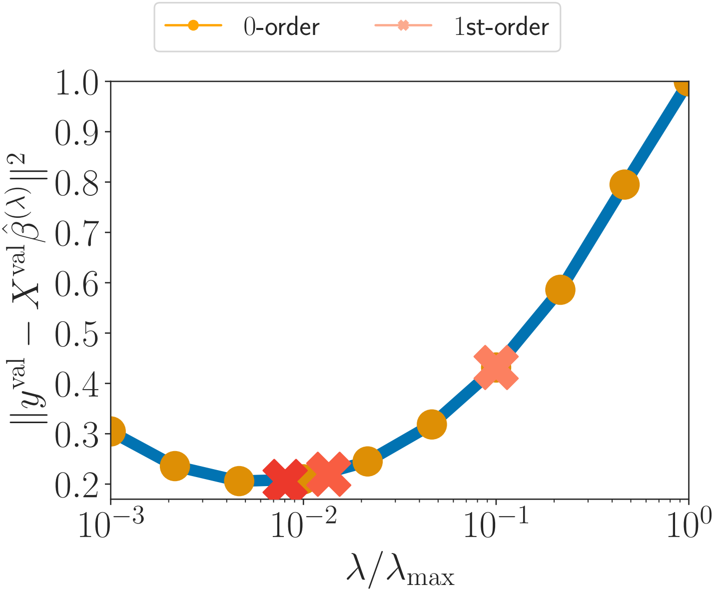

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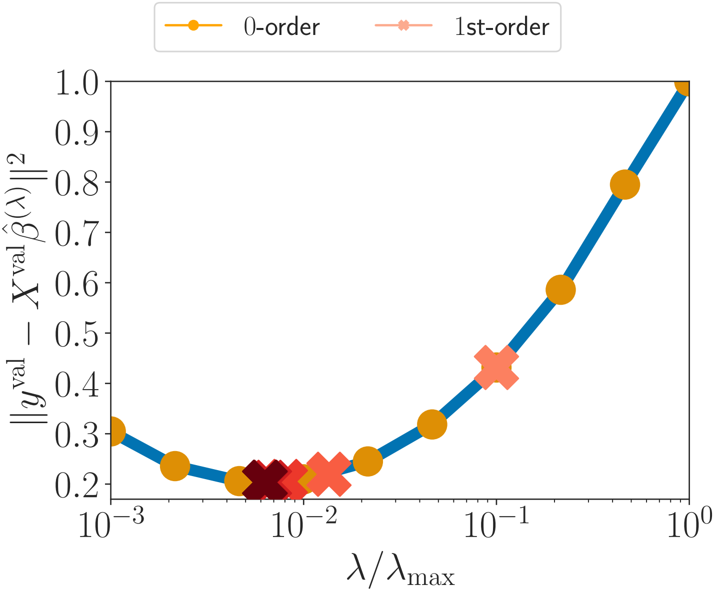

