Contributions to stochastic bilevel optimization

Mathieu DAGRÉOU

Under the supervision of Pierre Ablin, Thomas Moreau and Samuel Vaiter

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	Peter Ochs	*Saarland University*
	Émilie Chouzenoux	*Inria Saclay*
	Julien Mairal	*Inria Grenoble*
	Édouard Pauwels	*Toulouse School of Economics*

Bilevel optimization in machine learning

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- Mathematical formalism where the problem we want to solve depends on the solution of another problem

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DARTS: DIFFERENTIABLE ARCHITECTURE SEARCH

Hanxiao Liu*	**Karen Simonyan**	**Yiming Yang**
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Bilevel Optimization to Learn Training Distributions for Language Modeling under Domain Shift

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Deep Equilibrium Models

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Meta-Learning with Implicit Gradients

Aravind Rajeswaran[*,1] **Chelsea Finn**[*,2] **Sham Kakade**[1] **Sergey Levine**[2]
[1] University of Washington Seattle [2] University of California Berkeley

Bilevel optimization

Bilevel Optimization Problem

Bilevel optimization

Bilevel Optimization Problem

$$\min_{\lambda \in \mathbb{R}^{d_\lambda}} \Phi(\lambda) \triangleq f(\lambda, \theta^*(\lambda))$$

$$\theta^*(\lambda) = \operatorname*{argmin}_{\theta \in \mathbb{R}^{d_\theta}} g(\lambda, \theta)$$

Bilevel optimization

Value function

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Bilevel optimization

Value function Outer function

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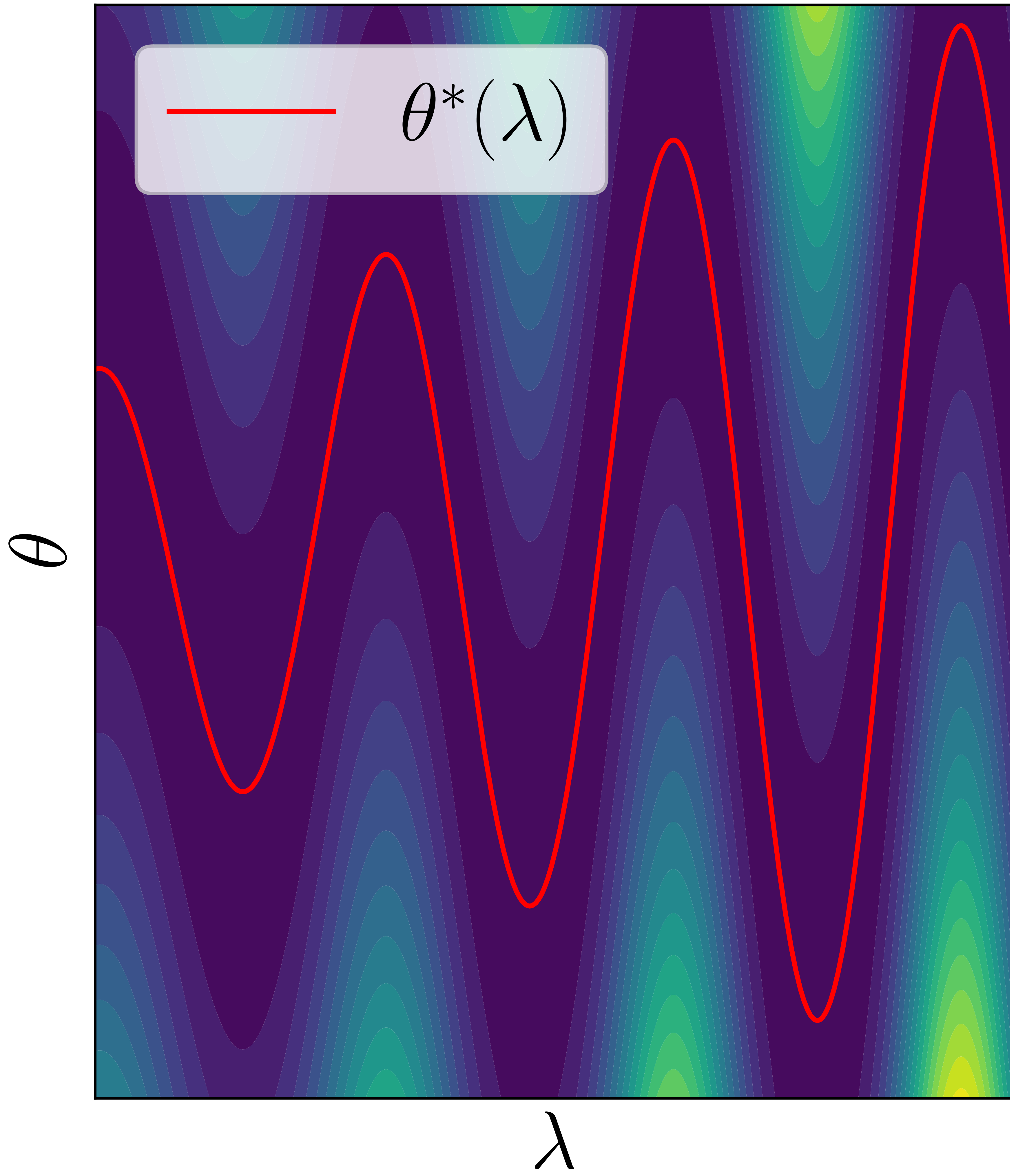
Inner function

Contour of g



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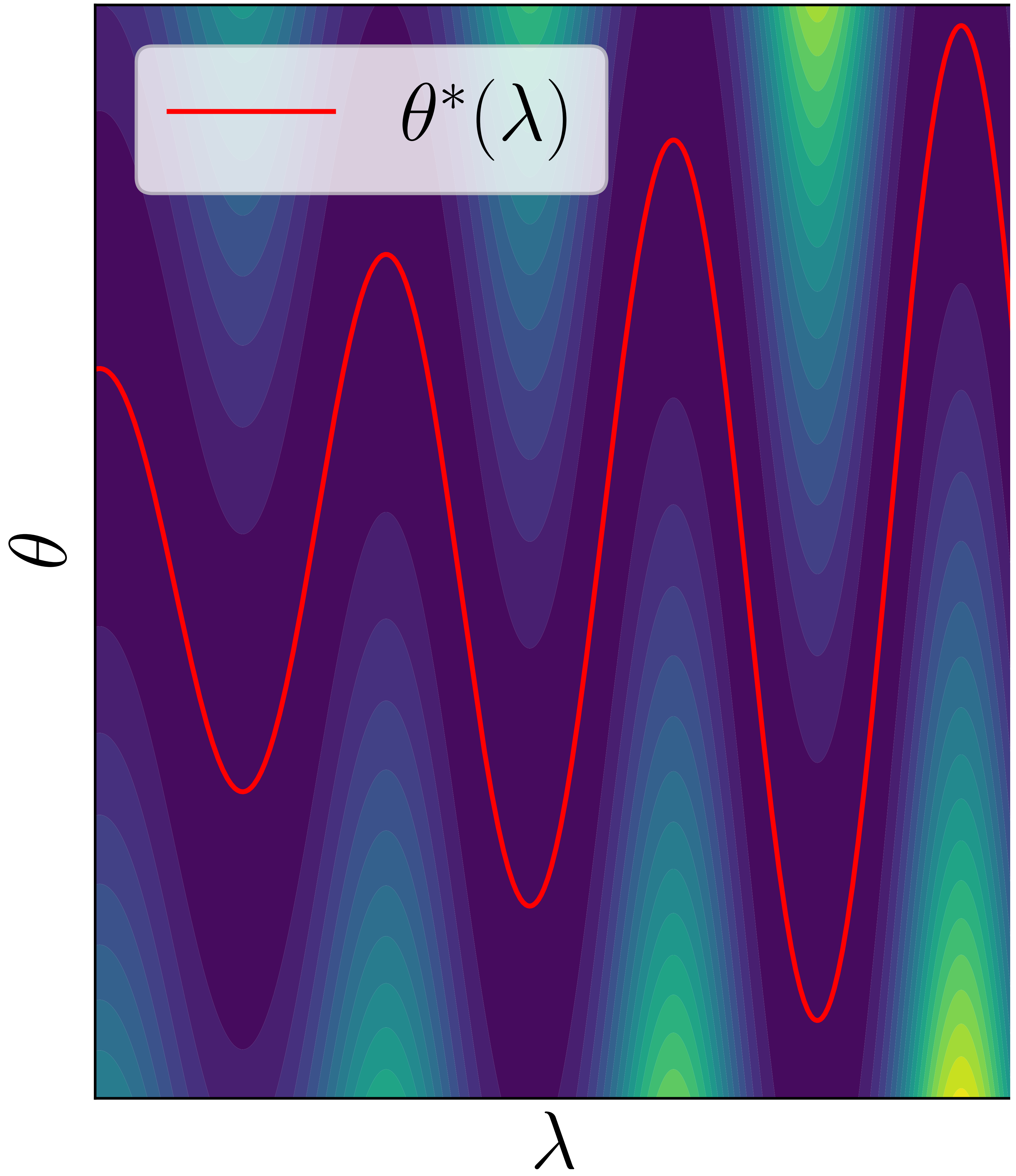
Inner variable

Inner function

Contour of g



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Value function
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Inner function
Outer variable
Inner variable

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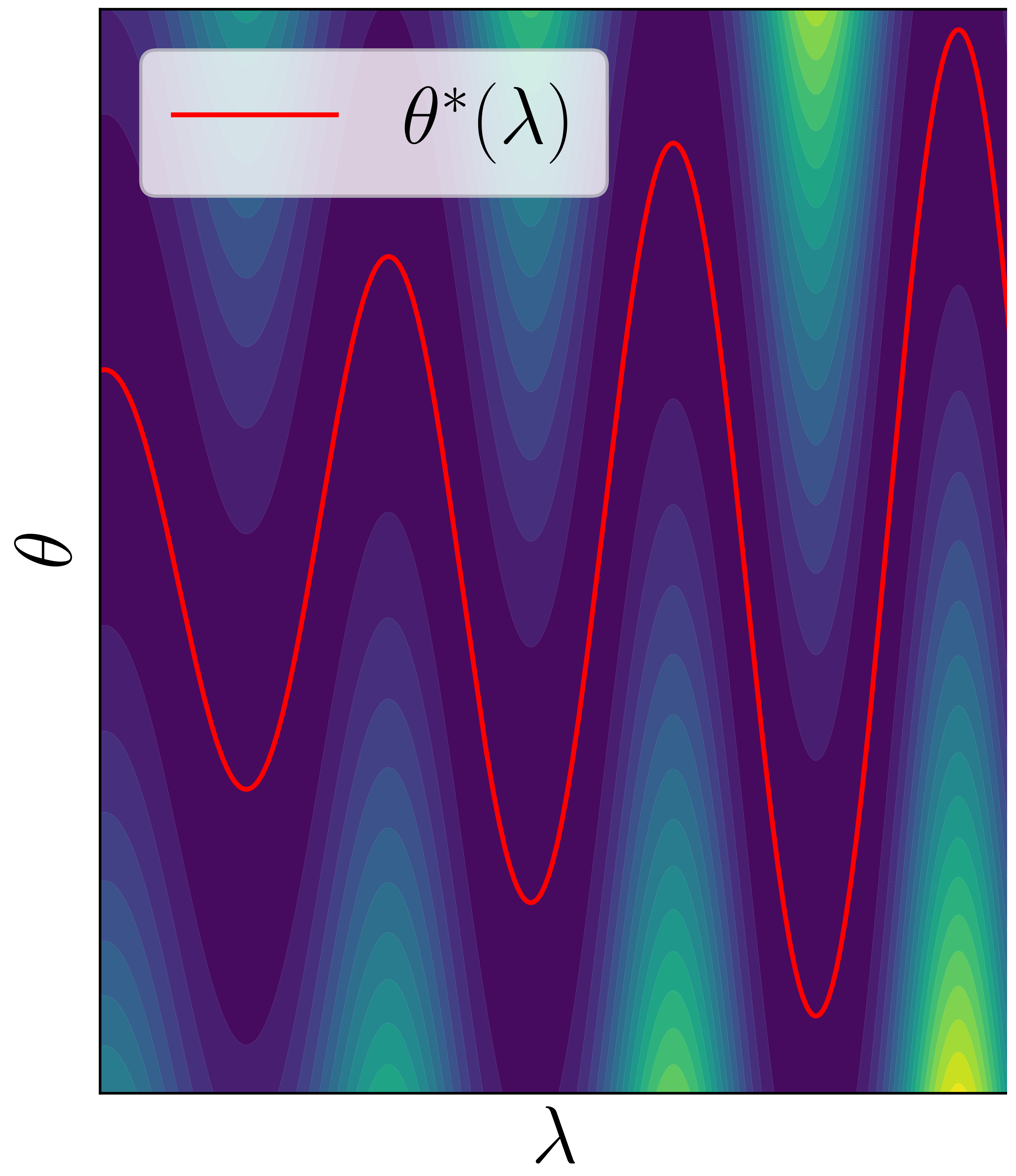

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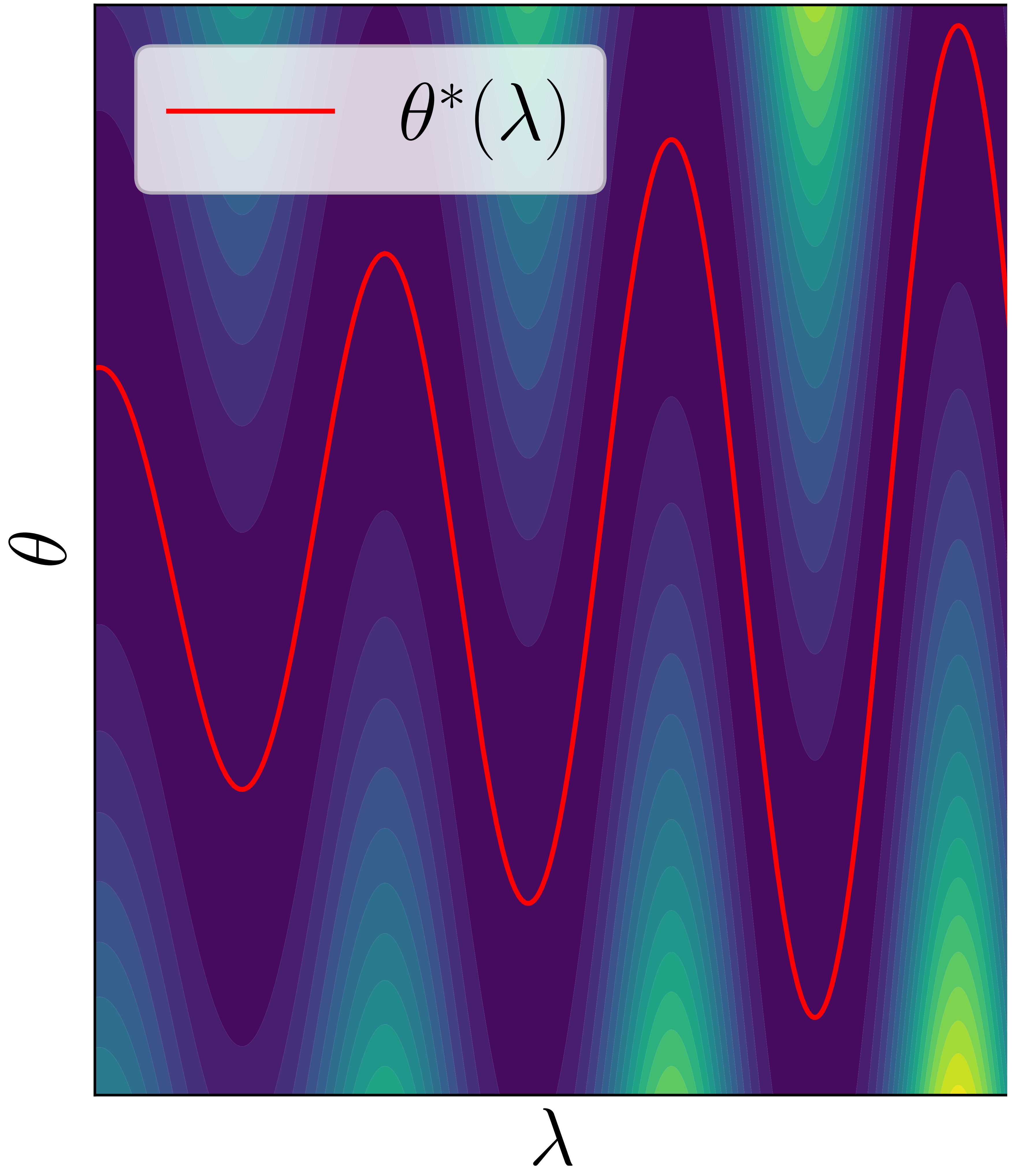
Inner variable

