Data-Driven Performance Guarantees for Classical and Learned Optimizers

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Collaborators

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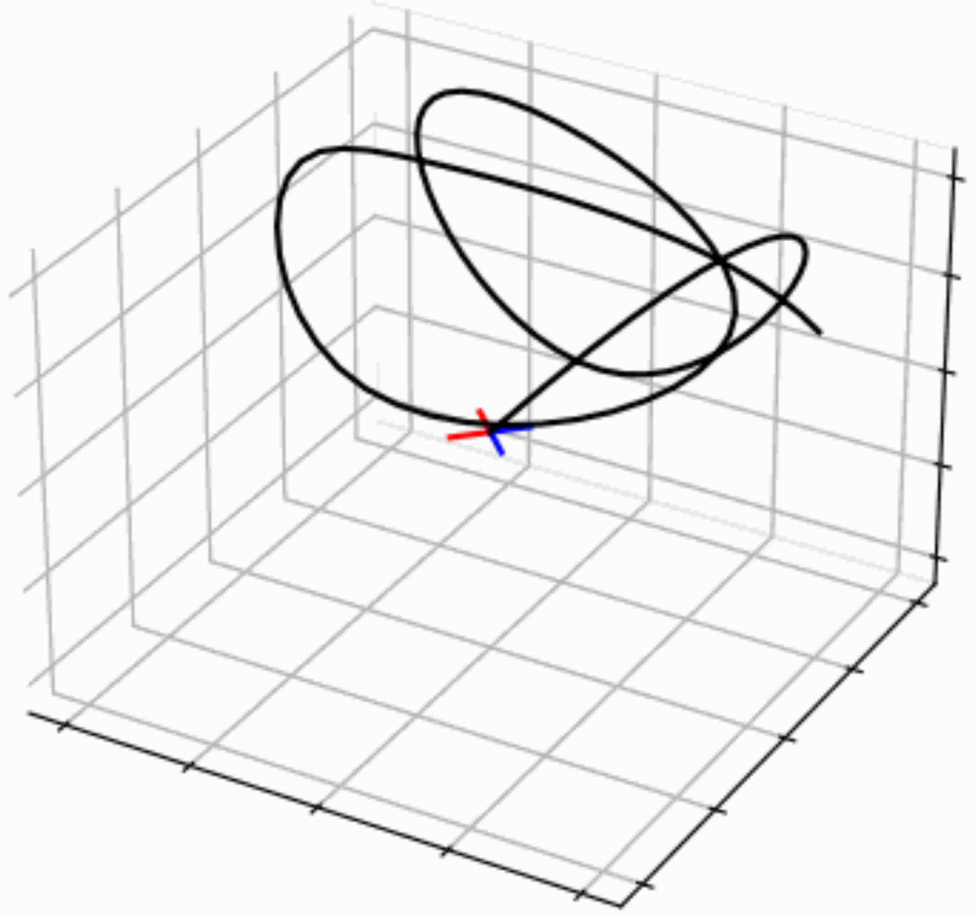
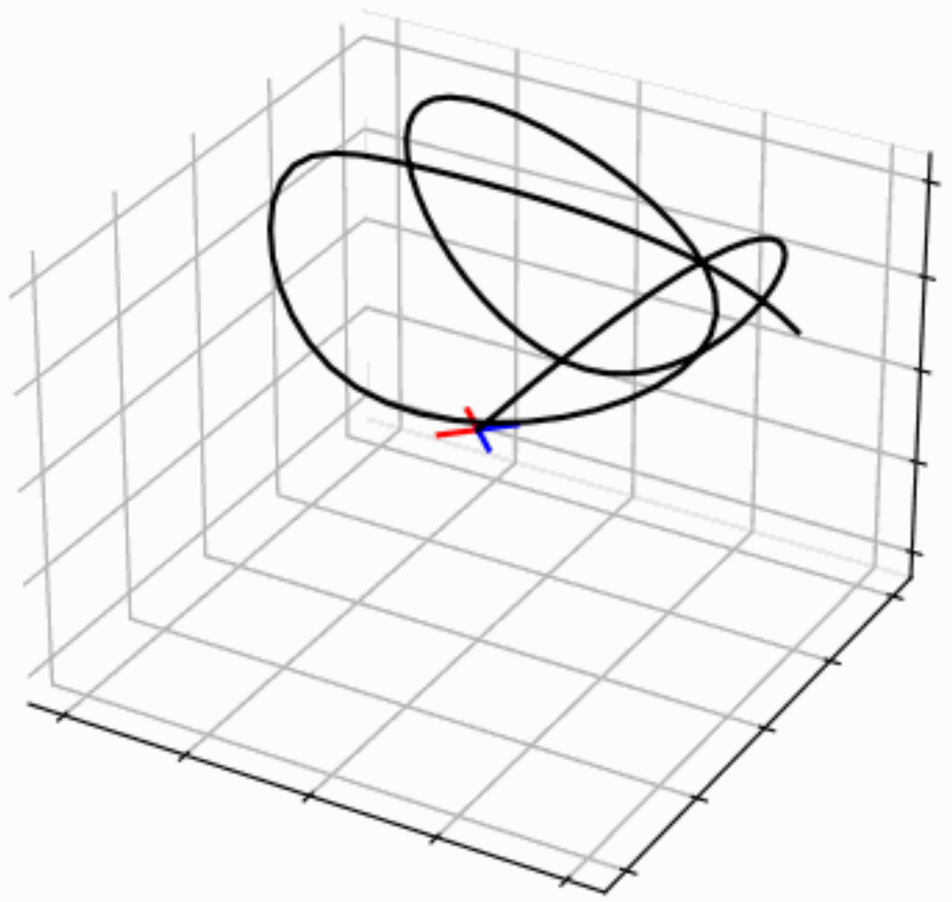
Tracking a reference trajectory with a quadcopter