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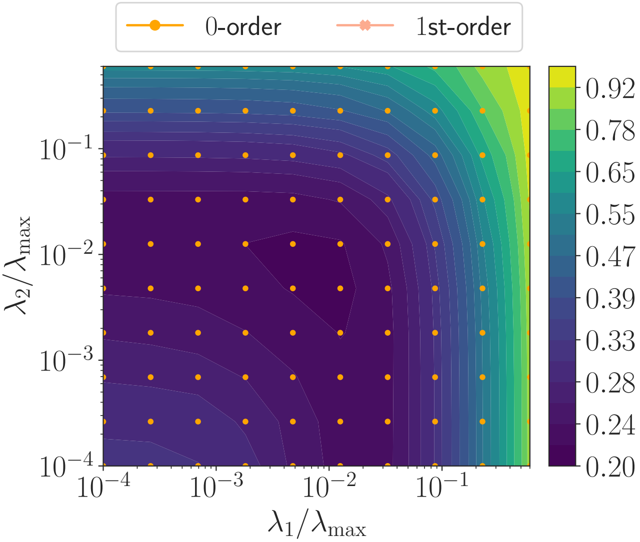
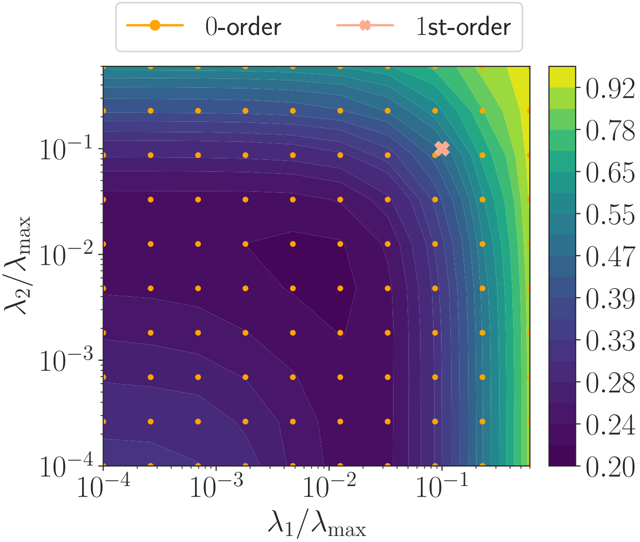
First-order optimization in λ, Enet



Real-sim dataset, level sets of the validation loss (hold-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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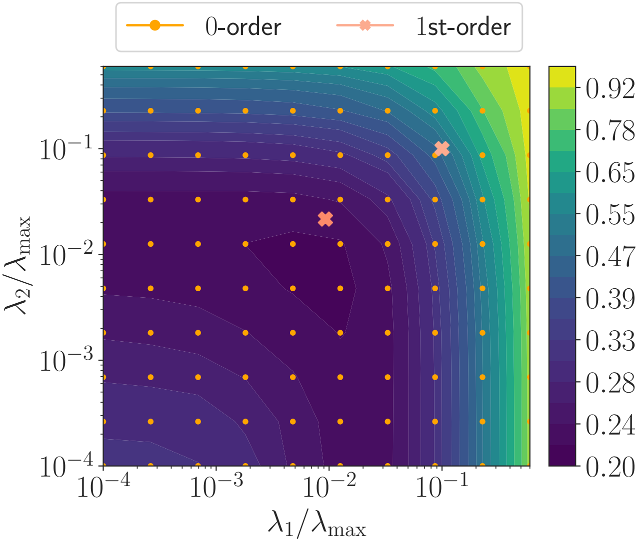
First-order optimization in λ, Enet



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

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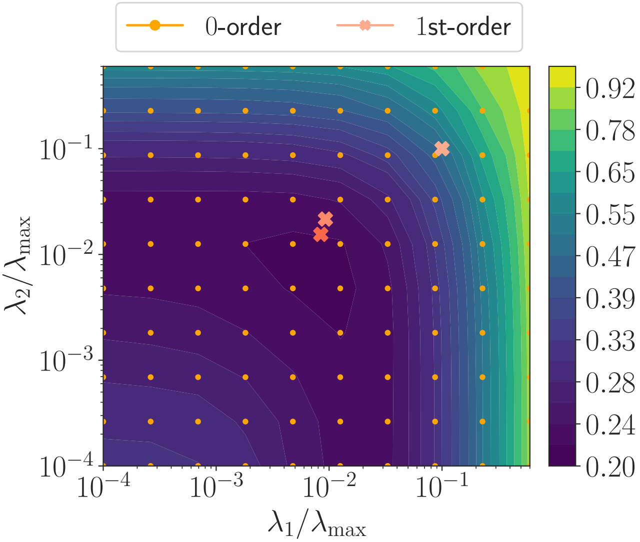