Inner function

Outer variable

- Generally nonconvex eventhough f and g are convex

Contour of g



Bilevel optimization

Value function Outer function

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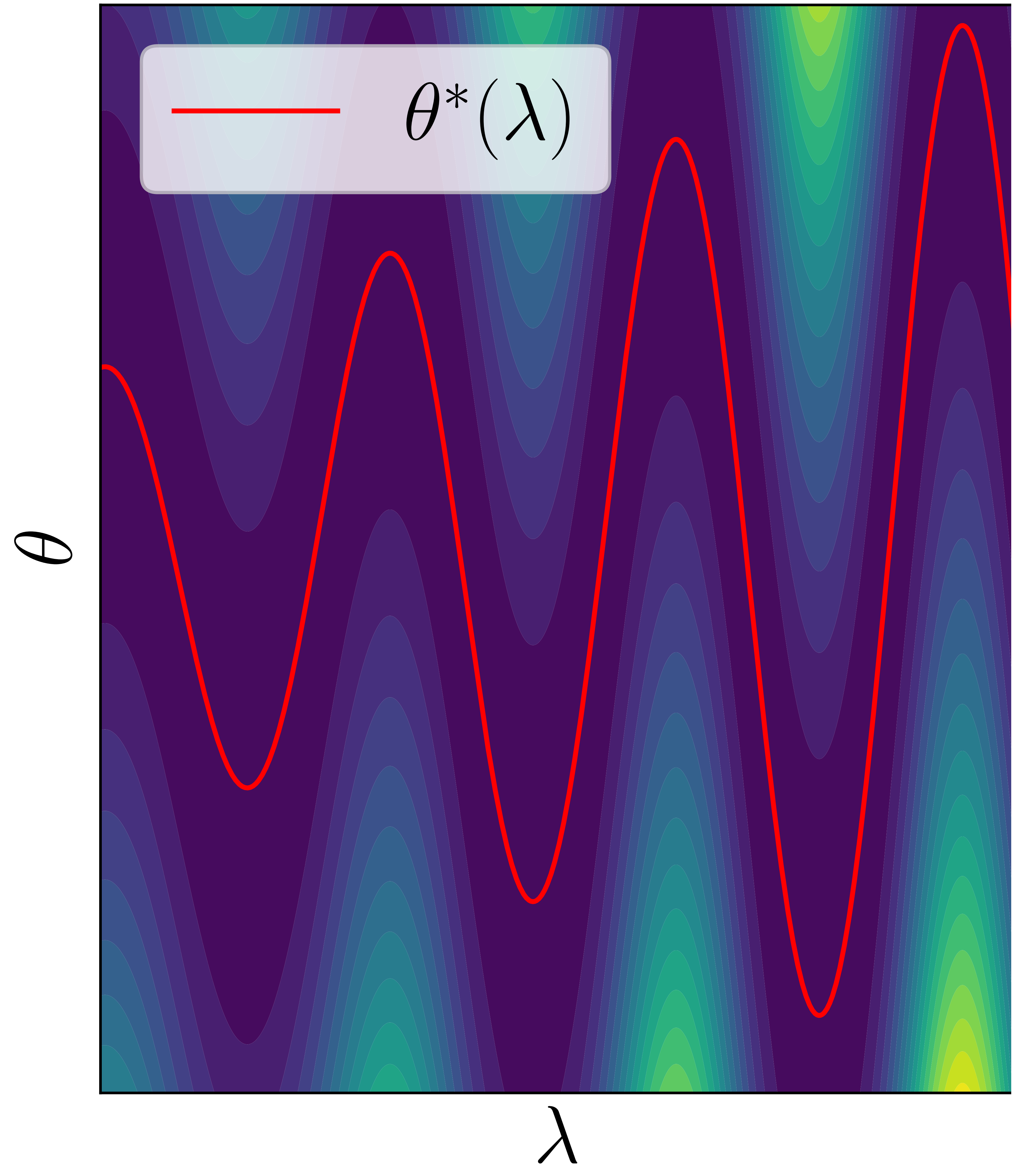
Inner function Outer variable Inner variable

- Generally nonconvex eventhough f and g are convex
- This definition assumes the uniqueness of the inner solution

Contour of g



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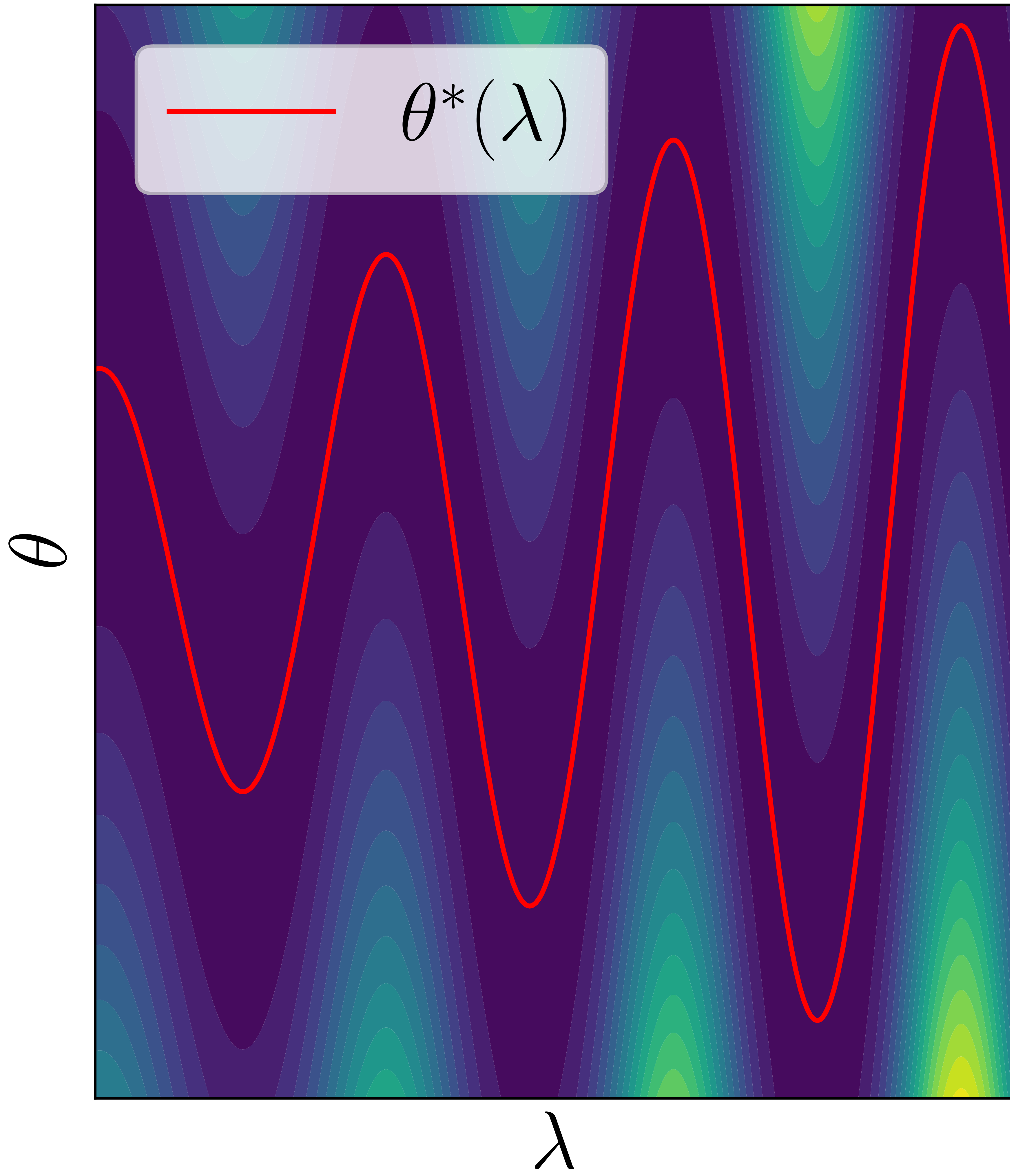
Inner variable

Inner function

Outer variable

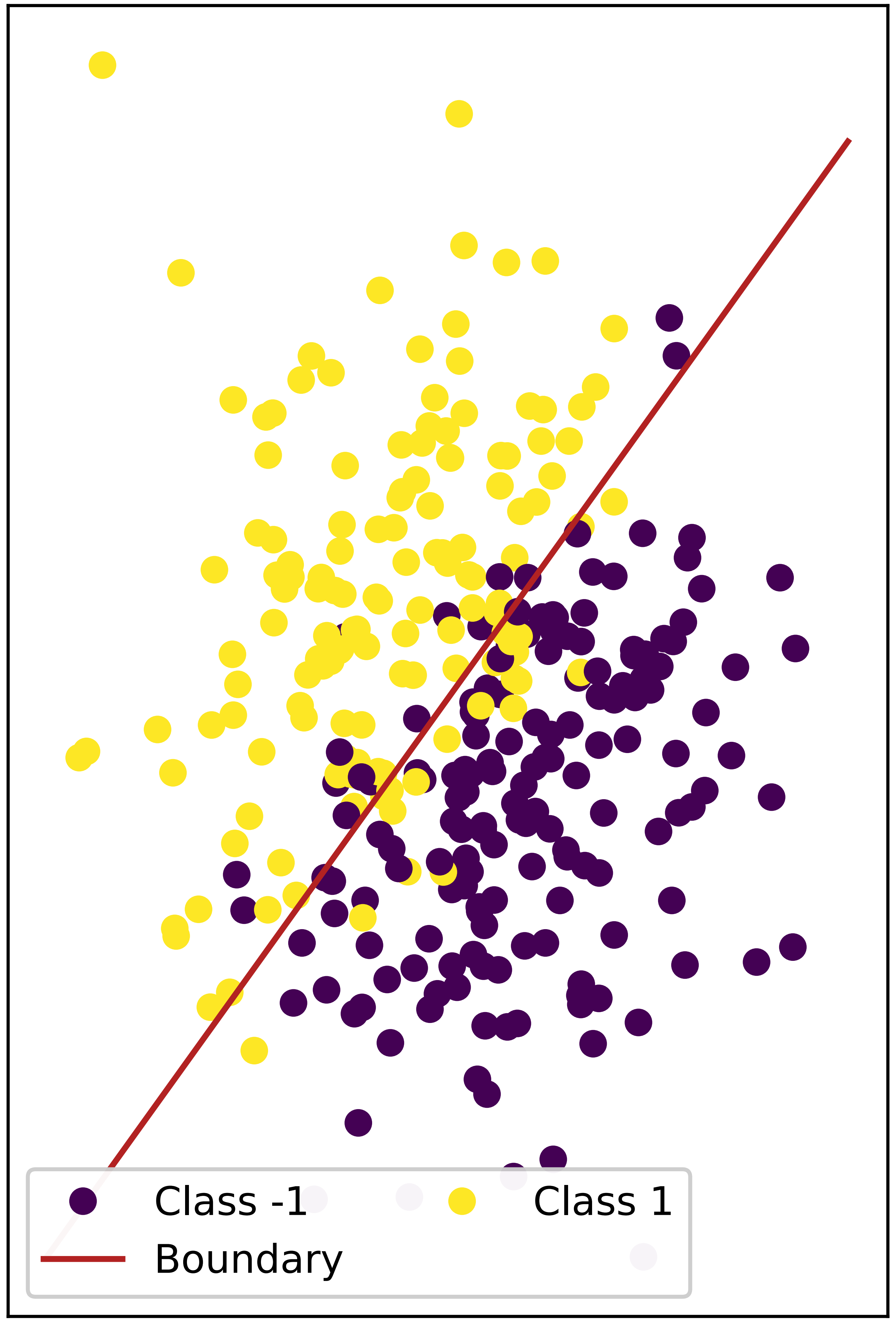
- Generally nonconvex eventhough f and g are convex
- This definition assumes the uniqueness of the inner solution
- Non-uniqueness leads to dramatically hard problems[Bolte et al. ’24]

Contour of g



Hyperparameter selection[Larsen ’96, Bennett et al. ’06]

Learning = Solving an optimization problem



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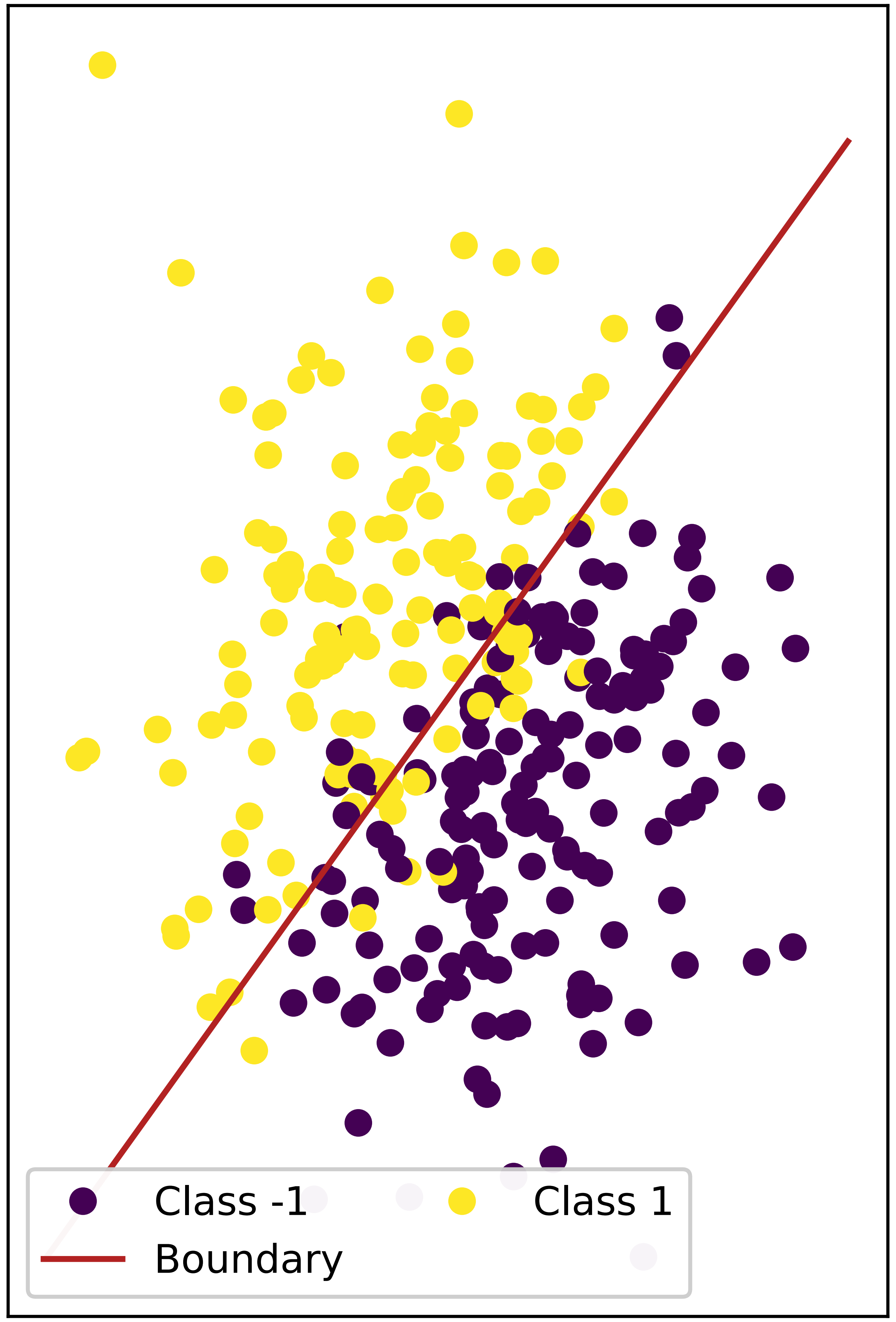

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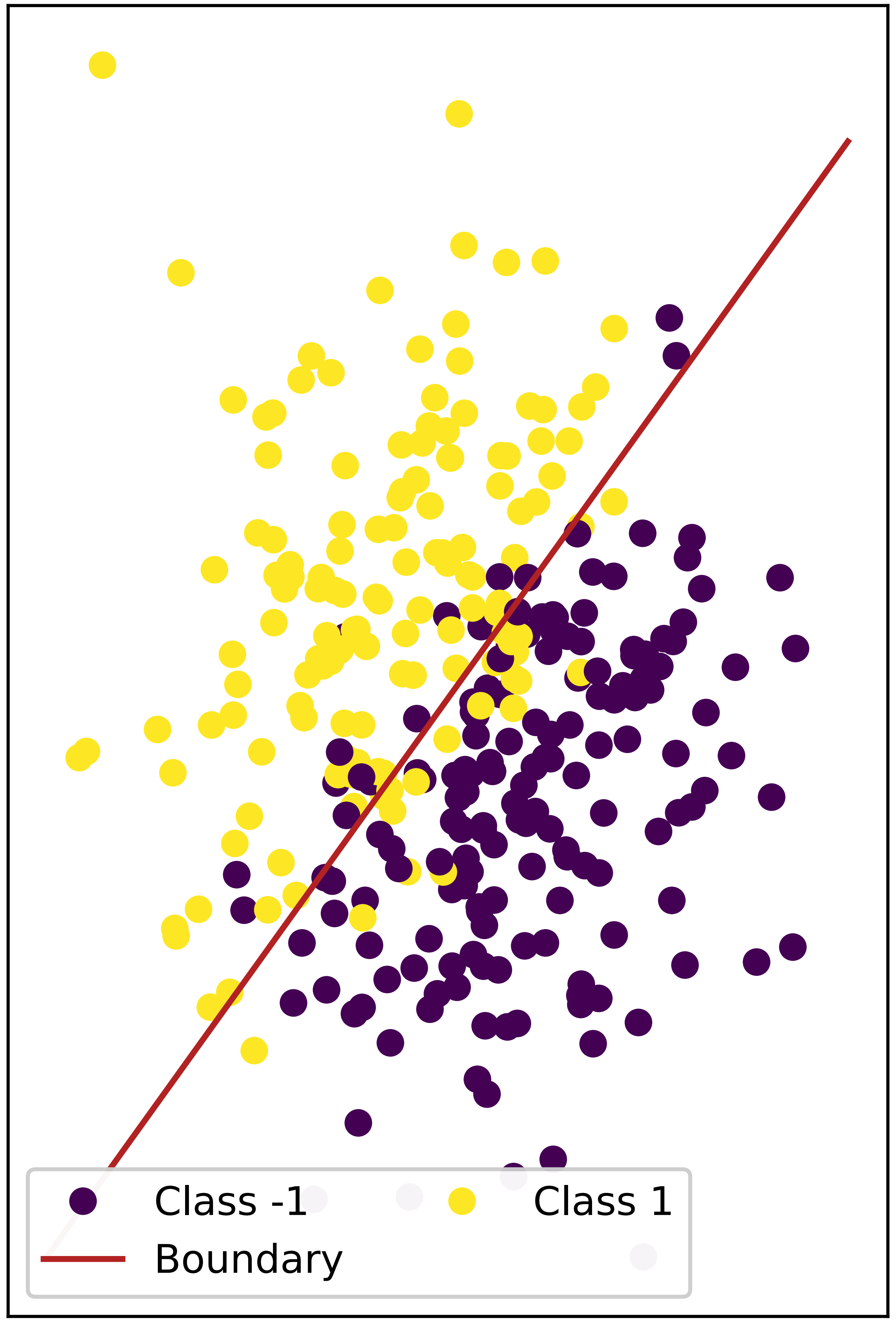