Success!
(If given enough time)



Failure: not enough time to solve

Model predictive control

optimize over a smaller horizon (T steps),
implement first control,
repeat

Current state,
reference trajectory

Model predictive controller

$$
\begin{array}{ll}
\text{minimize} & \sum_{t=1}^{T} \|x_t - x_t^{\text{ref}}\|_2^2 \\
\text{subject to} & x_{t+1} = Ax_t + Bu_t \\
& x_t \in \mathcal{X}, \quad u_t \in \mathcal{U} \\
& x_0 = x_{\text{init}}
\end{array}
$$

Control
inputs

Challenge: we need faster methods for optimization

Empirically **Guarantees**

Claim: real-world optimization is parametric

Parameter
θ $\longrightarrow$

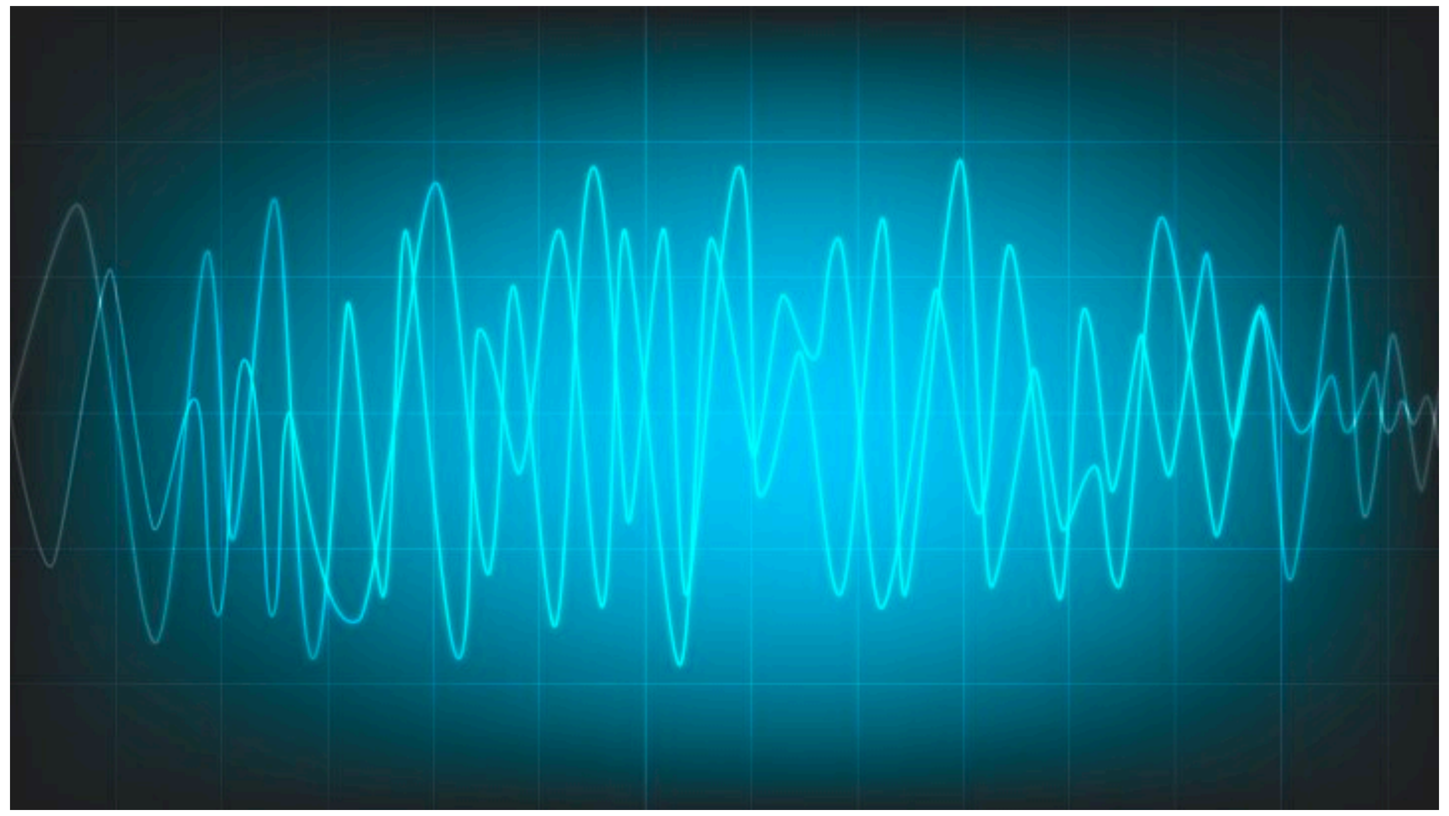
$$\begin{array}{ll} \text{minimize} & f_\theta(z) \\ \text{subject to} & g_\theta(z) \leq 0 \end{array}$$

