Data-Driven Algorithm Design and Verification for Parametric Convex Optimization

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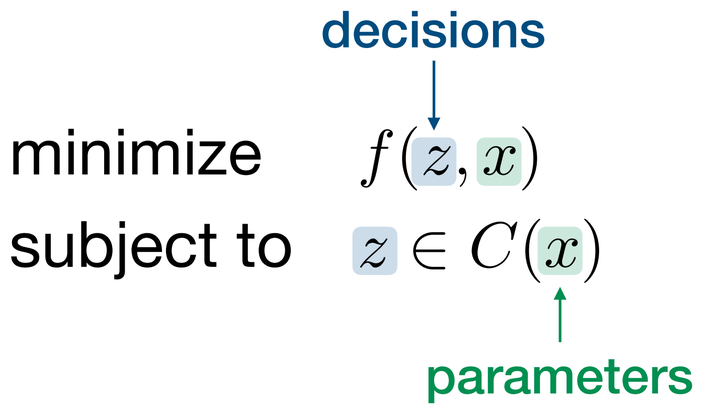
Most applications require fast and effective decisions in real-time

Real-time optimization can help us



objective f: energy consumption, costs
constraints C: dynamics, physical limits

re-planning in real-time is the key to effective decision-making

How do we solve such problems?

First-order methods are now widely popular…

use only **first-order information** (e.g., gradients)
to solve optimization problems

example
projected gradient descent

minimize $f(z, x)$
subject to $z \in C(x)$

$$z^{k+1} = \Pi_{C(x)}(z^k - \theta \nabla f(z^k, x))$$

projection gradient step

benefits of first-order methods

✓cheap iterations
✓easy to warm-start

embedded optimization

large-scale optimization

…and they can solve many constrained convex problems!

Linear Programs

PDLP

Applegate, Díaz, Hinder, Lu, Lubin, O'Donoghue, Schudy (2021)

Quadratic Programs

OSQP

Stellato, Banjac, Goulart, Bemporad, Boyd (2020)

Conic Programs

SCS

SPLITTING CONIC SOLVER

O'Donoghue, Chu, Parikh, Boyd (2016)

But they can converge slowly

major issue in safety-critical applications with

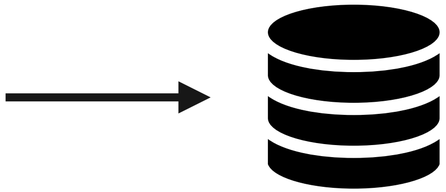
real-time requirements

limited computing power

💡 main idea

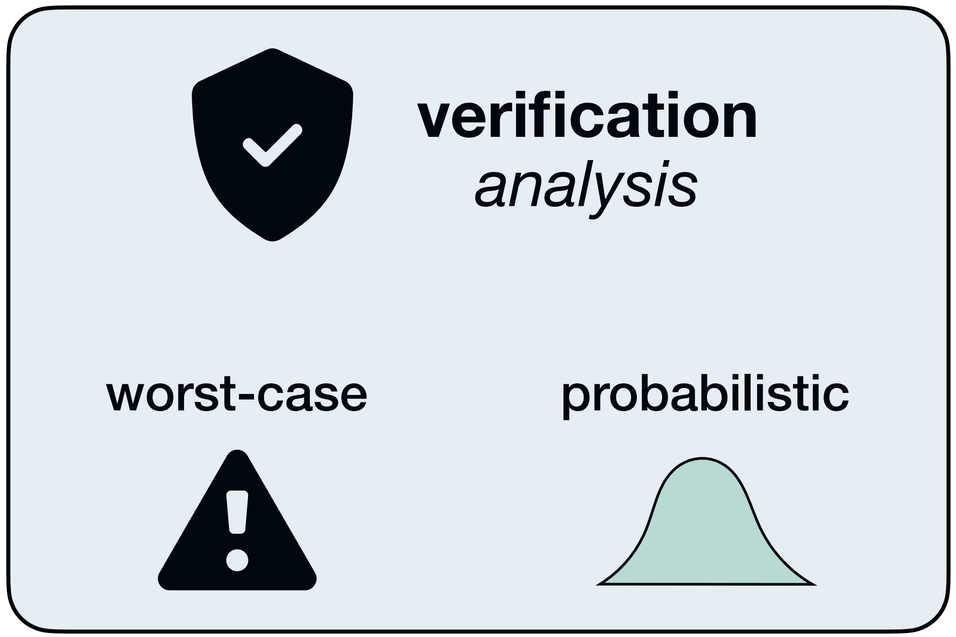
in most applications we repeatedly solve the same problem with varying parameters