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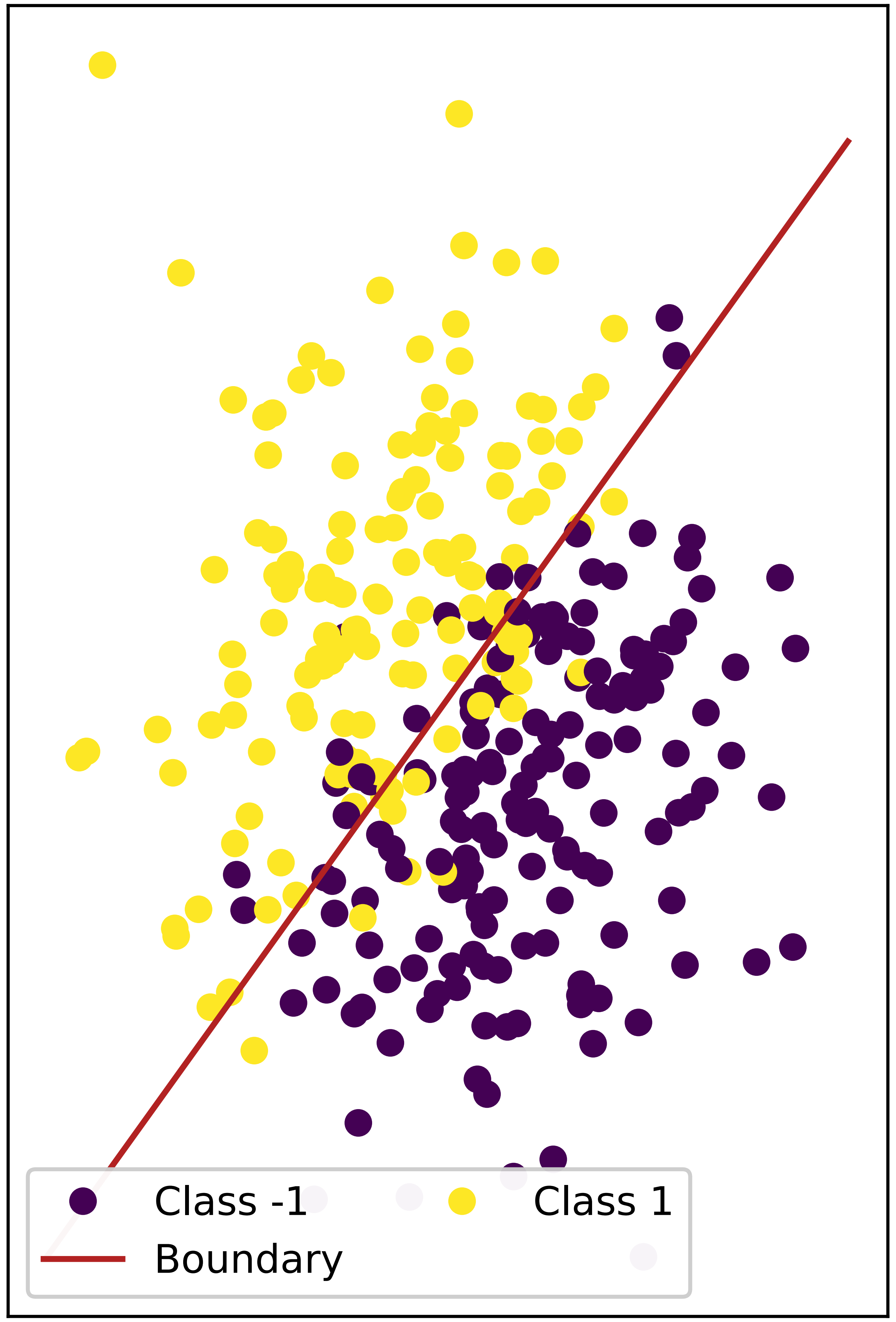

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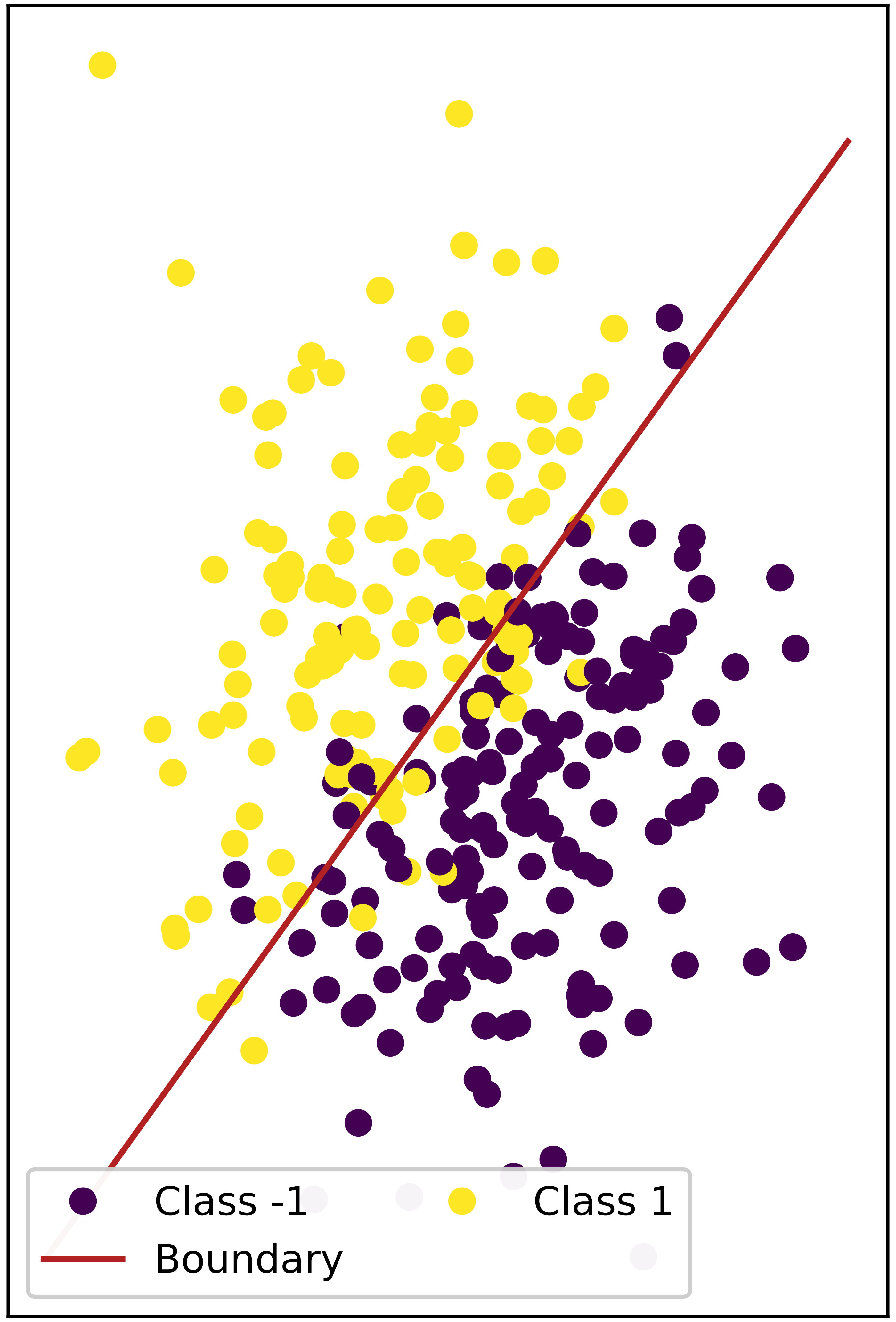

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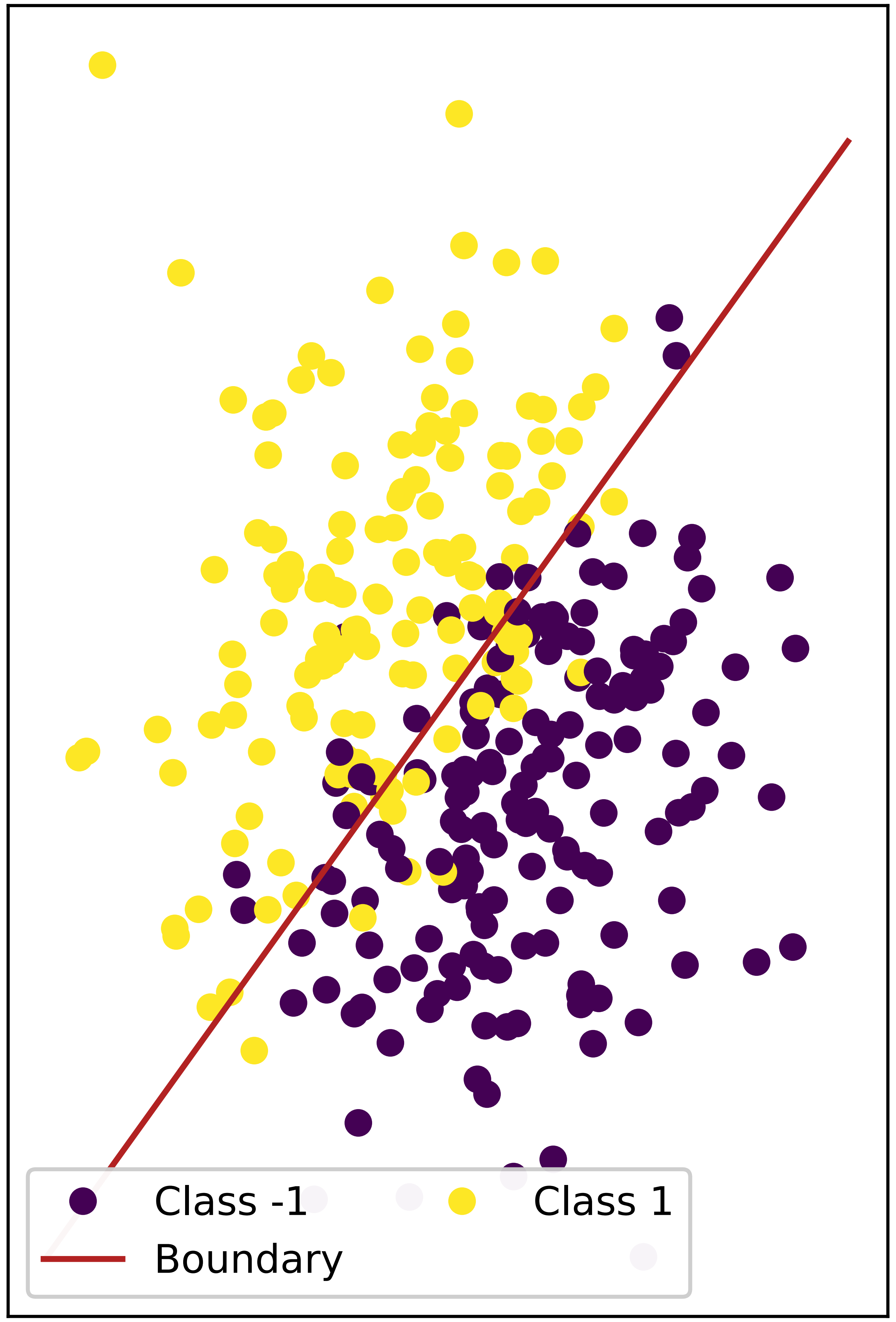

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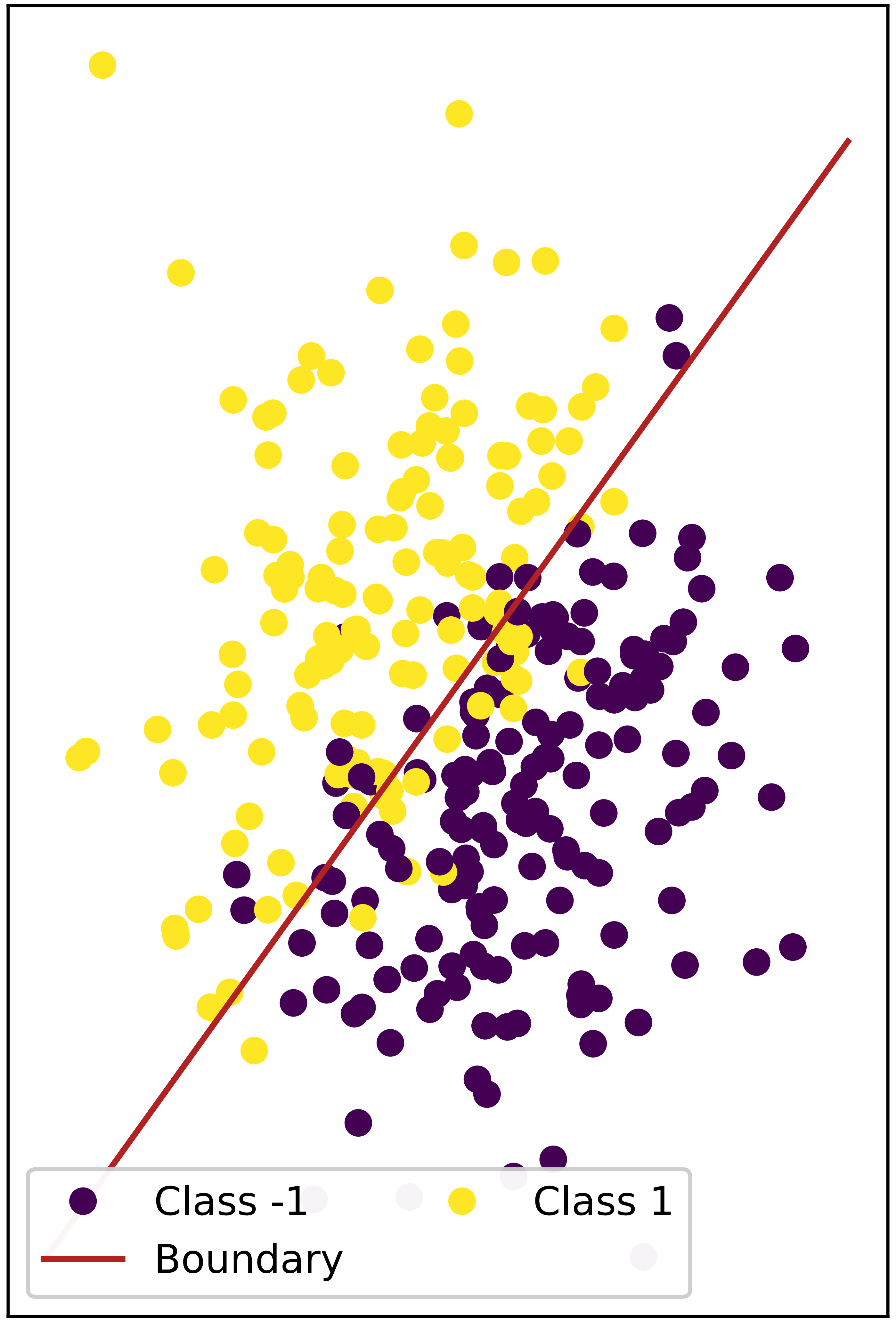
- The learnt parameter $\theta^*(\lambda)$ depends on λ
- λ selected by minimizing the validation loss

$$f(\theta^*(\lambda)) = \frac{1}{m} \sum_{j=1}^m \ell(y_i^{\text{val}}, h_{\theta^*(\lambda)}(x_i^{\text{val}}))$$



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Bilevel problem

$$\min_\lambda f(\theta^*(\lambda))$$

$$\theta^*(\lambda) = \operatorname*{argmin}_{\theta \in \mathbb{R}^{d_\theta}} g(\lambda, \theta)$$