$\longrightarrow$ Optimal solution
$z^\star(\theta)$

Robotics and control

Energy

Signal processing



Data-Driven Performance Guarantees for Classical and Learned Optimizers

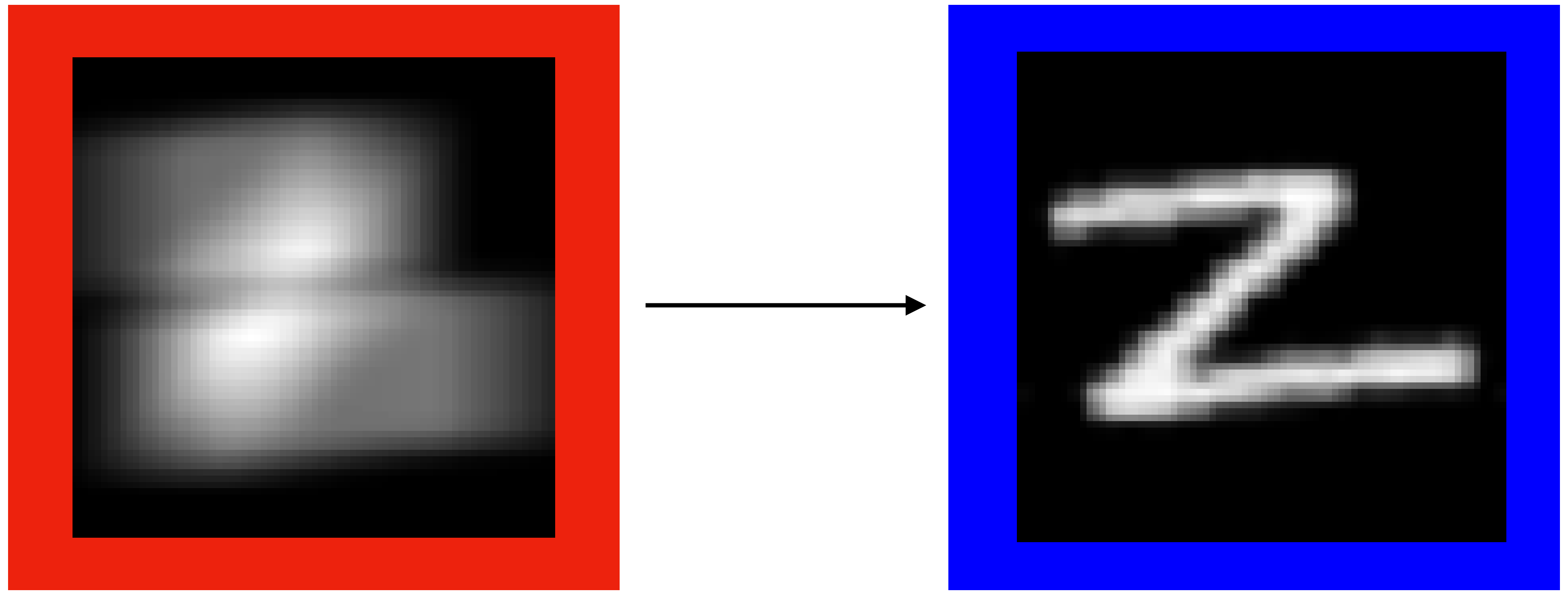
Parametric setting ✓

Faster optimization methods

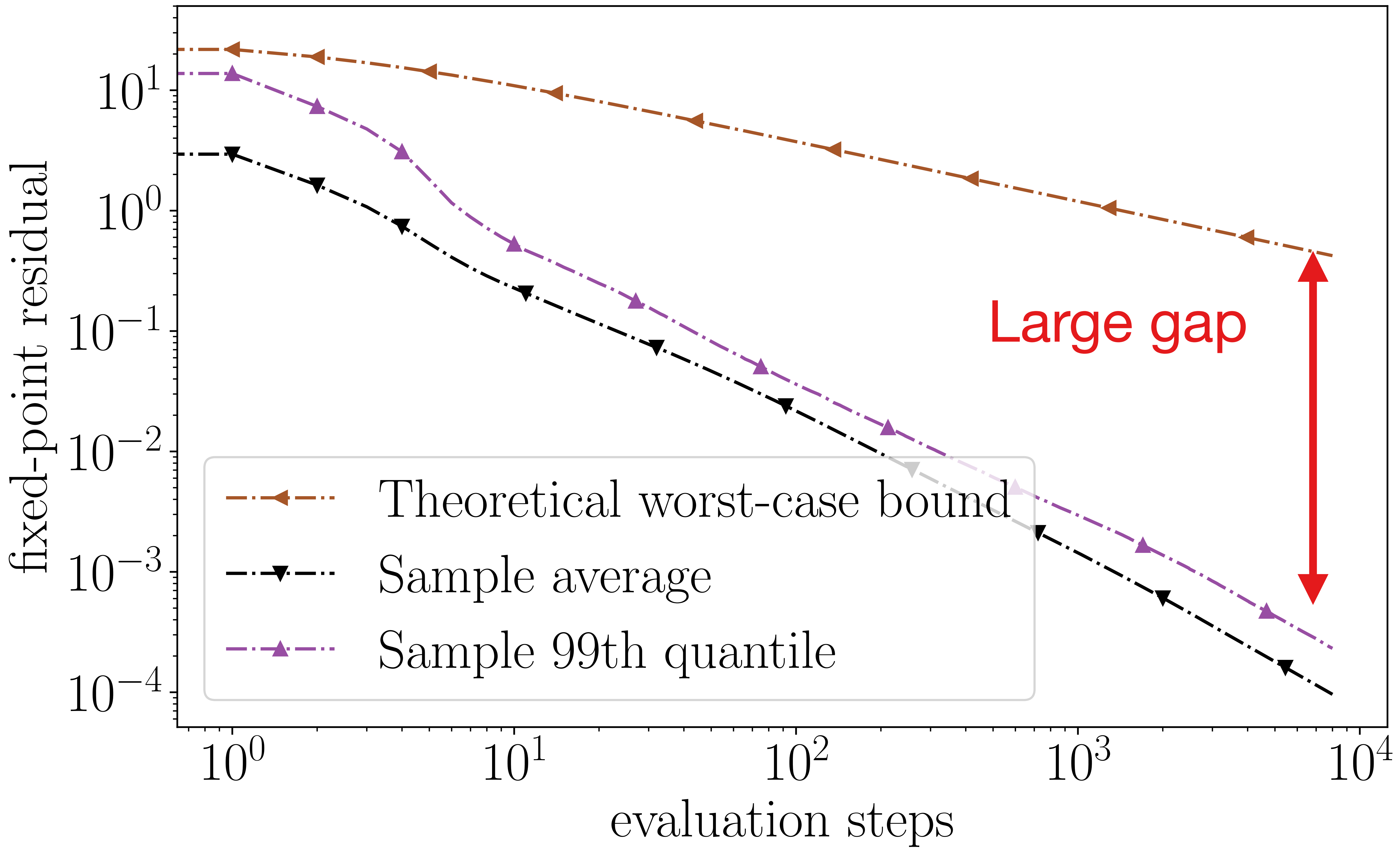
~~Empirical~~ Guarantees

Worst-case bounds can be very loose

Example: image deblurring



1000 problems solved with OSQP



Quadratic program

minimize $\|Ax - b\|_2^2 + \lambda \|x\|_1$

subject to $0 \le x \le 1$

Worst-case bounds are pessimistic and do not consider the parametric structure

Approach: probabilistically bound over the parametric distribution

Our recipe for guarantees for classical optimizers

algorithm steps

tolerance

$$e(\theta) = \mathbf{1}(\ell^{k}(\theta) > \epsilon)$$

Any metric
(*e.g.*, fixed-point residual)