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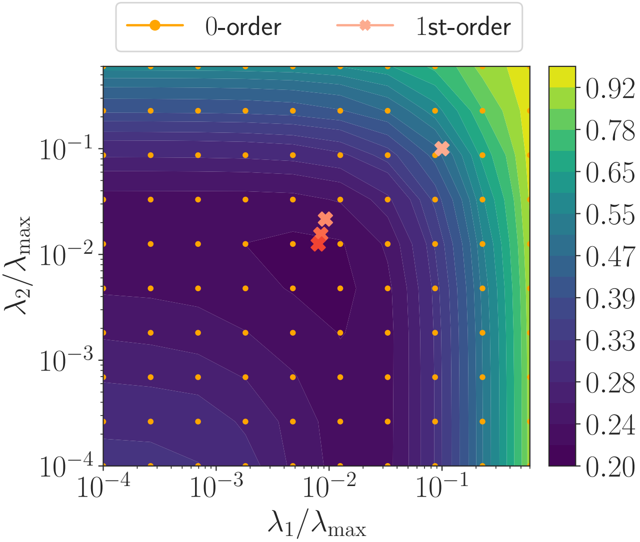

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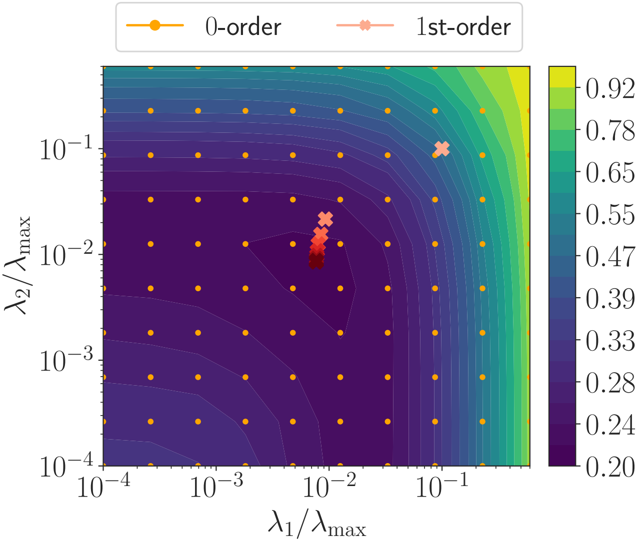

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What's hard? Computing $\nabla_\lambda \mathcal{L}(\lambda)$

$$\operatorname*{arg\,min}_{\lambda \in \mathbb{R}} \left\{ \mathcal{L}(\lambda) := C(\hat\beta^{(\lambda)}) := \| y^{\mathsf{val}} - X^{\mathsf{val}} \hat\beta^{(\lambda)} \|^2 \right\}$$

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Once $\nabla_\lambda \mathcal{L}(\lambda)$ is computed, let's pretend "life is easy":

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

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Chain rule and Jacobian:

$$\nabla_\lambda \mathcal{L}(\lambda) = \underbrace{\hat{\mathcal{J}}_{(\lambda)}^\top}_{\substack{:=(\nabla_\lambda \hat{\beta}_1^{(\lambda)}, \dots, \nabla_\lambda \hat{\beta}_p^{(\lambda)}) \\ \to \text{main challenge}}} \nabla_\beta C(\hat{\beta}^{(\lambda)})$$

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"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 *reverse*[16] mode

(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.

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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 proximal algorithms
- $\hat{\mathcal{J}}_{(\lambda)} := (\nabla_\lambda \hat{\beta}_1^{(\lambda)}, \dots, \nabla_\lambda \hat{\beta}_p^{(\lambda)})^\top$ shares $\hat{\beta}^{(\lambda)}$'s **sparsity pattern**

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

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Forward-mode differentiation of PGD

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

Algorithm: Proximal gradient descent PGD

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

for $\text{iter} = 1, \ldots,$ **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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  $\quad + \partial_\lambda \, \mathrm{prox}_{\lambda g/L}(z)$ `// do not forget this term!`

return β, $\mathcal{J}$

Forward-mode differentiation of PCD

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

- Forward-mode differentiation can be applied on **proximal coordinate descent** (PCD)
- **Convergence** of the Jacobian sequence $\mathcal{J}$?