Solving bilevel problems

Zeroth-order methods

Grid search

Zeroth-order methods

Grid search

1. Define a grid of candidates $\lambda_1, \ldots, \lambda_K$

Zeroth-order methods

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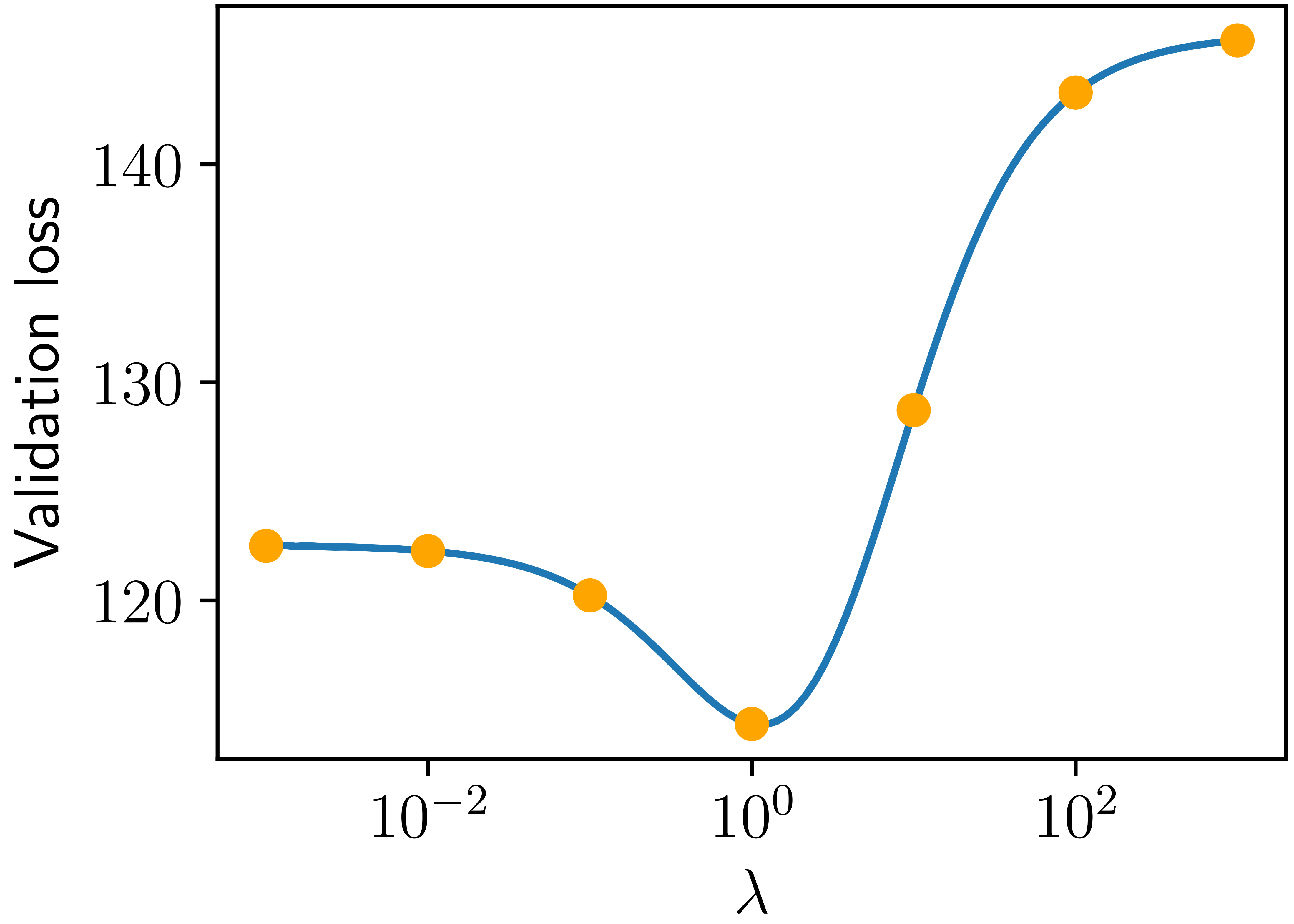
1. Define a grid of candidates $\lambda_1, \ldots, \lambda_K$
2. Train the model to get $\theta^*(\lambda_1), \ldots, \theta^*(\lambda_K)$

Zeroth-order methods

Grid search

1. Define a grid of candidates $\lambda_1, \ldots, \lambda_K$
2. Train the model to get $\theta^*(\lambda_1), \ldots, \theta^*(\lambda_K)$
3. Select the one that minimizes the value function $\Phi(\lambda) = f(\lambda, \theta^*(\lambda))$

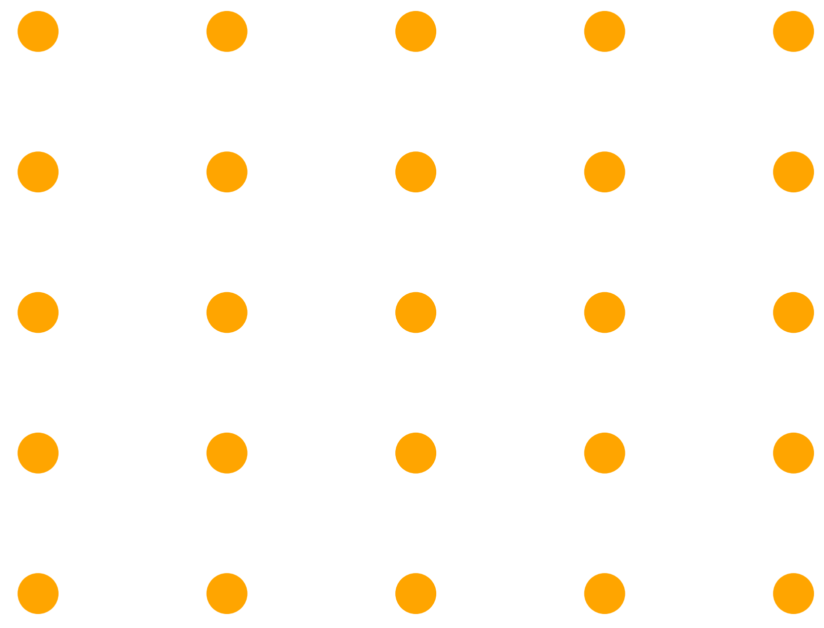


The problem with the grid search

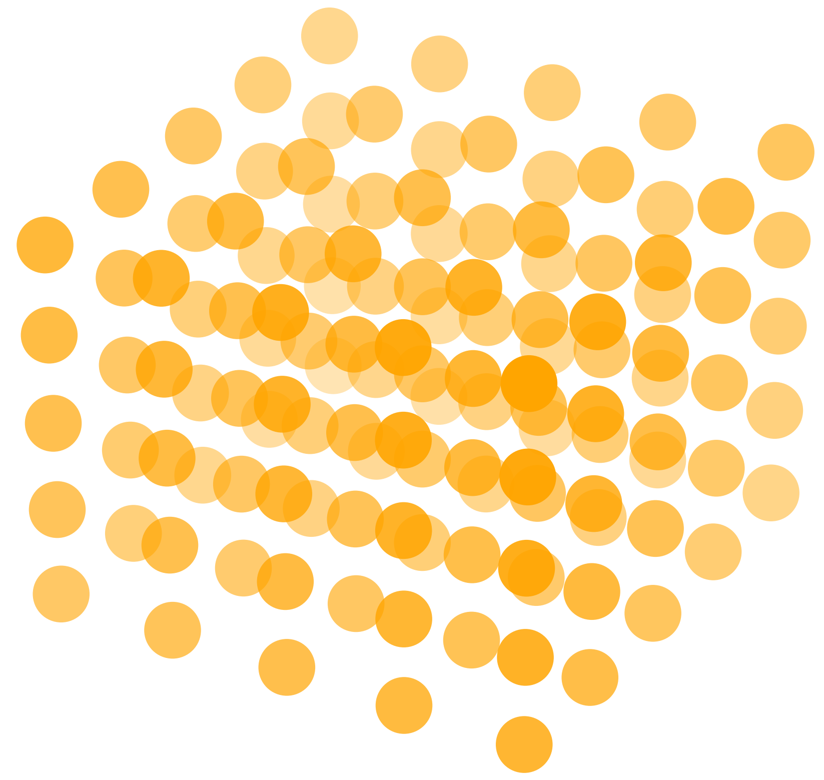
Grid search

1. Define a grid of candidates $\lambda_1, \ldots, \lambda_K$
2. Train the model to get $\theta^*(\lambda_1), \ldots, \theta^*(\lambda_K)$
3. Select the one that minimizes the value function

$$\left|\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}\}\right| = 5$$



$$\left|\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}\}^2\right| = 5^2 = 25$$



$$\left|\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}\}^3\right| = 5^3 = 125$$

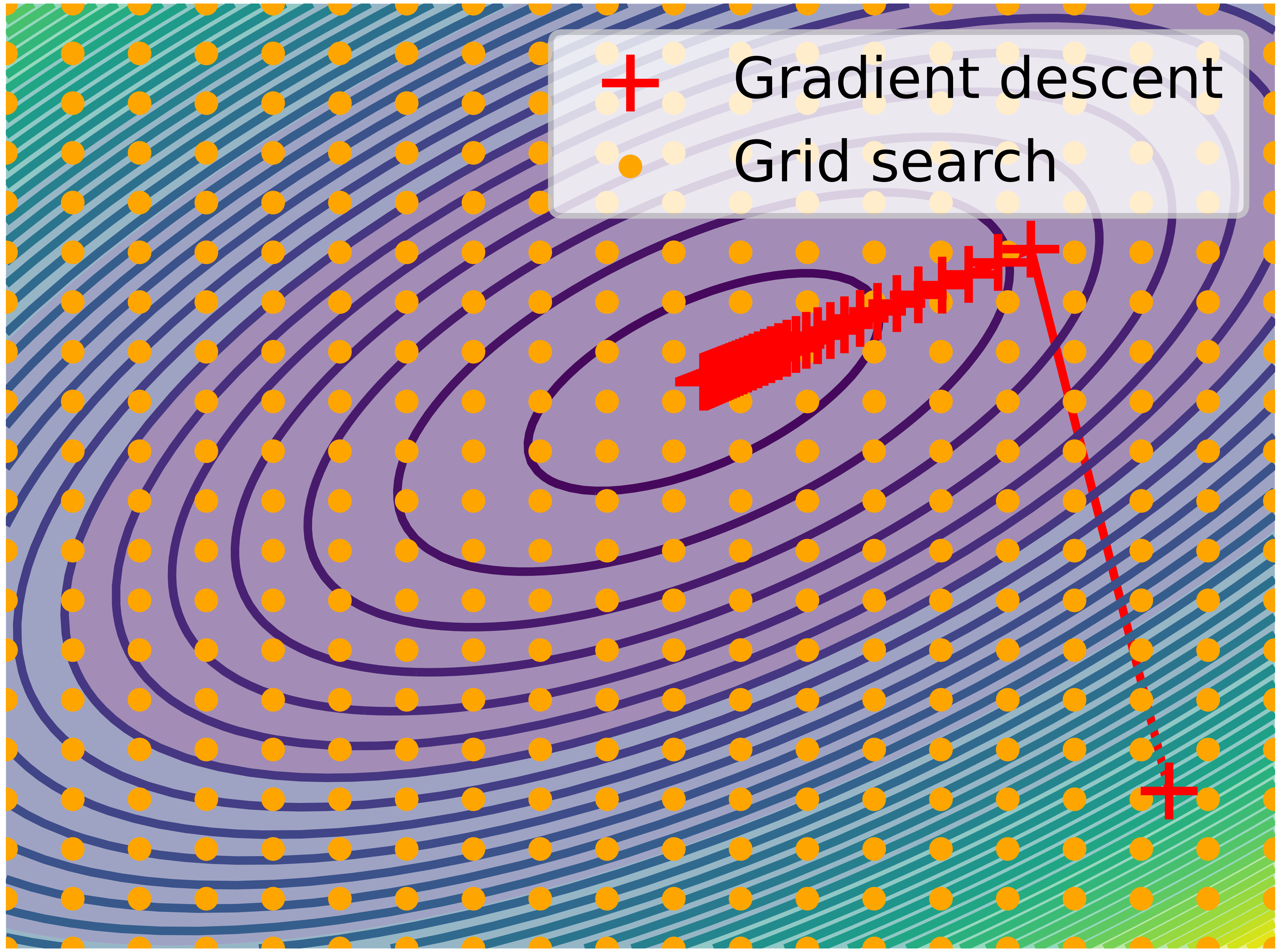
Curse of dimensionality

The number of function evaluations scales exponentially with the dimension

First-order optimization

Gradient descent on Φ

$$\lambda^{t+1} = \lambda^t - \gamma \nabla \Phi(\lambda^t)$$



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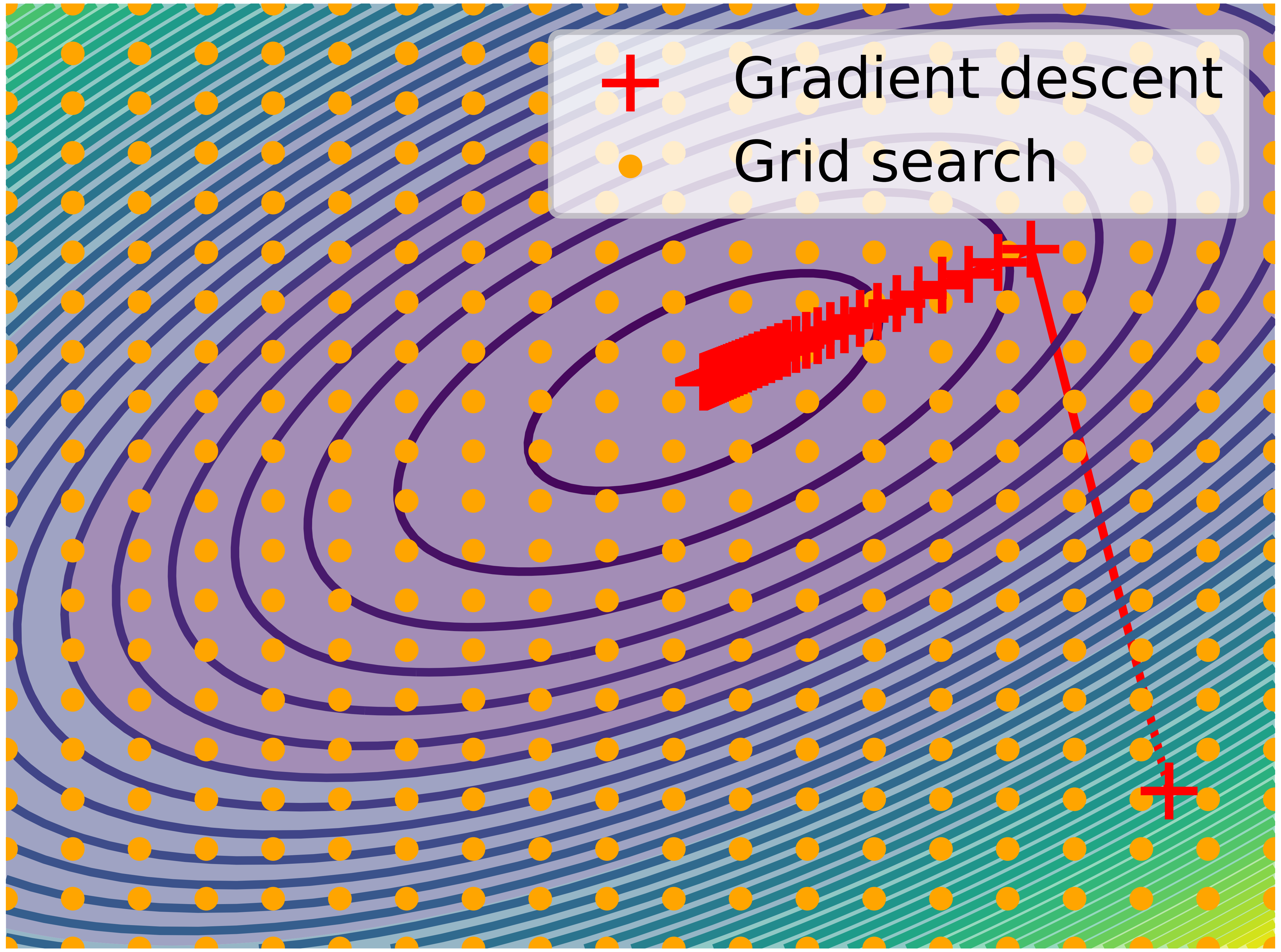
Complexity