Step 1
Run k steps
for N parametric problems

Parameters

Candidate solutions

θ

Run k steps

$z^{k}(\theta)$

Step 2
Evaluate the empirical risk

$$\frac{1}{N}\sum_{i=1}^{N} e(\theta_i)$$

Step 3
Bound the risk
(Next slide)

risk $= \mathbf{E}_{\theta \sim \mathcal{X}} e(\theta) \leq$ bound

Statistical learning theory can bound the risk

algorithm steps

tolerance

$$e(\theta) = \mathbf{1}(\ell^{k}(\theta) > \epsilon)$$

Any metric
(*e.g.*, fixed-point residual)

Sample convergence bound: with probability $1-\delta$ [Langford et. al 2001]

$$\mathbf{E}_{\theta\sim\mathcal{X}} e(\theta) \leq \mathrm{KL}^{-1}\left(\frac{1}{N}\sum_{i=1}^{N} e(\theta_i) \middle| \frac{\log(2/\delta)}{N}\right)$$

$\mathbf{P}(\ell^k(\theta) > \epsilon) =$ risk $\leq \mathrm{KL}^{-1}$ (empirical risk | regularizer)

"With probability $1-\delta$, 90% of the time the fixed-point residual is below $\epsilon = 0.01$ after $k = 20$ steps"

Image deblurring guarantees

With 1000 samples, we provide strong probabilistic guarantees on the 99th quantile