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Contribution

- Proved Jacobian sequence convergence for PGD and PCD

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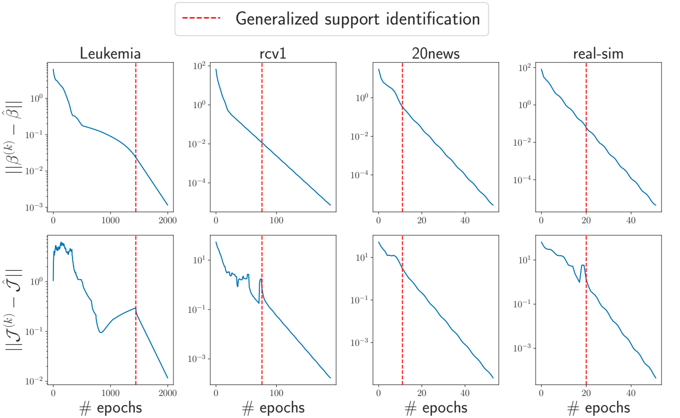
- Proved Jacobian sequence convergence for PGD and PCD

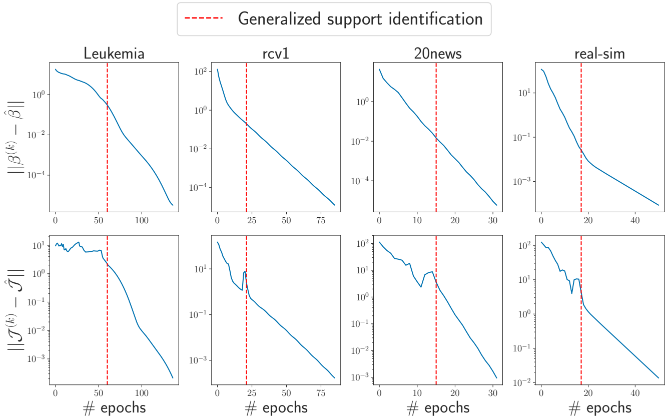
Local linear convergence of the Jacobian (I)

Proposition: forward diff. convergence (Lasso)

Assuming that the Lasso inner optimization has a unique minimizer, then the Jacobian sequence based on forward diff. of PCD 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)



Example: sparse logistic regression

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

Implicit differentiation (smooth ψ)

$$\hat{\beta}^{(\lambda)} \in \underset{\beta \in \mathbb{R}^p}{\arg\min}\, \psi(\beta, \lambda)$$

$$\nabla_\beta \psi\left(\hat{\beta}^{(\lambda)}, \lambda\right) = 0$$

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- Need to solve a linear **system of size** p

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Implicit differentiation ($f + \lambda \sum_j |\beta_j|$)

$$\hat{\beta}^{(\lambda)} \in \arg\min_{\beta \in \mathbb{R}^p} f(\beta) + \lambda \sum_j |\beta_j|$$

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$$+ \partial_\lambda \, \mathrm{ST}\left(\hat{\beta}^{(\lambda)} - \frac{1}{L}\nabla f(\hat{\beta}^{(\lambda)}), \frac{\lambda}{L}\right)$$

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Key observation, if $\hat{\beta}_j^{(\lambda)} = 0$:

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With $\mathcal{S} = \left\{j \in [p] \,:\, \hat\beta_j^{(\lambda)} = 0\right\}$ we have $\hat{\mathcal{J}}_{\mathcal{S}^c} = 0$