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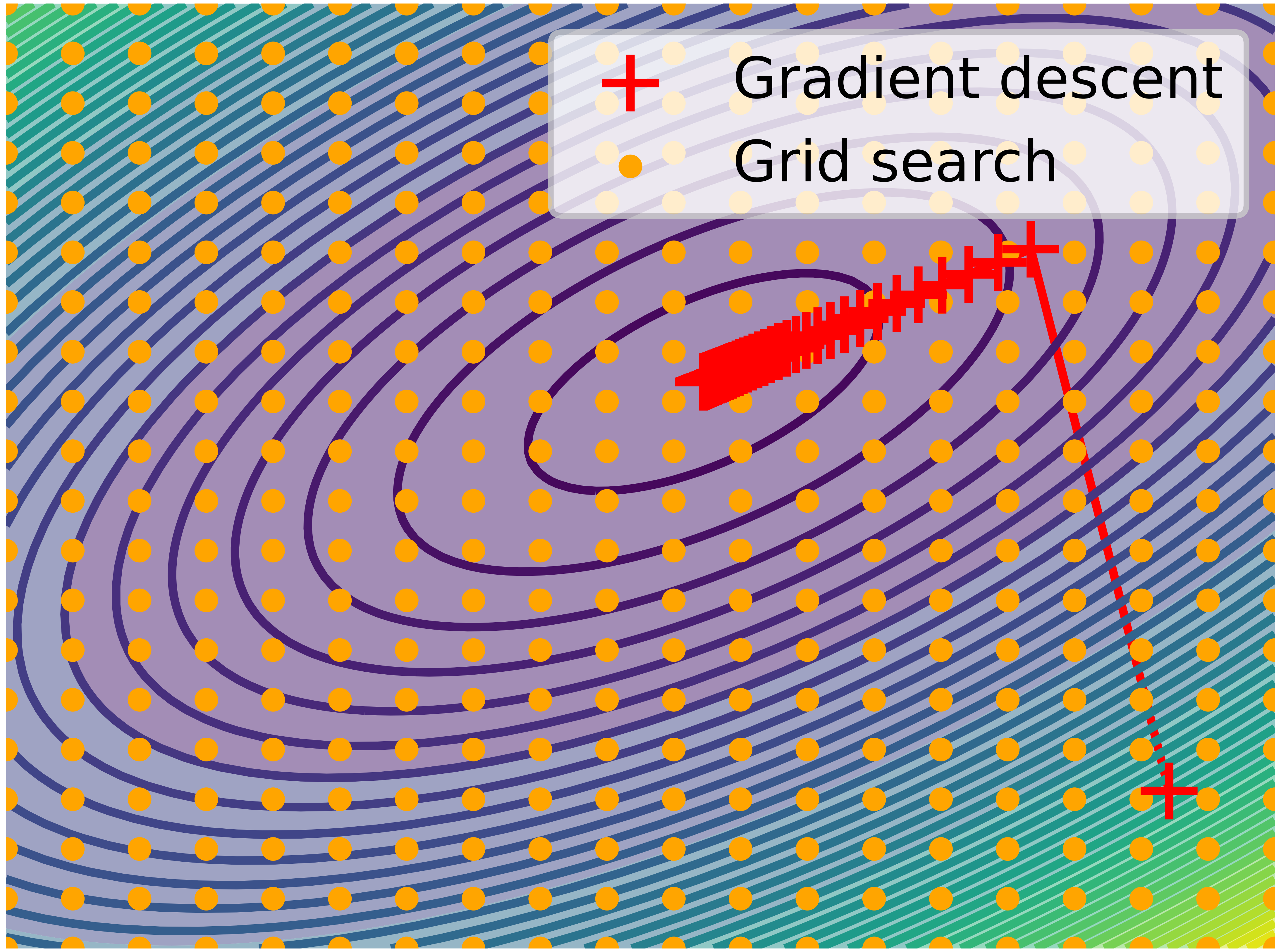
Complexity

✓ Number of gradient computations to reach an ϵ-stationary point if Φ is smooth:

$$\mathcal{O}(\epsilon^{-1})$$



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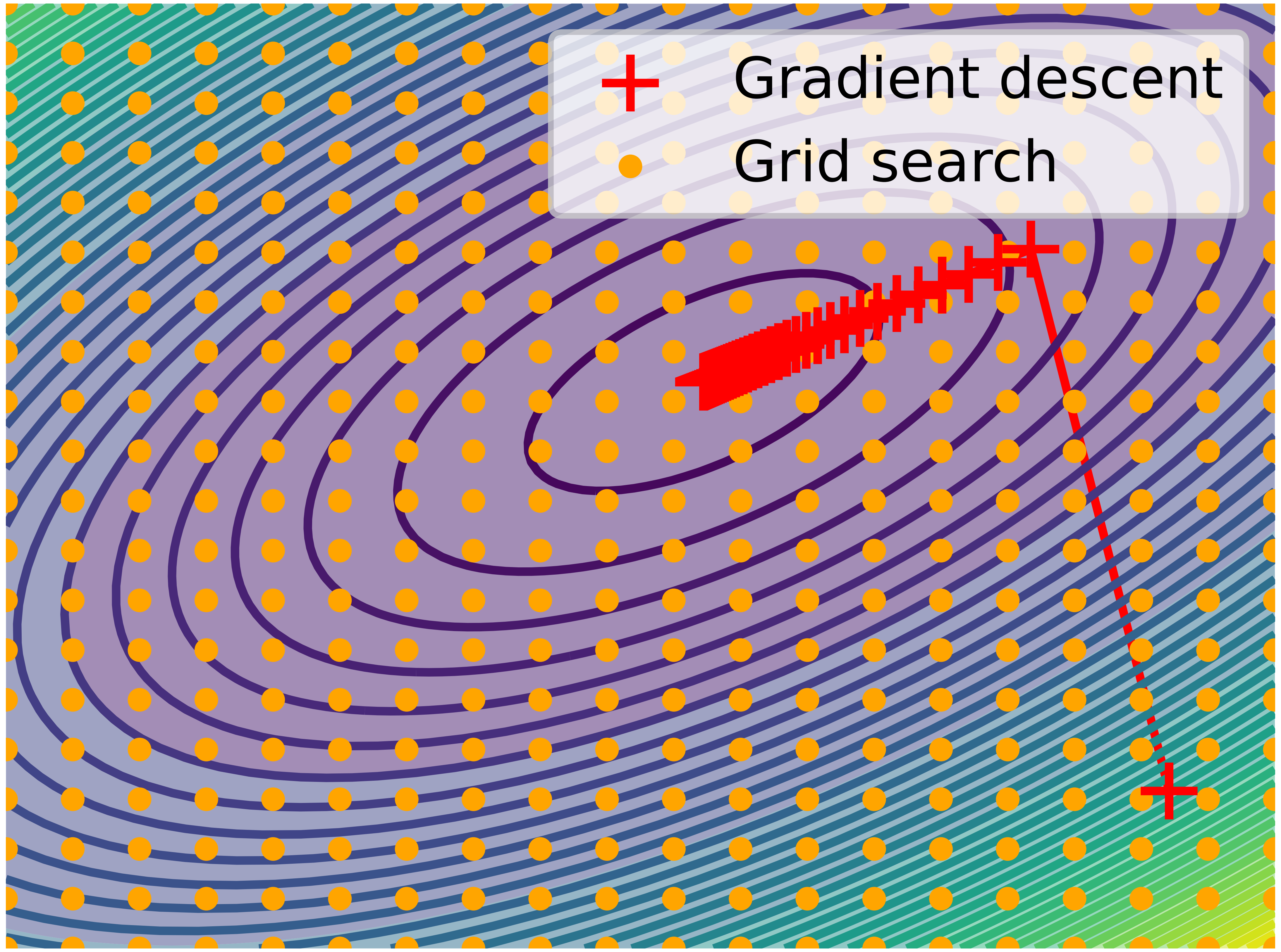

First-order optimization

Differentiable?

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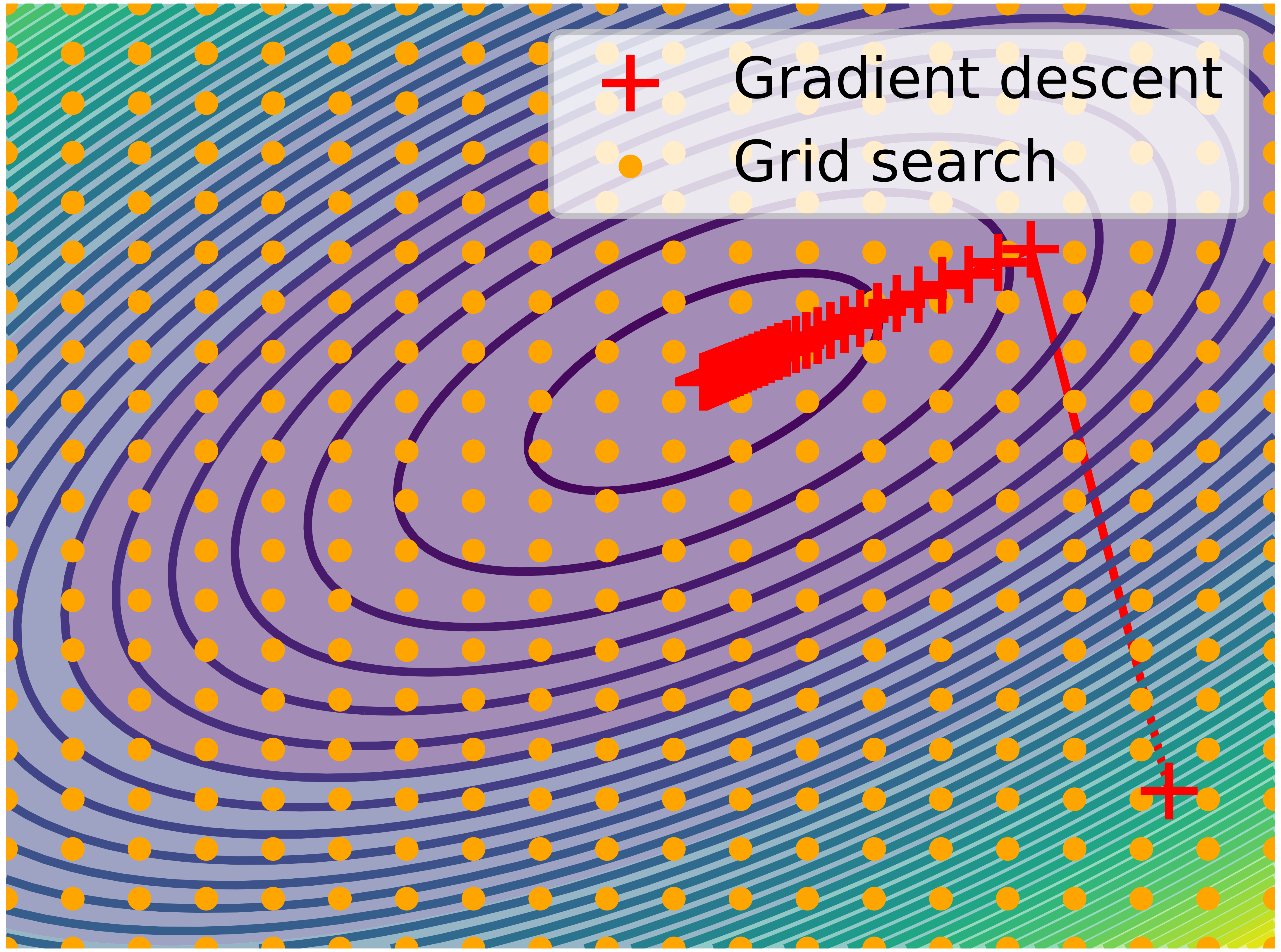

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Differentiable?

Gradient descent on Φ

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How to compute it?

Complexity

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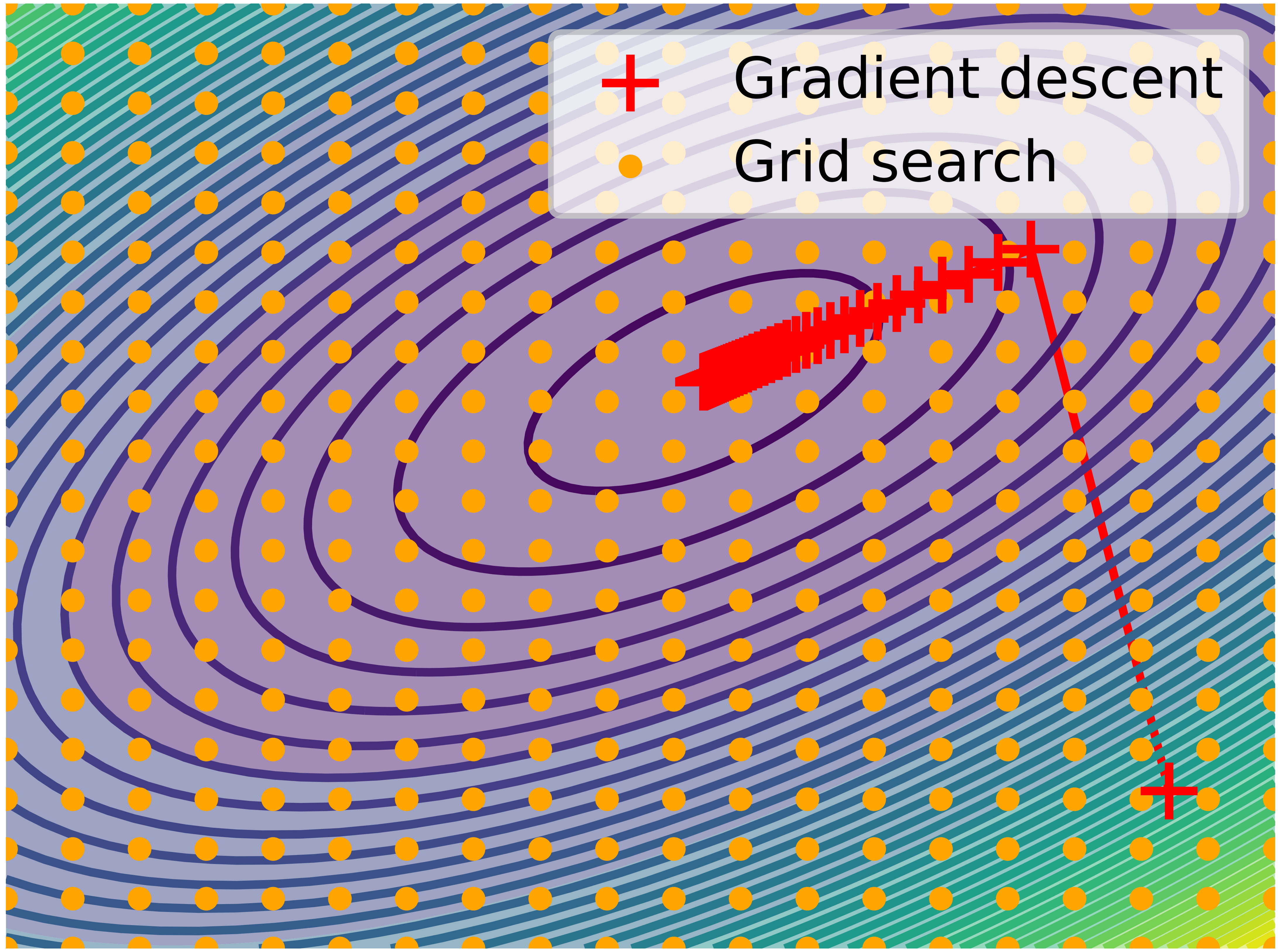

Implicit differentiation [Jongen et al. ’90, Dempe ‘93, Larsen ’96, Dempe ’98]

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Twice differentiable and strongly convex

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Twice differentiable and strongly convex

Chain rule

$$\nabla \Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \mathrm{d}\theta^*(\lambda)^\top \nabla_\theta f(\lambda, \theta^*(\lambda))$$

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Differentiable

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$$\theta^*(\lambda) = \underset{\theta \in \mathbb{R}^{d_\theta}}{\operatorname{argmin}}\, g(\lambda, \theta)$$

Twice differentiable and strongly convex

First-order condition

$$\nabla_\theta g(\lambda, \theta^*(\lambda)) = 0$$

Chain rule

$$\nabla \Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \mathrm{d}\theta^*(\lambda)^\top \nabla_\theta f(\lambda, \theta^*(\lambda))$$

Implicit differentiation [Jongen et al. '90, Dempe '93, Larsen '96, Dempe '98]

Differentiable

Bilevel problem

$$\min_{\lambda \in \mathbb{R}^{d_\lambda}} \Phi(\lambda) \triangleq f(\lambda, \theta^*(\lambda))$$

$$\theta^*(\lambda) = \operatorname*{argmin}_{\theta \in \mathbb{R}^{d_\theta}} g(\lambda, \theta)$$

Twice differentiable and strongly convex

First-order condition

$$\nabla_\theta g(\lambda, \theta^*(\lambda)) = 0$$

$$\frac{\partial}{\partial \lambda}$$

$$\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda)) \mathrm{d}\theta^*(\lambda) + \nabla^2_{\theta,\lambda} g(\lambda, \theta^*(\lambda)) = 0$$

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$$\nabla_\theta g(\lambda, \theta^*(\lambda)) = 0$$

$$\Big\downarrow \frac{\partial}{\partial \lambda}$$

$$\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda)) \mathrm{d}\theta^*(\lambda) + \nabla^2_{\theta,\lambda} g(\lambda, \theta^*(\lambda)) = 0$$

$$\mathrm{d}\theta^*(\lambda) = -\left[\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda))\right]^{-1} \nabla^2_{\theta,\lambda} g(\lambda, \theta^*(\lambda))$$

Chain rule

$$\nabla \Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \mathrm{d}\theta^*(\lambda)^\top \nabla_\theta f(\lambda, \theta^*(\lambda))$$

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strongly convex

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Implicit differentiation in practice

Implicit gradient

$$\nabla\Phi(\lambda) = \nabla_\lambda f(\lambda,\ \theta^*(\lambda)\ ) - \nabla^2_{\lambda,\theta} g(\lambda,\ \theta^*(\lambda)\ )\left[\nabla^2_{\theta,\theta} g(\lambda,\ \theta^*(\lambda)\ )\right]^{-1}\nabla_\theta f(\lambda,\ \theta^*(\lambda)\ )$$

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Bottlenecks

Implicit differentiation in practice

Implicit gradient

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Bottlenecks

- Solution of the inner problem

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Bottlenecks

- Solution of the inner problem
- Solution of a linear system

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Bottlenecks

- Solution of the inner problem
- Solution of a linear system
- Computing a gradient is expensive

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Bottlenecks

- Solution of the inner problem
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ML setting: Empirical Risk Minimization

$$f(\lambda, \theta) = \frac{1}{m}\sum_{j=1}^{m} f_j(\lambda, \theta), \quad g(\lambda, \theta) = \frac{1}{n}\sum_{i=1}^{n} g_i(\lambda, \theta)$$

Implicit differentiation in practice

Implicit gradient

$$\nabla \Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) - \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) \boxed{\left[\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda))\right]^{-1} \nabla_\theta f(\lambda, \theta^*(\lambda))}$$

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Stochastic optimization [Robbins & Monro '51]

$$\lambda^{t+1} = \lambda^t - \gamma^t d^t$$

Cheap estimator of $\nabla \Phi(\lambda^t)$

Implicit differentiation in practice

Implicit gradient

$$\nabla\Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) - \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) \boxed{\left[\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda))\right]^{-1} \nabla_\theta f(\lambda, \theta^*(\lambda))}$$

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Can we build an unbiased estimate of $\nabla\Phi(\lambda)$?

