Bi-level optimization in Machine Learning

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PARIETAL

Inria informatics mathematics

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$\Rightarrow$ The 1 000 000€ question: How to select λ, f, X_{tr}, ...?

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$\Rightarrow$ This is a bi-level optimization problem.

Bi-level problem: Optimization problem with two levels

$$\min_{x} h(\lambda) = F(\lambda, \theta^*(x))$$

$$s.t. \quad \theta^*(\lambda) = \operatorname*{argmin}_{\theta} G(\lambda, \theta)$$

Outer function

Value function

Inner function/Problem

Goal: Optimize the value function h whose value depends on the result of another optimization problem.

$\Rightarrow$ Challenging to theoretically and practically.

Other bi-level optimization problems: Model selection

Selecting the best model: G is the training loss and θ are the parameters of the model. The goal is to optimize λ to get the best validation loss F,

- *Hyperparameter optimization:* λ are the regularisation parameters, or the number of trees, ...

  [Pedregosa 2016, Lorraine et al. 2020]

- *Automatic Data Augmentation:* λ are the parameters of data augmentation used to train the model.

  [Cubuk et al. 2019; Rommel et al. 2022]

- *Neural Architecture Search:* λ are the parameter of a Neural Network architecture.

  [Liu et al. 2018, Zhang et al. 2021]

Other bi-level optimization problems: Representation Learning

Generative Adversarial Network: G is the discriminator loss, that classify between generated and natural samples. Then $F = -G$ and one aims to solve [Goodfellow et al. 2014]

$$\max_{\lambda} G(\lambda, \theta^*) \quad s.t. \quad \theta^* = \min_{\theta} G(\lambda, \theta)$$

Here θ are the parameter of the discriminator and λ of the generator.

Dictionary Learning: $F = G$ are the reconstruction loss and one looks for the dictionary D that minimizes [Malezieux et al. 2022]

$$\min_{D} \|X - D\theta^*\| \quad s.t. \quad \theta^* = \operatorname*{argmin}_{\theta} \|X - D\theta\| + \lambda\|\theta\|_1$$

Here, θ^* is a sparse representation of the input sample X.

Other bi-level optimization problems: Implicit Deep Learning

Deep Equilibrium Network: G is a fixed point equation that defines the output of a layer and F is the training loss of the network, [Bai et al. 2019]

$$\max_{\lambda} F(\lambda, \theta^*) \quad s.t. \quad G(\lambda, \theta) = \theta - g(\theta, \lambda) = 0$$

These networks micmic infinite depth network as θ^* can be seen as applying the transfer function g infinitly many times if it is contractive.

Black box methods: Take $\{\lambda_k\}_k$ and compute $\min_k h(\lambda_k)$

- Grid-Search
- Random-Search
- Bayesian-Optimization

Solving bi-level optimization

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First order methods: Compute the gradient of h

$$\lambda^{t+1} = \lambda^t - \rho^t \underbrace{\frac{\partial F(\lambda, \theta^*(\lambda))}{\partial \lambda}}_{\nabla h(\lambda)}$$

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- Can we compute the gradient of h?
- Do we need to compute $\theta^*(\lambda)$?
- How to efficiently approximate $\nabla h(\lambda)$?

Implicit Gradient

Computing the gradient of the value function h

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Value Function's Gradient

First order methods on h needs to compute the gradient of h.

Chain rule:

$$\nabla_\lambda h(\lambda) = \frac{\partial F}{\partial \lambda}(\lambda, \theta^*(\lambda)) + \frac{\partial F}{\partial \theta}(\lambda, \theta^*(\lambda)) \frac{\partial \theta^*}{\partial \lambda}(\lambda)$$

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$\Rightarrow$ Need to compute $\theta^*(\lambda)$ and an inverse hvp.

Do we need to compute them precisely?

Idea: Approximate $\theta^*(\lambda^t)$ and $v^*(\lambda^t) = -\frac{\partial^2 G}{\partial \theta^2}^{-1} \frac{\partial F}{\partial \theta}(\lambda^t, \theta^*(\lambda^t))$

HOAG - Approximating $\theta^*(\lambda^t)$ [Pedregosa 2016]