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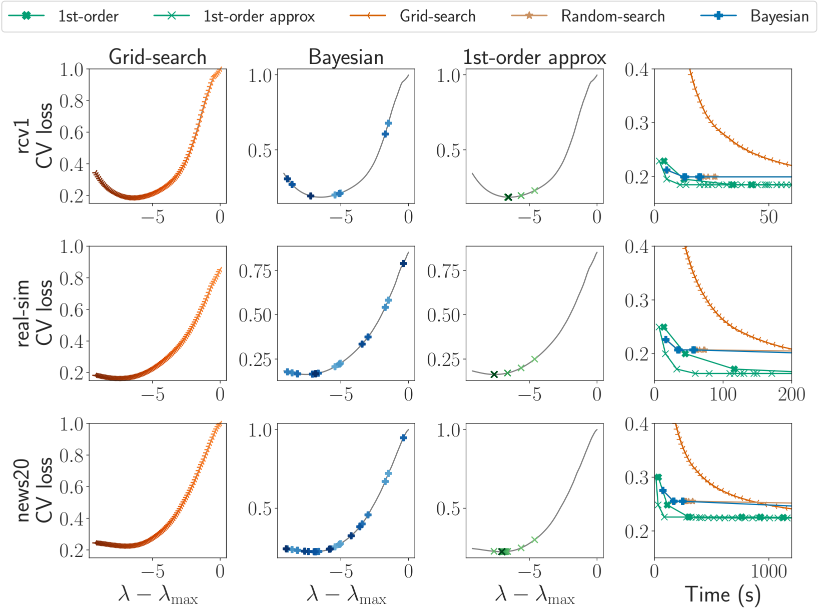
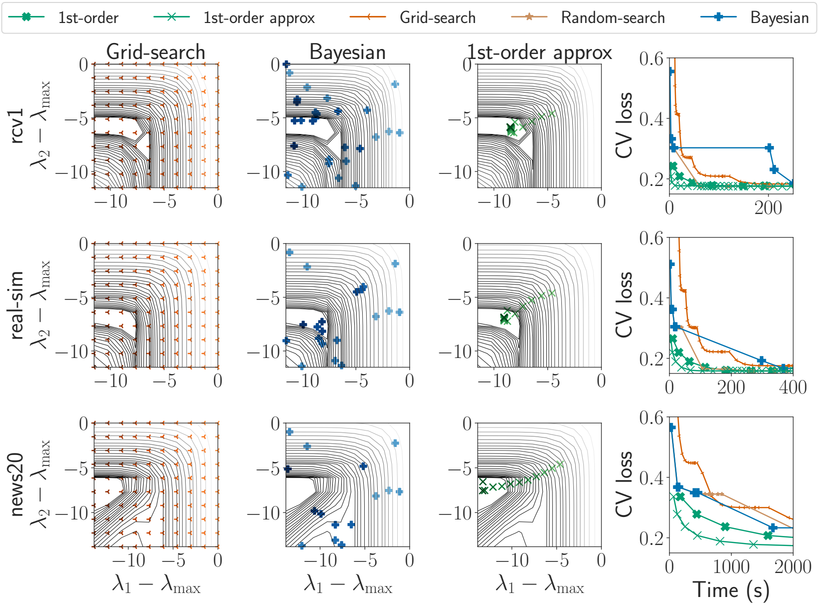
Experiments I - Lasso cross-validation

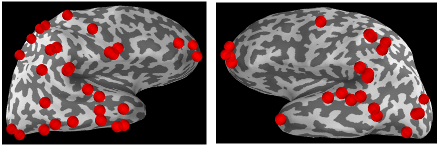


Experiments II - Enet cross-validation



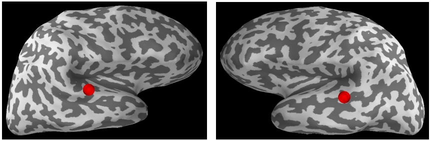
Experiments III - Real MEEG data

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



Vanilla Lasso (1 parameter)

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



Weighted Lasso (p parameters)

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

Limitations

- 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
- Potentially slow and handy **outer solver**

[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

Contributions:

- 1st-order optimization with nonsmooth inner problem
- **Local linear convergence** of the Jacobian
- **Leverage sparsity** to speed up hypergradient computation

Future work:

- Convergence of the bilevel procedure
- Smarter outer solver

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References:

- Paper `https://proceedings.icml.cc/paper/2020/file/e0ab531ec312161511493b002f9be2ee-Paper.pdf`
- Open source package `https://github.com/QB3/sparse-ho`

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