Implicit differentiation in practice

Implicit gradient

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Cheap estimator of $\nabla \Phi(\lambda^t)$

Can we build an unbiased estimate of $\nabla \Phi(\lambda)$?

No straightforward answer since…

$$\left[\sum_{i=1}^{n} \nabla^2_{\theta,\theta} g_i\right]^{-1} \neq \sum_{i=1}^{n} \left[\nabla^2_{\theta,\theta} g_i\right]^{-1}$$

A framework for bilevel optimization that enables stochastic and global variance reduction algorithms

M. Dagréou, P. Ablin, S. Vaiter, T. Moreau. A framework for bilevel optimization that enables stochastic and global variance reduction algorithm. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2022. *Oral*

Framework for bilevel optimization

Implicit gradient

$$\nabla \Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) - \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) \left[\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda))\right]^{-1} \nabla_\theta f(\lambda, \theta^*(\lambda))$$

Framework for bilevel optimization

Implicit gradient

$$\nabla\Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) v^*(\lambda)$$

$$v^*(\lambda) \triangleq -\left[\nabla^2_{\theta,\theta} g(\lambda, \theta^*(\lambda))\right]^{-1} \nabla_\theta f(\lambda, \theta^*(\lambda))$$

Framework for bilevel optimization

Implicit gradient

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Main idea: Update θ, v and λ in the following directions:

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Main idea: Update θ, v and λ in the following directions:

- θ: $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$

Goes towards $\theta^*(\lambda)$

Framework for bilevel optimization

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- θ: $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$ — *Goes towards* $\theta^*(\lambda)$
- v: $D_v(\theta, v, \lambda) = \nabla^2_{\theta,\theta} g(\lambda, \theta) v + \nabla_\theta f(\lambda, \theta)$ — *Goes towards* $v^*(\lambda)$

Framework for bilevel optimization

Implicit gradient

$$\nabla\Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) v^*(\lambda)$$

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$$\longrightarrow D_\lambda(\theta^*(\lambda), v^*(\lambda), \lambda) = \nabla\Phi(\lambda)$$

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Implicit gradient

$$\nabla\Phi(\lambda) = \nabla_\lambda f(\lambda, \theta^*(\lambda)) + \nabla^2_{\lambda,\theta} g(\lambda, \theta^*(\lambda)) v^*(\lambda)$$

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$$\rightarrow \quad D_\lambda(\theta^*(\lambda), v^*(\lambda), \lambda) = \nabla\Phi(\lambda)$$

Bilevel Dynamics

$$\begin{bmatrix} \theta^{t+1} \\ v^{t+1} \\ \lambda^{t+1} \end{bmatrix} = \begin{bmatrix} \theta^t - \rho^t D_\theta(\theta^t, v^t, \lambda^t) \\ v^t - \rho^t D_v(\theta^t, v^t, \lambda^t) \\ \lambda^t - \gamma^t D_\lambda(\theta^t, v^t, \lambda^t) \end{bmatrix}$$

Same step size in θ and v because same conditioning

Framework for *stochastic* bilevel optimization

Update directions

- $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$
- $D_v(\theta, v, \lambda) = \nabla^2_{\theta,\theta} g(\lambda, \theta) v + \nabla_\theta f(\lambda, \theta)$
- $D_\lambda(\theta, v, \lambda) = \nabla^2_{\lambda,\theta} g(\lambda, \theta) v + \nabla_\lambda f(\lambda, \theta)$

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ERM

$$f(\lambda, \theta) = \frac{1}{m} \sum_{j=1}^{m} f_j(\lambda, \theta), \quad g(\lambda, \theta) = \frac{1}{n} \sum_{i=1}^{n} g_i(\lambda, \theta)$$

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Linear in f and g

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Framework for *stochastic* bilevel optimization

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- $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$
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Stochastic estimators of $D_\theta(\theta^t, v^t, \lambda^t)$, $D_v(\theta^t, v^t, \lambda^t)$ and $D_\lambda(\theta^t, v^t, \lambda^t)$

Framework for *stochastic* bilevel optimization

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- $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$
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SOBA directions

Sample $i \in \{1, \ldots, n\}$ and $j \in \{1, \ldots, m\}$and set

$$D^t_\theta = \nabla_\theta g_i(\lambda^t, \theta^t)$$
$$D^t_v = \nabla^2_{\theta,\theta} g_i(\lambda^t, \theta^t) v^t + \nabla_\theta f_j(\lambda^t, \theta^t)$$
$$D^t_\lambda = \nabla^2_{\lambda,\theta} g_i(\lambda^t, \theta^t) v^t + \nabla_\lambda f_j(\lambda^t, \theta^t)$$

SOBA (StOchastic Bilevel Algorithm) in details

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Sample $i \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$ and set

$$D_\theta^t = \nabla_\theta g_i(\lambda^t, \theta^t)$$
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Iteration cost

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Iteration cost

- Gradients: computed efficiently by reverse mode automatic differentiation [Linnainmaa et al. '70]

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Iteration cost

- Gradients: computed efficiently by reverse mode automatic differentiation [Linnainmaa et al. '70]
- HVPs: At first sight 😱 😱 😱 😱, but…

How to compute Hessian-vector products?

M. Dagréou, P. Ablin, S. Vaiter, T. Moreau. How to compute Hessian-vector products? In *ICLR blogpost track*, 2024. *Spotlight*

Efficient computation by automatic differentiation [Pearlmutter ’94]

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$$\nabla^2_{\theta,\theta} g_i(\lambda^t, \theta^t) v^t = \nabla_\theta \left[\langle \nabla_\theta g_i(\lambda^t, \theta^t), v^t \rangle\right]$$

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- reverse-over-reverse: « grad of the JVP »

```
jax.grad(lambda y: jnp.vdot(jax.grad(g)(y), v))(params)
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```
jax.grad(lambda y: jax.jvp(g, (y, ), (v, ))[1])(params)
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- reverse-over-forward: « grad of the JVP »

```
jax.grad(lambda y: jax.jvp(g, (y, ), (v, ))[1])(params)
```

- forward-over-reverse: « JVP of the grad »

```
jax.jvp(jax.grad(g), (params, ), (v, ))[1]
```

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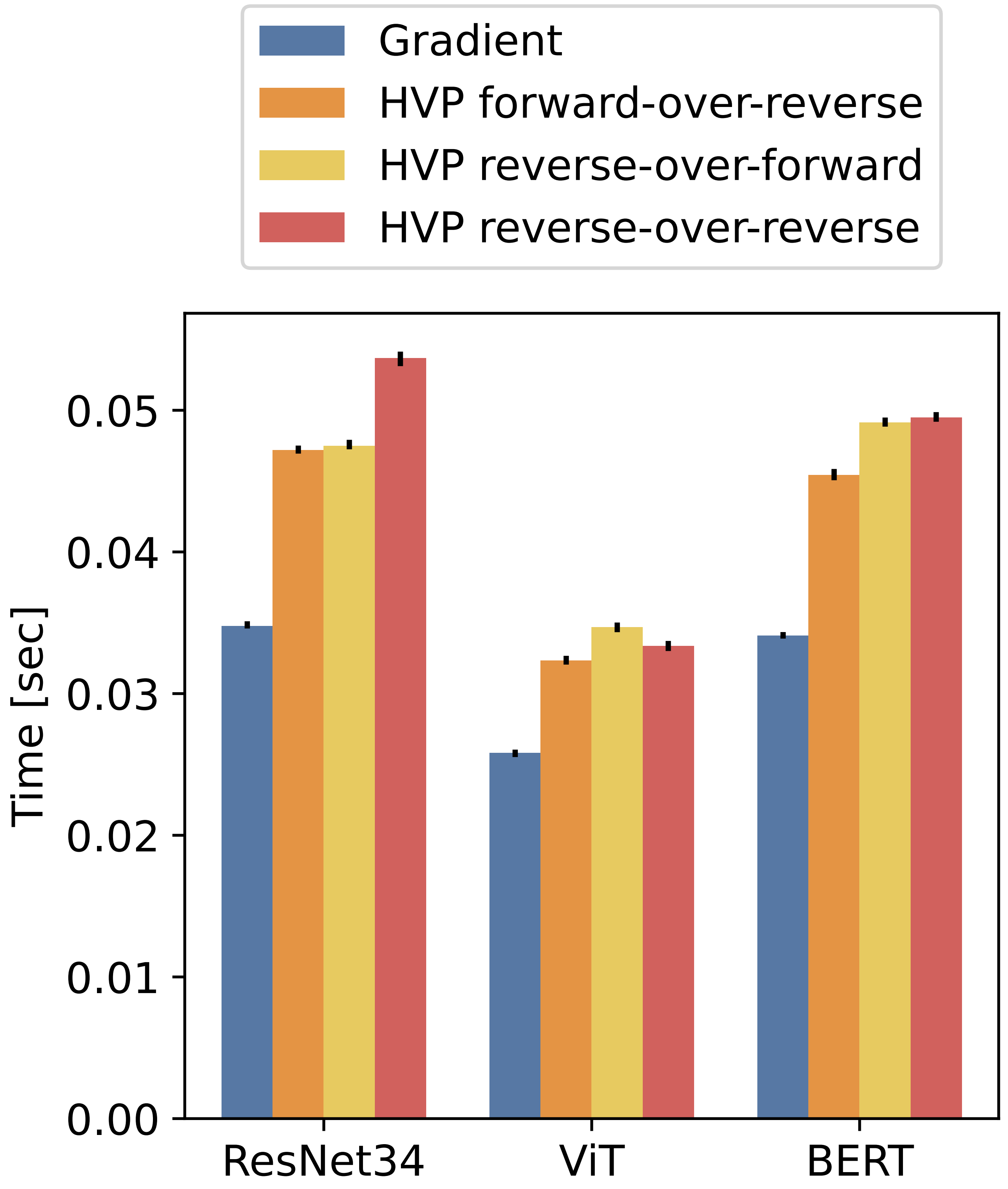
```
jax.grad(lambda y: jax.jvp(g, (y, ), (v, ))[1])(params)
```

- forward-over-reverse: « JVP of the grad »

```
jax.jvp(jax.grad(g), (params, ), (v, ))[1]
```



How to compute Hessian-vector products?

M. Dagréou, P. Ablin, S. Vaiter, T. Moreau. How to compute Hessian-vector products? In *ICLR blogpost track*, 2024. *Spotlight*

Efficient computation by automatic differentiation [Pearlmutter '94]

$$\nabla^2_{\theta,\theta} g_i(\lambda^t, \theta^t) v^t = \nabla_\theta \left[\langle \nabla_\theta g_i(\lambda^t, \theta^t), v^t \rangle \right]$$

- reverse-over-reverse: « grad of the JVP »

```
jax.grad(lambda y: jnp.vdot(jax.grad(g)(y), v))(params)
```

- reverse-over-forward: « grad of the JVP »