Data-Driven Performance Guarantees for Classical and Learned Optimizers

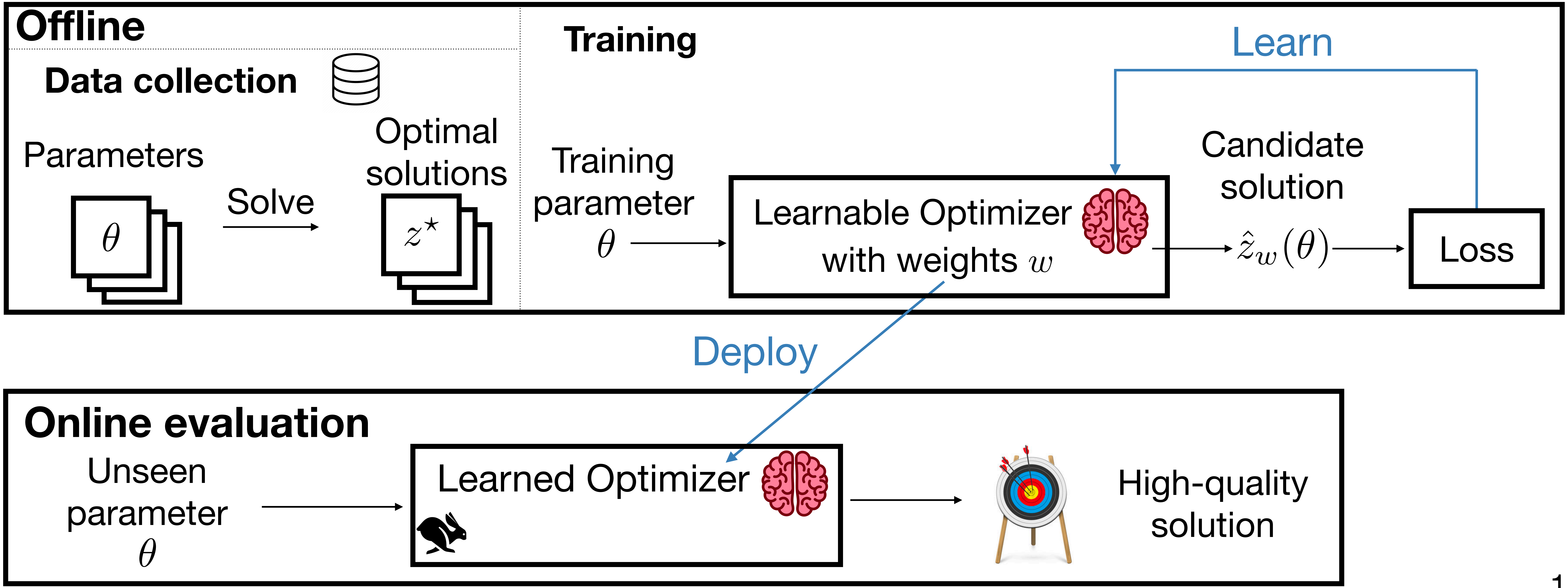
Parametric setting ✓

Uses machine learning to accelerate the optimizer

The learning to optimize paradigm

Goal: solve the parametric optimization problem fast

$$\begin{array}{ll} \text{minimize} & f_\theta(z) \\ \text{subject to} & g_\theta(z) \leq 0 \end{array}$$



Data-Driven Performance Guarantees for Classical and Learned Optimizers

Parametric setting ✓

Faster optimization methods

Empirical

Guarantees

Goal: endow learned optimizers with generalization guarantees

PAC-Bayes guarantees for learned optimizers

algorithm steps

tolerance

$$e_w(\theta) = \mathbf{1}(\ell_w^k(\theta) > \epsilon)$$

learnable weights

McAllester bound: given posterior and prior distributions [McAllester et. al 2003] P and P_0, with probability $1-\delta$

$$\mathbf{E}_{\theta\sim\mathcal{X}}\mathbf{E}_{w\sim P}e_w(\theta) \leq \boxed{\mathrm{KL}^{-1}\left(\frac{1}{N}\sum_{i=1}^{N}\mathbf{E}_{w\sim P}e_w(\theta_i)\middle|\frac{1}{N}\left(\mathrm{KL}(\mathrm{P}\parallel\mathrm{P}_0)+\log(\mathrm{N}/\delta)\right)\right)}$$

risk $\leq \mathrm{KL}^{-1}$ (empirical risk | regularizer)

Optimize the bounds directly

Learned algorithms for sparse coding

Noisy measurements
$\theta = b$

→

Sparse coding

Recover sparse $z^\star$ from $b = Dz^\star + \sigma$

→

Ground truth sparse signal
$z^\star$

D: dictionary, σ: noise

Standard technique

minimize $\|Dz - b\|_2^2 + \lambda \|z\|_1$

ISTA (iterative shrinkage thresholding algorithm)

(Classical optimizer)

$$z^{j+1} = \text{soft threshold}_{\frac{\lambda}{L}}\left(z^j - \frac{1}{L}D^T(Dz^j - b)\right)$$

Learned ISTA

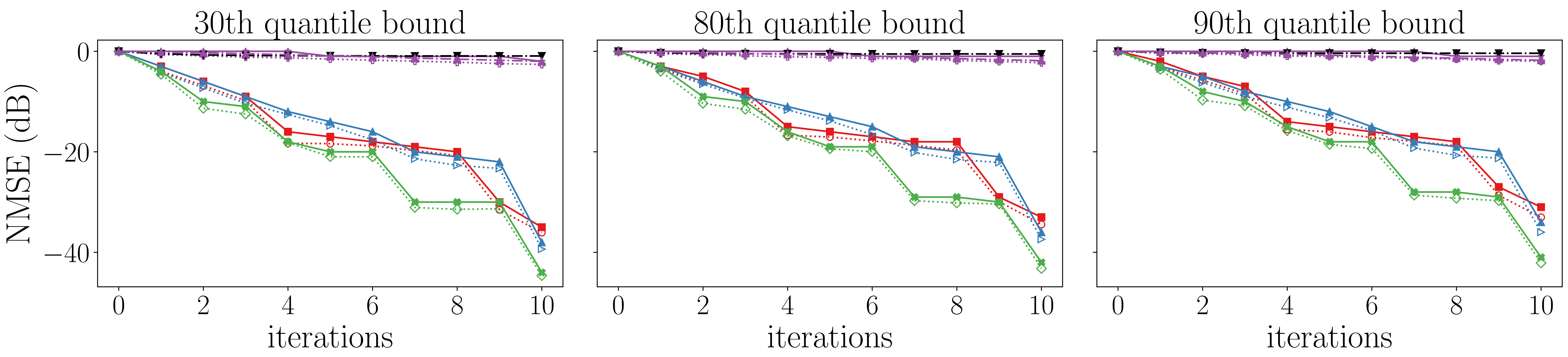
(Learned optimizer)