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- Compute θ^t such that $\|\theta^t - \theta^*(\lambda^t)\|_2 \leq \epsilon_t$,
  iterative solver *e.g.* L-BFGS
- Compute v^t such that $\|\frac{\partial^2 G}{\partial \theta^2}(\lambda^t, \theta^t)v^t + \frac{\partial F}{\partial \theta}(\lambda^t, \theta^t)\|_2 \leq \epsilon_t$,
  L-BFGS or CG
- Compute the approximate gradient $g_t = \frac{\partial F}{\partial \lambda}(\lambda^t, \theta^t) + \frac{\partial^2 G}{\partial \theta \partial \lambda}(\lambda^t, \theta^t)v^t$
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Theorem: If $\sum_t \epsilon_t < \infty$ and the step are chosen appropriatly, then the algorithm converges to a stationary point *i.e.*

$$\|\nabla h(\lambda^t)\|_2 \to 0 \ .$$

Further approximation of the Inverse Hvp

Solving the linear system for $v^*(\lambda^t)$,

- Core idea is to not inverse the hessian $\frac{\partial^2 G}{\partial \theta^2}(\lambda^t, \theta^t)$,

  We are only interested in one direction.

- Only rely on Hessian-vector product (Hvp).

  Can be computed efficiently

Proposed Methods:

- L-BFGS
- Conjugate Gradient
- Jacobian-Free method

$$\frac{\partial^2 G}{\partial \theta^2}(\lambda^t, \theta^t) \approx Id$$

- Neumann iterations

$$\frac{\partial^2 G}{\partial \theta^2}(\lambda^t, \theta^t)^{-1} \approx \sum_k (Id - \frac{\partial^2 G}{\partial \theta^2}(\lambda^t, \theta^t))^k$$

[Pedregosa 2016, Lorraine et al. 2020, Luketina et al. 2016]

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Newton Method

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$$x^{t+1} = x^t - B_t^{-1}\frac{\partial f}{\partial x}(x^t)$$

B_n: low-rank approx. of the Hessian.

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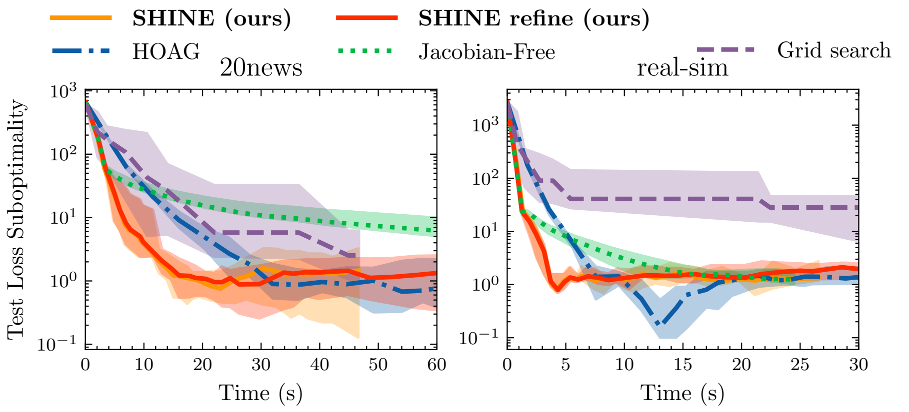
$\Rightarrow$ Use B_n^{-1} as the inverse of the Hessian for v^*

Logistic Regression with ℓ_2-regularisation on 2 datasets:



$\Rightarrow$ Theoretically grounded, can be further refined, large scale experiments on DEQs.

Algorithm Unrolling

Differentiable inner problem solvers

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- Malézieux, B., Moreau, T., and Kowalski, M. (2022). Understanding approximate and Unrolled Dictionary Learning for Pattern Recovery. In *International Conference on Learning Representations (ICLR)*, online

Differentiable unrolling of θ^t

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For the gradient descent algorithm:

$$\theta^{t+1} = \theta^t - \rho \frac{\partial G}{\partial \theta}(\lambda, \theta^t)$$

The Jacobian reads,

$$\frac{\partial \theta^{t+1}}{\partial \lambda}(\lambda) = \left(Id - \rho \frac{\partial^2 G}{\partial \theta^2}(\lambda, \theta^t) \right) \frac{\partial \theta^t}{\partial \lambda}(\lambda) - \rho \frac{\partial^2 G}{\partial \theta \partial \lambda}(\lambda, \theta^t)$$

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$\Rightarrow$ Under smoothness conditions, if θ^t converges to θ^*, this converges toward $\frac{\partial \theta^*}{\partial \lambda}(\lambda)$

Context: min-min problems where $F = G$

$$\Rightarrow \text{Here, } \frac{\partial F}{\partial \theta}(\lambda, \theta^*) = 0$$

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We consider the 3 gradient estimates:

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- $g_2 = \frac{\partial G}{\partial \lambda}(\lambda, \theta^t) + \frac{\partial G}{\partial \theta}(\lambda, \theta^t)\frac{\partial \theta^t}{\partial \lambda}$ — Automatic
- $g_3 = \frac{\partial G}{\partial \lambda}(\lambda, \theta^t) - \frac{\partial G}{\partial \theta}(\lambda, \theta^t)\frac{\partial^2 G}{\partial \theta^2}^{-1}(\lambda, \theta^t)\frac{\partial^2 G}{\partial \theta \partial \lambda}(\lambda, \theta^t)$ — Implicit

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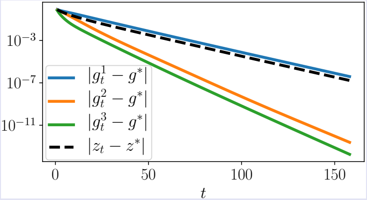
Convergence rates: For G strongly convex in θ,

$$|g_t^1(x) - g^*(x)| = O\left(|\theta^t(\lambda) - \theta^*(\lambda)|\right),$$
$$|g_t^2(x) - g^*(x)| = o\left(|\theta^t(\lambda) - \theta^*(\lambda)|\right),$$
$$|g_t^3(x) - g^*(x)| = O\left(|\theta^t(\lambda) - \theta^*(\lambda)|^2\right).$$



Analysis for non-smooth min-min problems [Malezieux et al. 2022]

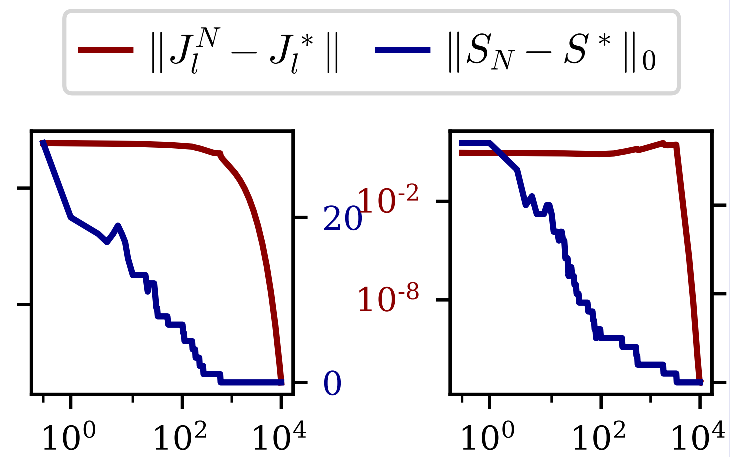
Context: dictionary learning, $F = G$ with an ℓ_1-regularization for θ.

Issue: The implicit gradient quality mostly depends on the support identifiaction,

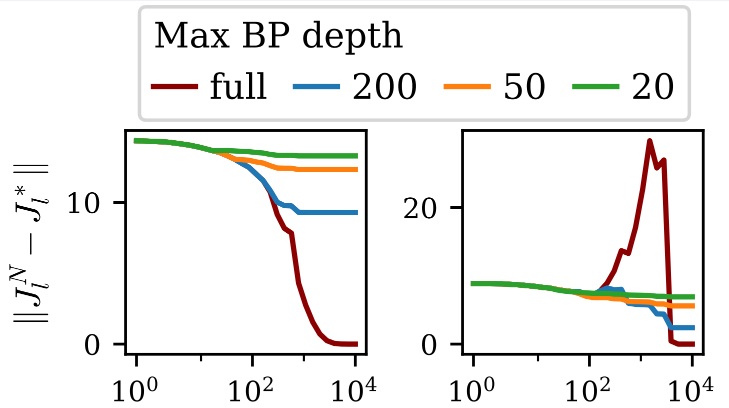
$$\left(\frac{\partial \theta^*}{\partial D_l}\right)_{S^*} = -(D_{:,S^*}^\top D_{:,S^*})^{-1}(D_l \theta^{*\top} + (D_l^\top \theta^* - y_l) Id_n)_{S^*} \ ,$$

$\Rightarrow$ Is the autodiff approach better than the analytic one?

On the support, the function is smooth and we recover the same convergence.



Outside of the support, errors can accumulate and the gradient can blow up.



Conclusion

- Bi-level optimization is intrinsic in many ML problems.
- Classical optimization method can be used once we know how to compute the gradient.
- The gradient can be computed either using implicit function theorem or algorithm unrolling.
- No clear winner, this depends on the problem at end!

Current work:

- Efficient and stochastic bi-level solvers,
- Application of bi-level solvers to Data-Augmentation problems for EEG.

$\Rightarrow$ Stay tuned!

Slides will be on my web page:

tommoral.github.io @tomamoral

Thanks to all my bi-level collaborators!