```
jax.grad(lambda y: jax.jvp(g, (y, ), (v, ))[1])(params)
```

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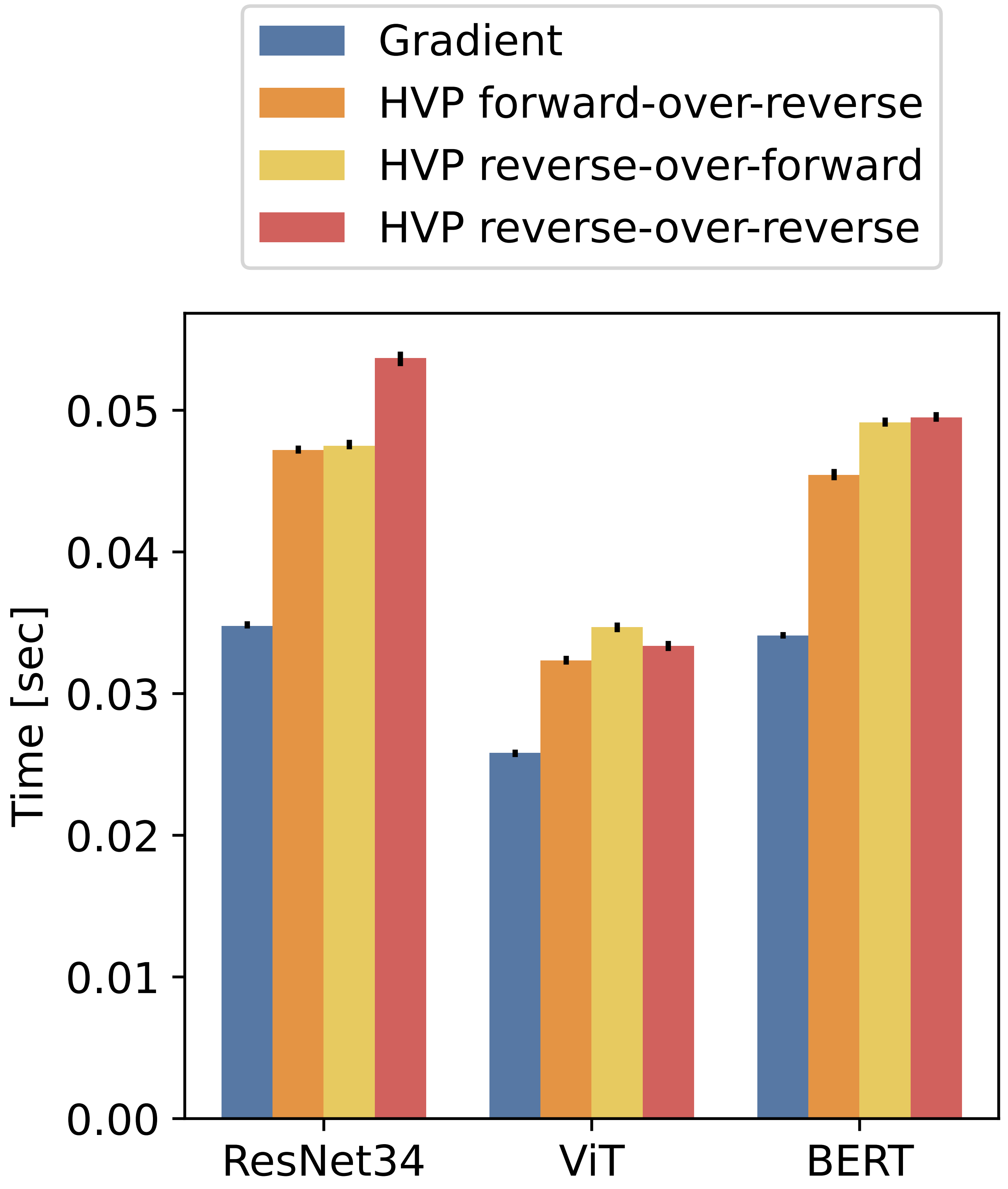

The HVP cost scales as the gradient cost!!!

Convergence of SOBA

Convergence of SOBA

Theorem

Assume that

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$$\mathbb{E}_t\left[\|D_\theta^t\|^2\right] \leq B_\theta(1 + \|D_\theta(\theta^t, v^t, \lambda^t)\|^2), \quad \mathbb{E}_t\left[\|D_v^t\|^2\right] \leq B_v(1 + \|D_v(\theta^t, v^t, \lambda^t)\|^2),$$

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Then, for step sizes $\rho^t \asymp t^{-\frac{1}{2}}$ and $\gamma^t \asymp t^{-\frac{1}{2}}$ it holds

$$\inf_{0 \leq t \leq T-1} \mathbb{E}[\|\nabla \Phi(\lambda^t)\|^2] \leq \mathcal{O}(\log(T) T^{-\frac{1}{2}})$$

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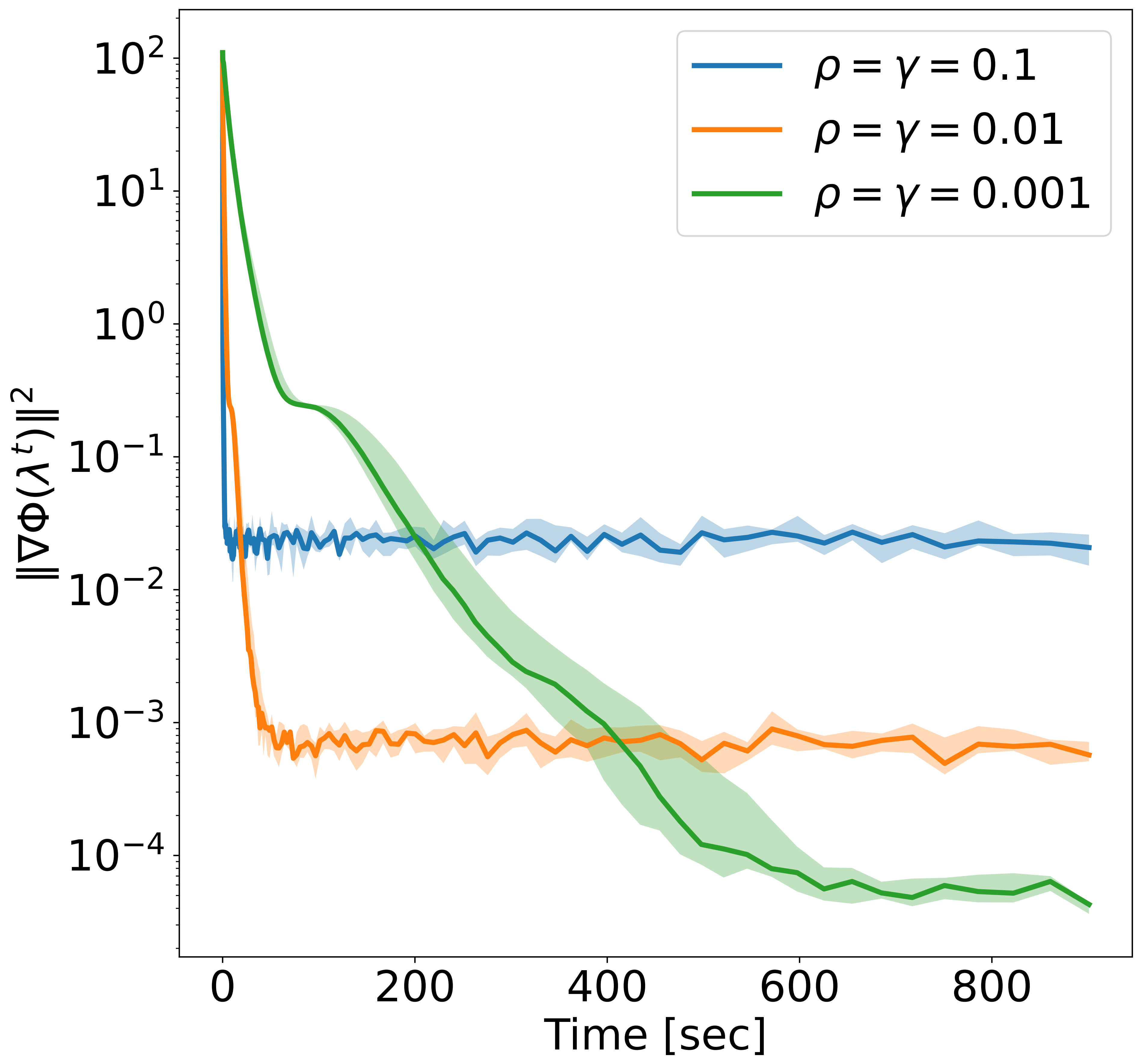
Similar to the rate of SGD for non-convex smooth functions [Ghadimi '13]

Why decreasing the step sizes?

Quadratic setting

$$f(\lambda, \theta) = \frac{1}{m} \sum_{j=1}^{m} \left\langle A_j^f \begin{bmatrix} \lambda \\ \theta \end{bmatrix}, \begin{bmatrix} \lambda \\ \theta \end{bmatrix} \right\rangle + \left\langle b_j^f, \begin{bmatrix} \lambda \\ \theta \end{bmatrix} \right\rangle + c_j^f$$

$$g(\lambda, \theta) = \frac{1}{n} \sum_{i=1}^{n} \left\langle A_i^g \begin{bmatrix} \lambda \\ \theta \end{bmatrix}, \begin{bmatrix} \lambda \\ \theta \end{bmatrix} \right\rangle + \left\langle b_i^g, \begin{bmatrix} \lambda \\ \theta \end{bmatrix} \right\rangle + c_i^g$$



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$$\delta_v^t = \mathbb{E}\left[\|v^t - v^*(\lambda^t)\|^2\right]$$

$$\Phi^t = \mathbb{E}[\Phi(\lambda^t)]$$

Fundamental descent lemma

$$\delta_\theta^{t+1} \leq (1-\rho\mu_g)\delta_\theta^t + \rho^2\mathbb{E}[\|D_\theta^t\|^2] + \rho^2\mathbb{E}[\|D_\lambda^t\|^2] + \frac{\gamma^2}{\rho}\mathbb{E}[\|D_\lambda(\theta^t, v^t, \lambda^t)\|^2]$$

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$$\Phi^{t+1} \leq \Phi^t - \gamma\mathbb{E}\left[\|\nabla\Phi(\lambda^t)\|^2\right] - \gamma\mathbb{E}[\|D_\lambda(\theta^t, v^t, \lambda^t)\|] + \gamma(\delta_\theta^t + \delta_v^t) + \gamma^2\mathbb{E}\left[\|D_\lambda^t\|^2\right]$$

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Variance terms prevent from converging if not converging towards 0

- Make the step sizes decreasing -> leads to slow convergence
- Make the variance decrease? -> Variance reduction algorithms[Johnson et al. 13, Defazio et al. ’14, Bietti & Mairal ‘17]

SRBA (Stochastic Recursive Bilevel Algorithm)

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General principle

- Adaptation of SARAH/SPIDER to bilevel setting [Nguyen et al. ’17, Fang et al. ’18]

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Recursive estimation of the directions

Sample $i \in \{1, \dots, n\}$ and $j \in \{1, \dots, m\}$ and set

$$
\begin{aligned}
D_\theta^{t,k} &= D_\theta^{i,j}(\theta^{t,k}, v^{t,k}, \lambda^{t,k}) - D_\theta^{i,j}(\theta^{t,k-1}, v^{t,k-1}, \lambda^{t,k-1}) + D_\theta^{t,k-1} \\
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Inner loop index

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Unbiased estimators of the directions

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- Recursive estimate of the directions
- Periodic reinitialization of the estimate

Reinitialization of estimate directions

$$D_\theta^{t,0} = D_\theta(\theta^{t,0}, v^{t,0}, \lambda^{t,0})$$
$$D_v^{t,0} = D_v(\theta^{t,0}, v^{t,0}, \lambda^{t,0})$$
$$D_\lambda^{t,0} = D_\lambda(\theta^{t,}, v^{t,0}, \lambda^{t,0})$$

Full batch directions

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Then, for constant step sizes proportional to $(n+m)^{-\frac{1}{2}}$,

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calls to oracles are sufficient to find an ϵ-stationary point

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Similar to the rate of SARAH for non-convex smooth finite sums [Nguyen '22]

Lower bound for bilevel empirical risk minimization

M. Dagréou, T. Moreau, S. Vaiter, P. Ablin. A Lower Bound and a Near-Optimal Algorithm for Bilevel Empirical Risk Minimization. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2024.

Complexity bounds in optimization

Question

What is the amount of oracle computations I need to solve bilevel ERM with smooth outer and strongly convex inner functions by only accessing individual gradient of the outer function and gradient/HVP/JVP of the inner function?

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Proxy of the total amount of elementary operations of an algorithm

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A detour by single-level optimization

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Finite sum minimization setting

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Upper bound [Nguyen '22]
There exists an algorithm which is able to find an ϵ-stationary point of any function h in less than

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Random variables in $\{1, \ldots, n\}$

Lower bound [Zhou et al. '19]

Given an algorithm A we can find a function h such that A requires at least

$$\Omega(\sqrt{n}\epsilon^{-1})$$

oracle calls to find an ϵ-stationary point.

Why does single-level results do not extend directly to bilevel problems?

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We need a specific algorithm class

Algorithm class