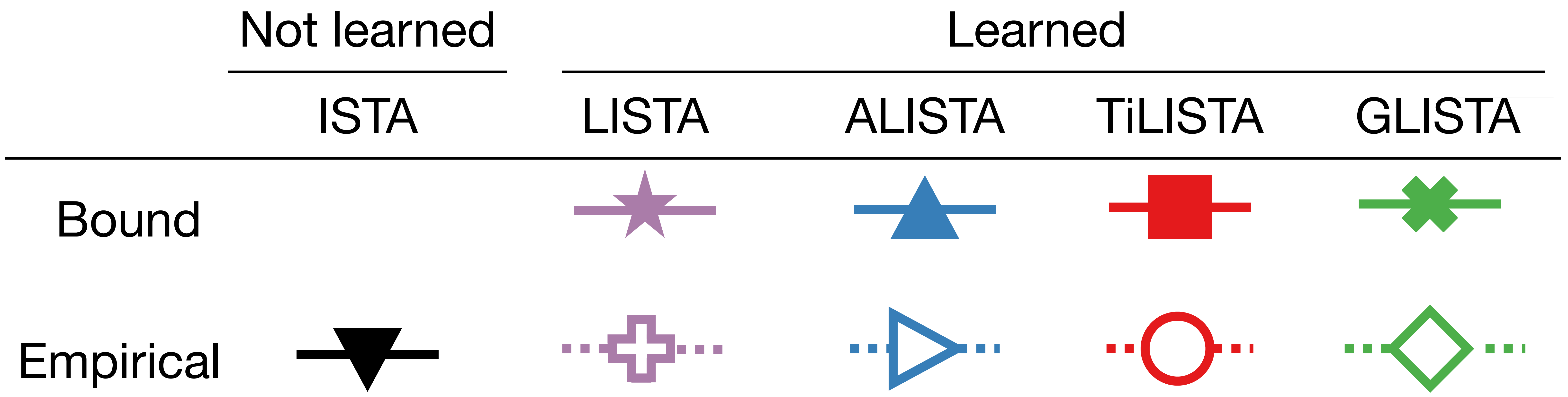
$$z^{j+1} = \text{soft threshold}_{\psi^j}\left(W_1^j z^j + W_2^j b\right)$$

+ variants [Gregor and LeCun 2010, Liu et. al 2019]