Update directions

- $D_\theta(\theta, v, \lambda) = \nabla_\theta g(\lambda, \theta)$
- $D_v(\theta, v, \lambda) = \nabla^2_{\theta,\theta} g(\lambda, \theta) v + \nabla_\theta f(\lambda, \theta)$
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Linear Bilevel Algorithm

$$\theta^{t+1} \in \theta^0 + \operatorname{span}\left\{\nabla_\theta g_{i_0}(\lambda^0, \theta^0), \ldots, \nabla_\theta g_{i_t}(\lambda^t, \theta^t)\right\}$$

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- Contains several several bilevel algorithms

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- Contains several several bilevel algorithms
- But excludes non-linear subroutines like Neumann iterations

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Problem class

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Bilevel Optimization Problem

$$\min_{\lambda \in \mathbb{R}^{d_\lambda}} \Phi(\lambda) \triangleq f(\lambda, \theta^*(\lambda))$$

$$\theta^*(\lambda) \in \operatorname*{argmin}_{\theta \in \mathbb{R}^{d_\theta}} g(\lambda, \theta)$$

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Empirical Risk Minimization

$$f(\lambda, \theta) = \frac{1}{m} \sum_{j=1}^{m} f_j(\lambda, \theta), \quad g(\lambda, \theta) = \frac{1}{n} \sum_{i=1}^{n} g_i(\lambda, \theta)$$

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Lipschitz gradient

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Lipschitz gradient

Twice differentiable,
Strongly convex

Lower bound for bilevel ERM

Theorem (informal)

For any linear bilevel algorithm, for a large enough dimension d_λ we can find an instantiation of bilevel ERM problem such that such that finding a point $\hat{\lambda} \in \mathbb{R}^{d_\lambda}$ that verifies

$$\mathbb{E}[\|\nabla\Phi(\hat{\lambda})\|^2] \leq \epsilon$$

requires at least $\Omega(m^{\frac{1}{2}}\epsilon^{-1})$ gradient/HVP/JVP computations.

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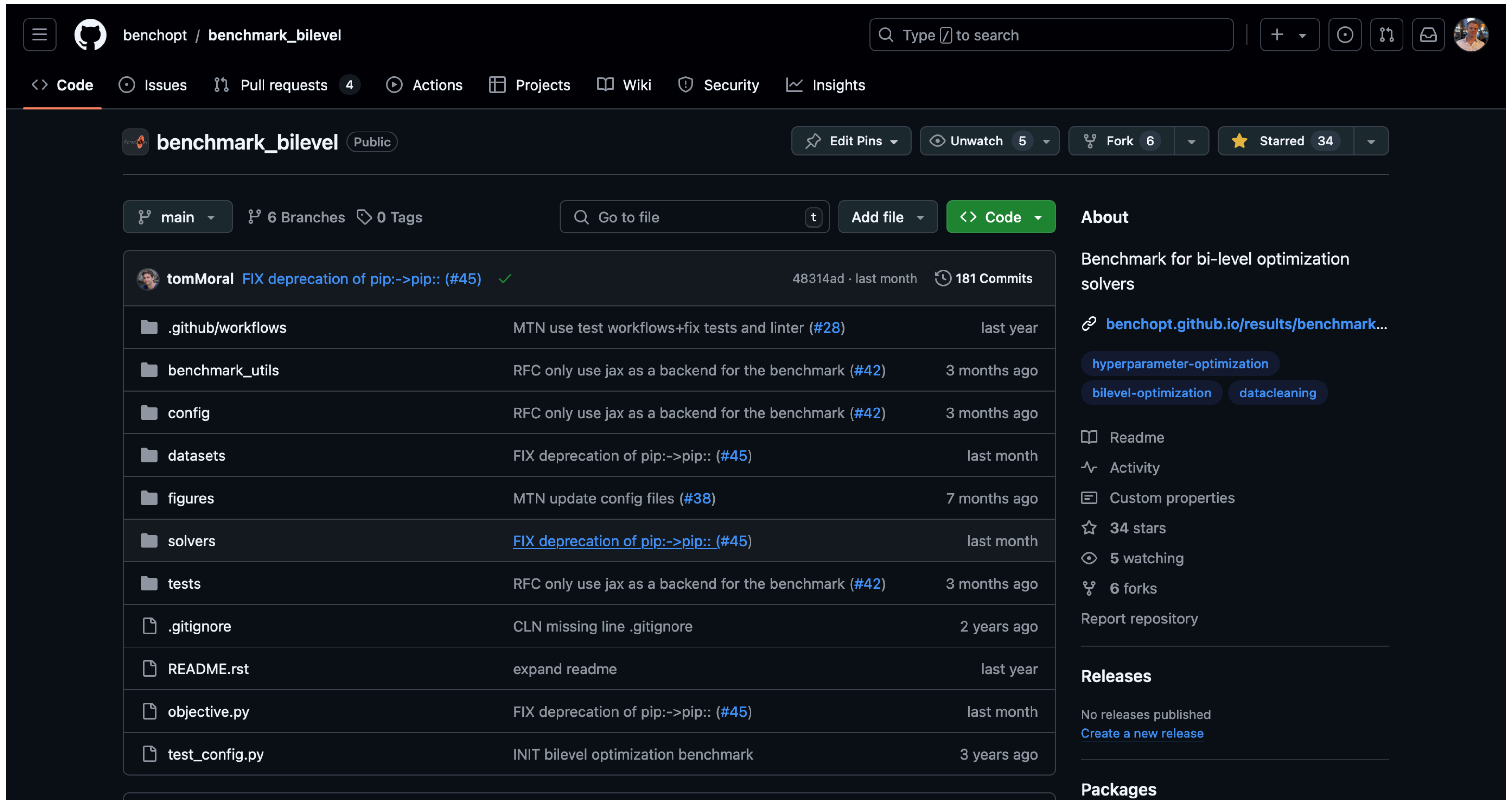
- Still missing the dependency on the inner number of samples

Numerical evaluation of bilevel algorithms

Benchmark of bilevel algorithms

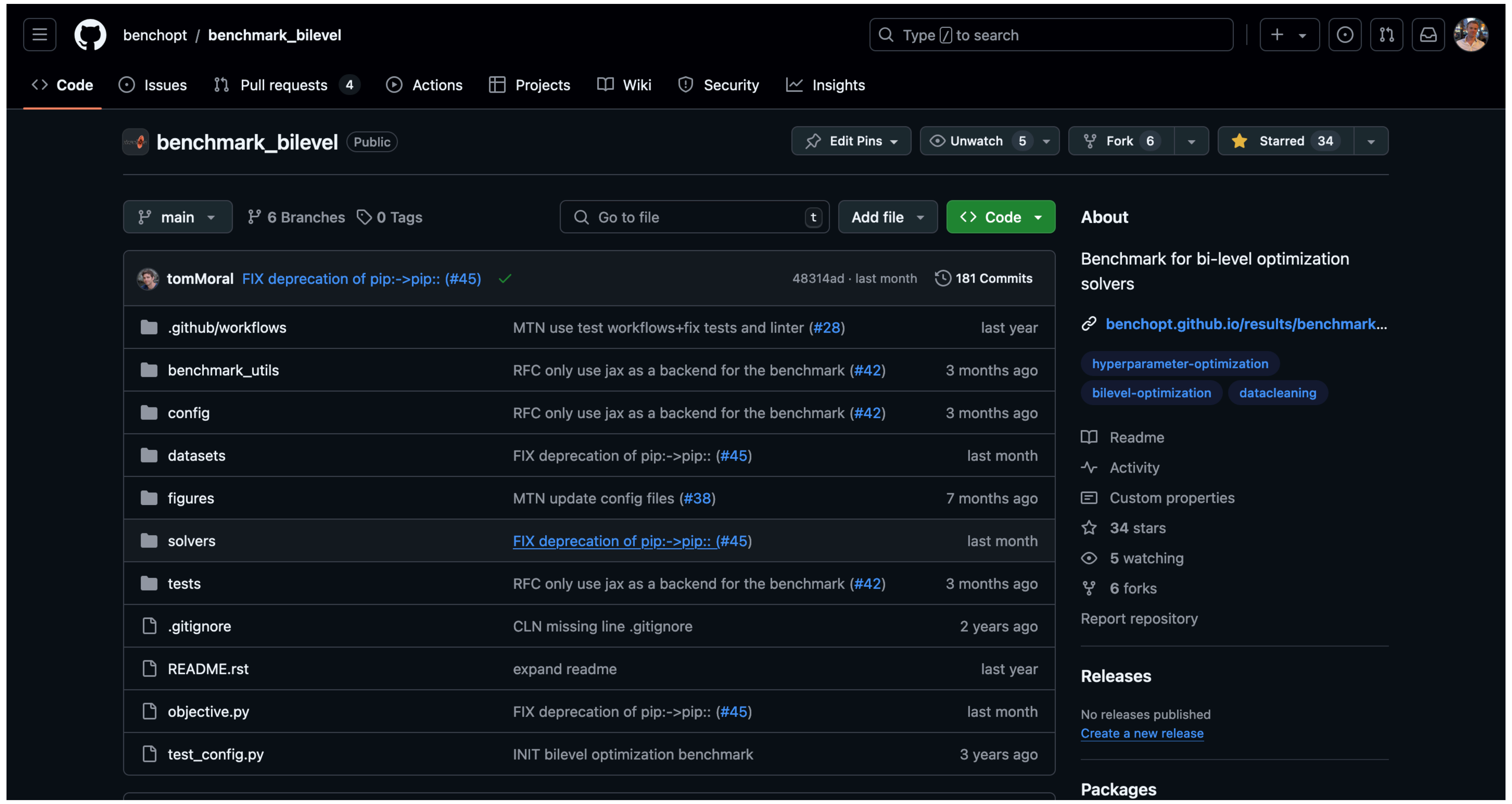
Benchmark of bilevel algorithms

- Open and reproducible benchmark



Benchmark of bilevel algorithms

- Open and reproducible benchmark
- Benchopt ecosystem, Jax framework



T. Moreau et al. *Benchopt: Reproducible, efficient and collaborative optimization benchmarks*. In Advances in Neural Information Processing Systems (NeurIPS), 2022.

Benchmark of bilevel algorithms

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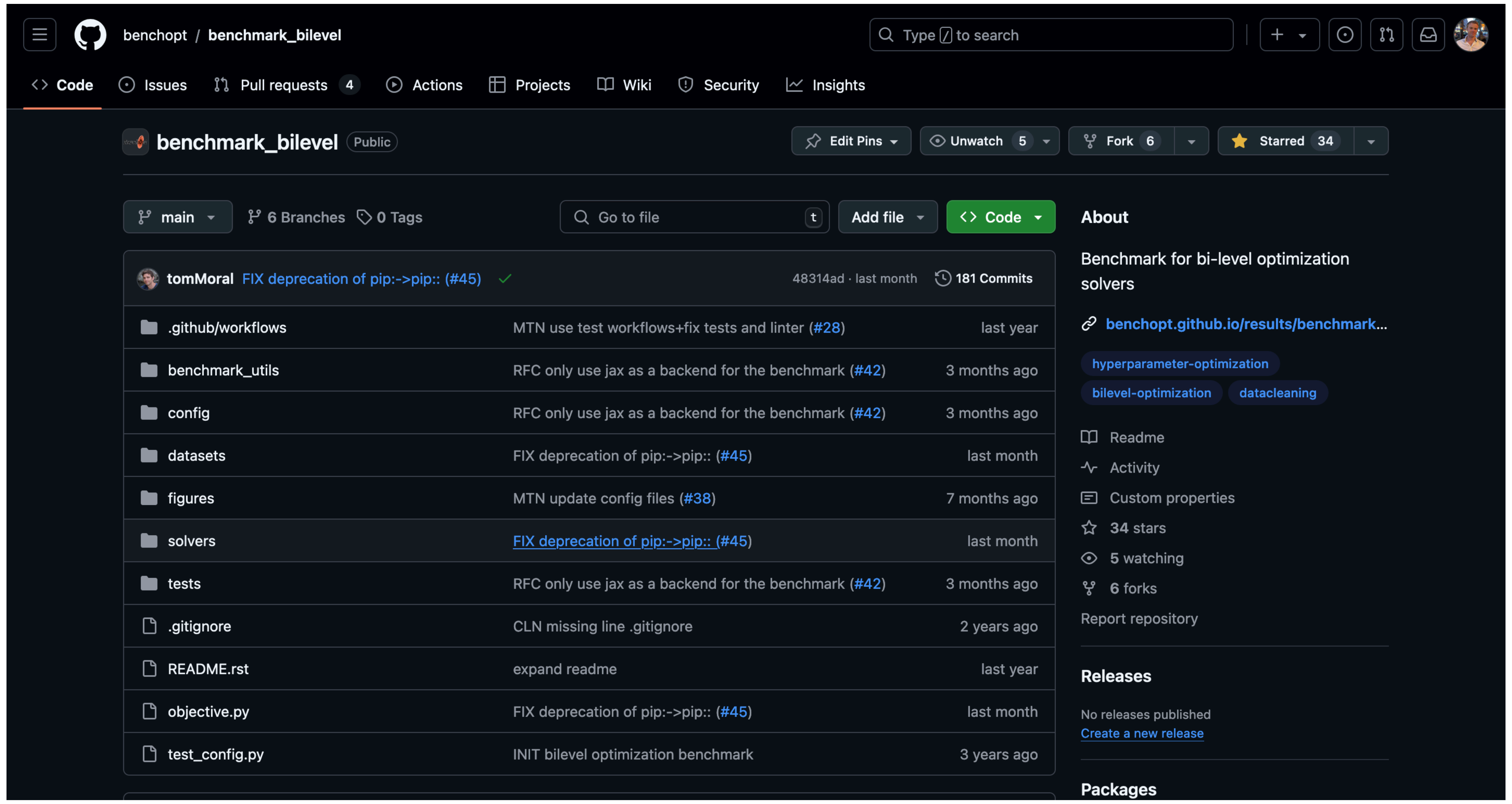

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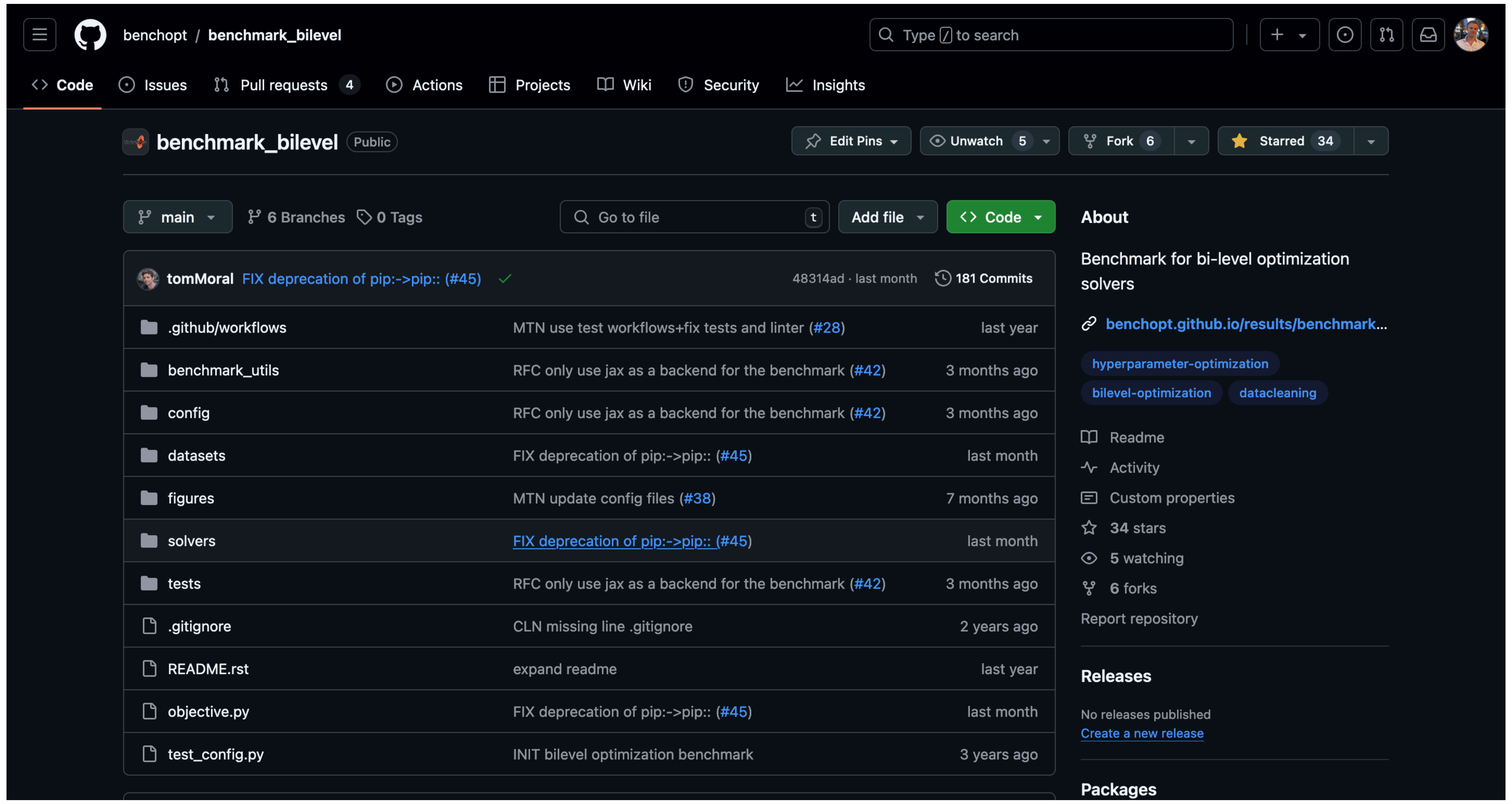
Benchmark of bilevel algorithms

Benchopt

- Open and reproducible benchmark
- Benchopt ecosystem, Jax framework
- 17 solvers: stochastic, deterministic, variance reduction, Hessian free…
- 4 tasks: quadratics, hyperparameter selection with ICJNN1 and COVTYPE, data hypercleaning with MNIST



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Data hypercleaning [Franceschi et al. '17]

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- Training samples with corrupted labels

Data hypercleaning [Franceschi et al. '17]

Setting

- Dataset: MNIST
- Training samples with corrupted labels
- Idea: Give more weight to uncorrupted samples

$$g(\lambda, \theta) = \frac{1}{n}\sum_{i=1}^{n} \sigma(\lambda_i)\ell(\theta x_i^{\text{train}}, y_i^{\text{train}}) + C_r \|\theta\|^2$$

with $\sigma(\lambda_i) \in [0, 1]$

Data hypercleaning [Franceschi et al. '17]

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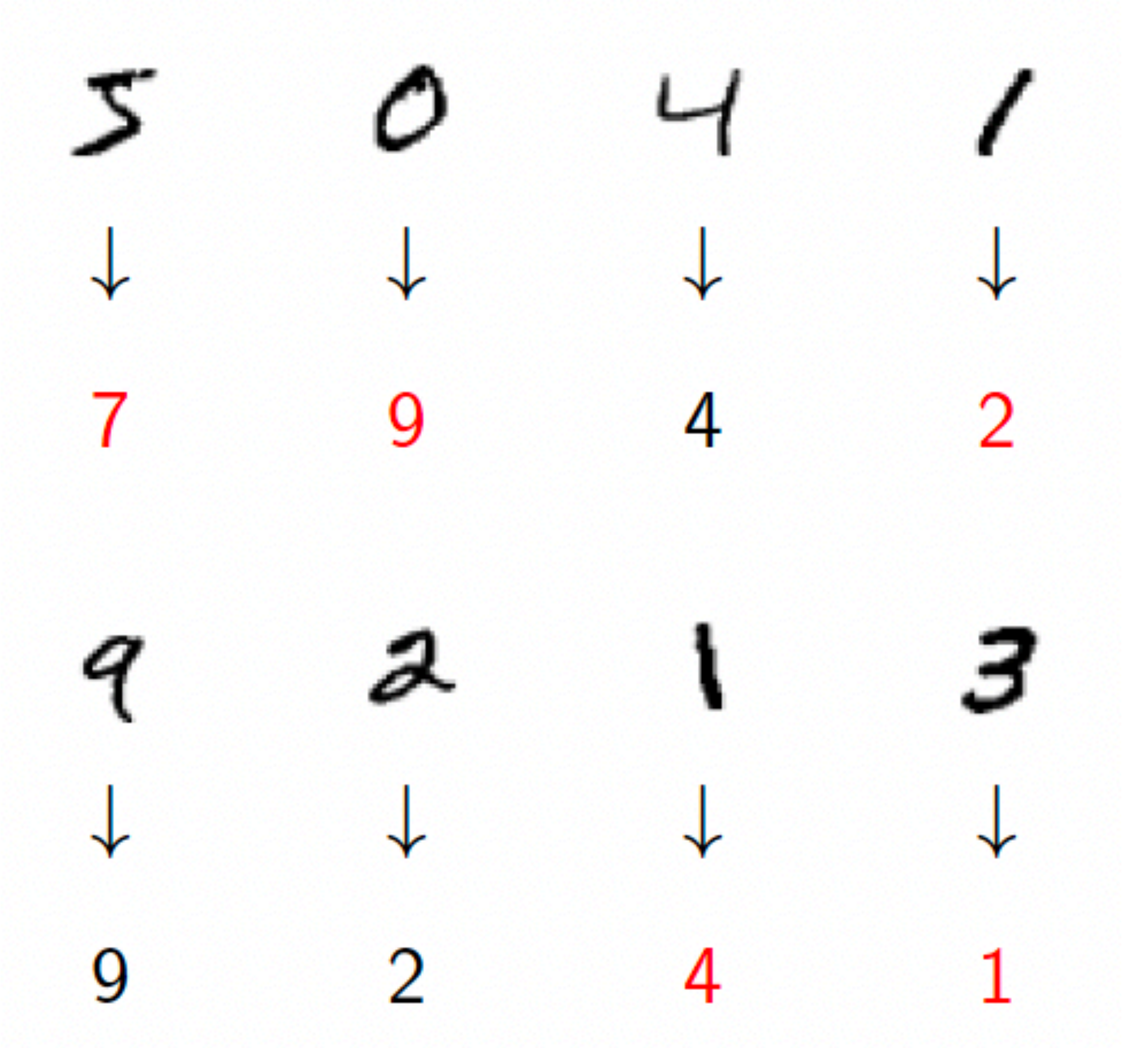
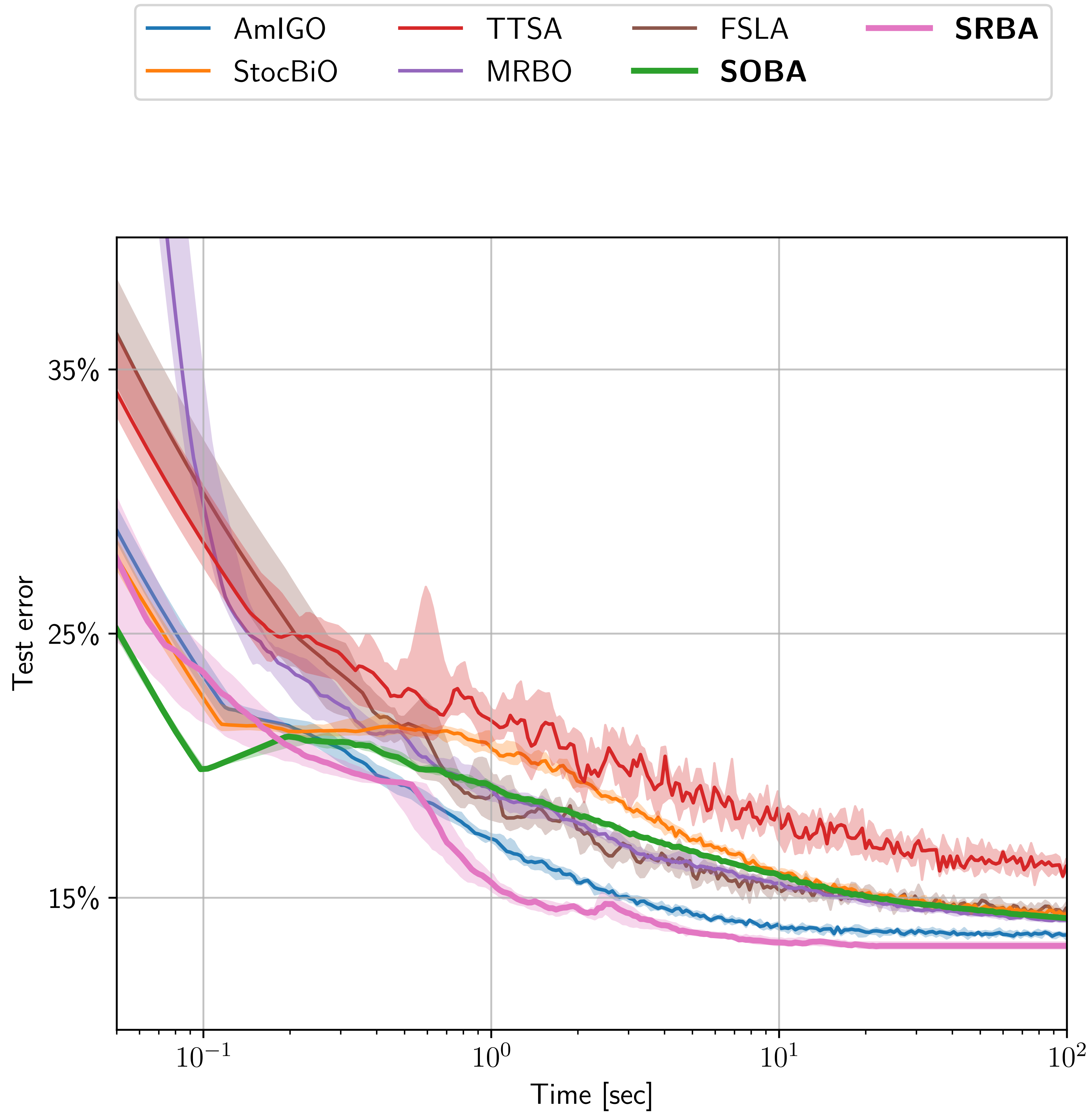
$$f(\theta^*(\lambda)) = \frac{1}{m} \sum_{j=1}^{m} \ell(\theta^*(\lambda) x_i^{\text{val}}, y_i^{\text{val}})$$

Correct labels



Data hypercleaning



Conclusion and perpectives

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- Instantiations of this framework yields similar oracle complexity to their single-level counterparts.
- Provided a complexity lower bound for bilevel problems.
- Provided an open benchmark to compare bilevel algorithms

Perspectives/Open questions

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- Sensitivity to the step sizes choice

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- Generalization performances of gradient-based hyperparameter selection procedures

Perspectives/Open questions

- Sensitivity to the step sizes choice
- Generalization performances of gradient-based hyperparameter selection procedures
- Understanding performances of implicit differentiation-based techniques when apply to problems with non-strongly convex inner functions

Thanks for your attention!!!

Conference papers

- **M. Dagréou**, P. Ablin, S. Vaiter, T. Moreau. A framework for bilevel optimization that enables stochastic and global variance reduction algorithm. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2022. *Oral*

- **M. Dagréou**, T. Moreau, S. Vaiter, P. Ablin. A Lower Bound and a Near-Optimal Algorithm for Bilevel Empirical Risk Minimization. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2024.

- T. Moreau et al. Benchopt: Reproducible, efficient and collaborative optimization benchmarks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2022.

Miscellaneous

- **M. Dagréou**, P. Ablin, S. Vaiter, T. Moreau. How to compute Hessian-vector products? In *ICLR blogpost track*, 2024. *Spotlight*