soft threshold$_\psi(z) = \textbf{sign}(z)\max(0, |z| - \psi)$

Learned ISTA results for sparse coding

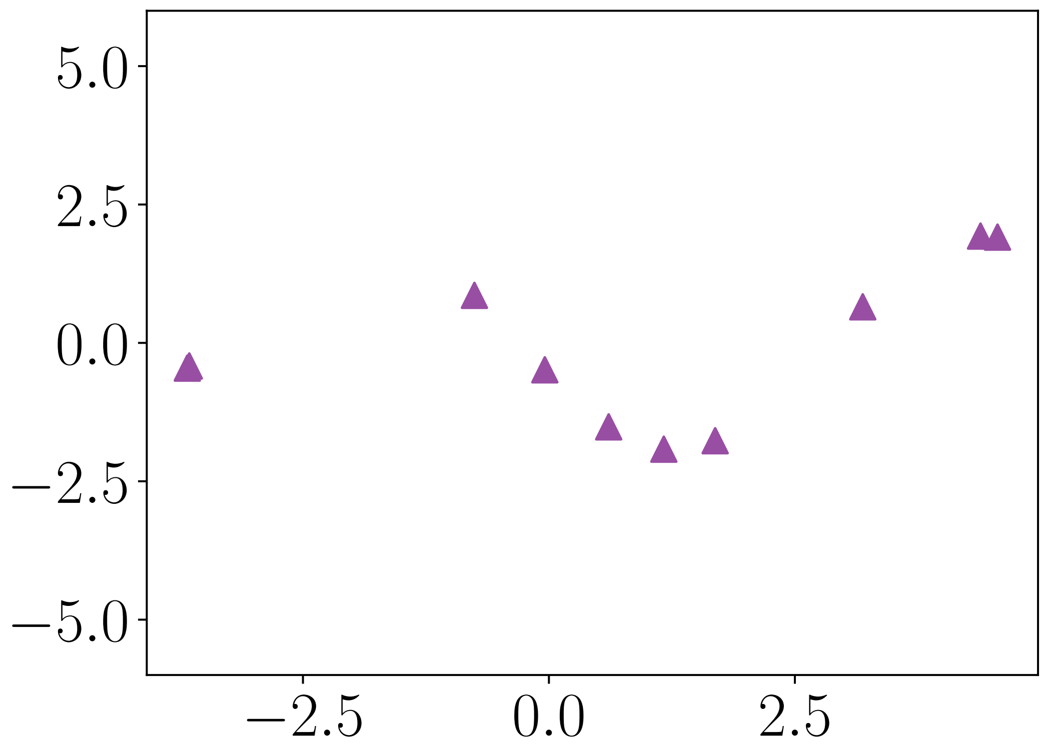




Our bounds are close to empirical performance

Learned optimizers provably perform well in just 10 steps

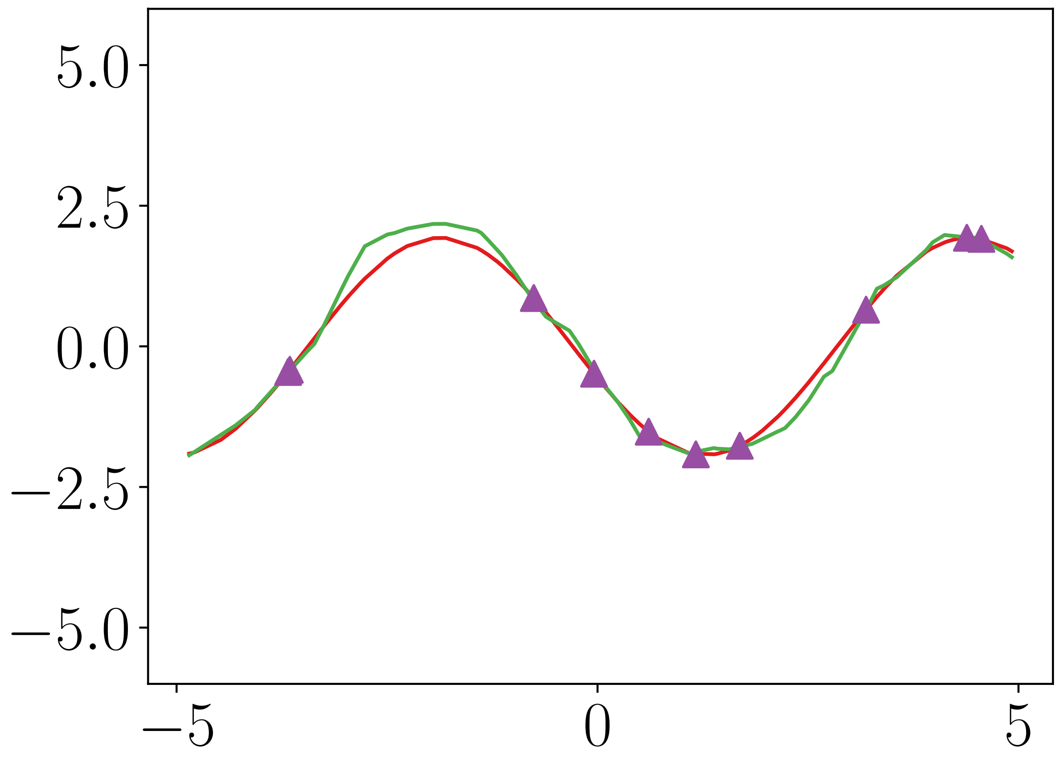
K-shot Meta-Learning for Sine Curves



Neural network learning

find weights z so that $g_z(x_i) \approx y_i$

predictor with weights z



Training dataset
with K points

$\mathcal{D}^{\text{train}}$

Gradient step

$$\hat{z} = z - \alpha \nabla_z \mathcal{L}(z, \mathcal{D}^{\text{train}})$$

Weights that generalize
to new points quickly

$\hat{z}$

Model-Agnostic Meta-Learning (MAML) [Finn et. al 2017]

MAML learns a shared initialization z so that $\hat{z}$ performs well on test data

Visualizing Guarantees: K-shot Meta-Learning for Sine Curves

With high probability, 87% of the time MAML stays within the band

The pretrained baseline only stays within the band 33% of the time

Conclusions: Data-Driven Performance Guarantees

- For **classical optimizers** our probabilistic bounds outperform worst-case guarantees
- We endow **learned optimizers** with strong generalization guarantees

Data can help us

- **Accelerate** optimization algorithms
- **Guarantee** their performance

Data-Driven Performance Guarantees for Classical and Learned Optimizers
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Submitted
https://arxiv.org/pdf/2404.13831.pdf

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