$$\begin{aligned} \text{minimize} \quad & f(z, x) \\ \text{subject to} \quad & z \in C(x) \end{aligned}$$



large amount of data
(e.g., instances, solutions)

First-order methods in parametric convex optimization



Performance verification

Convergence of first-order methods

iterations

$$z^{k+1} = T(z^k, x) \quad \text{for } k = 0, 1, \ldots$$

operator
(e.g., contractive, averaged)

goal: find fixed-points

$$z^\star = T(z^\star, x)$$

example
gradient descent

problem

minimize $f(z, x)$ ⟶ **optimality conditions** $\nabla f(z^\star, x) = 0$

iterations

$$z^{k+1} = z^k - \theta \nabla f(z^k, x)$$

fixed-points

$$z^\star = z^\star - \theta \nabla f(z^\star, x)$$

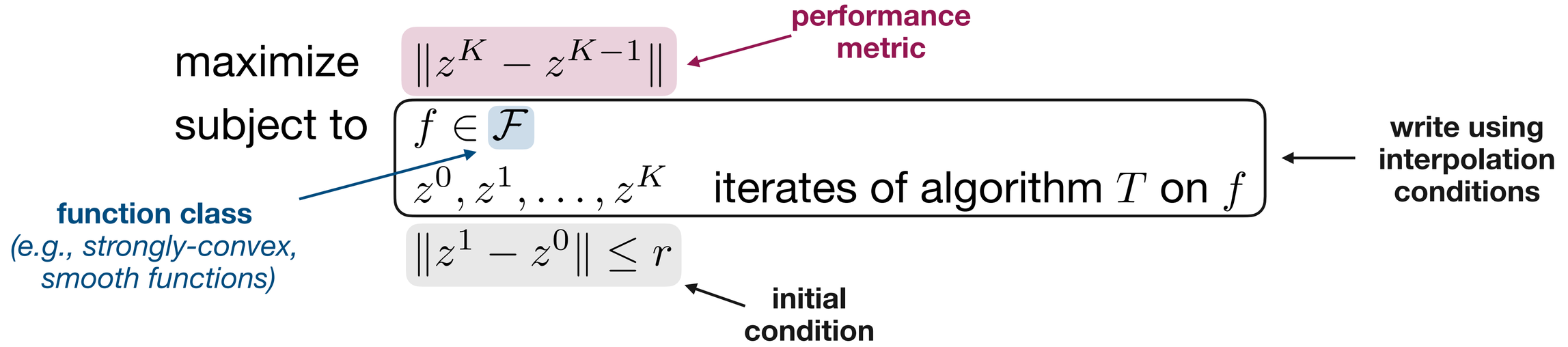
same as

performance metric

$$r^k(x) = \|T(z^{k-1}) - z^{k-1}\| = \|z^k - z^{k-1}\|$$

fixed-point residual
(converges to 0)

Classical convergence bounds via Performance Estimation



convex SDP
Gram matrix reformulation

$$G = \begin{bmatrix} \|z^1 - z^0\|_2^2 & (z^1 - z^0)^T g^1 & (z^1 - z^0)^T g^0 \\ (z^1 - z^0)^T g^1 & \|g^1\|_2^2 & (g^1)^T g^0 \\ (z^1 - z^0)^T g^0 & (g^1)^T g^0 & \|g^0\|_2^2 \\ & & \ddots \end{bmatrix}$$

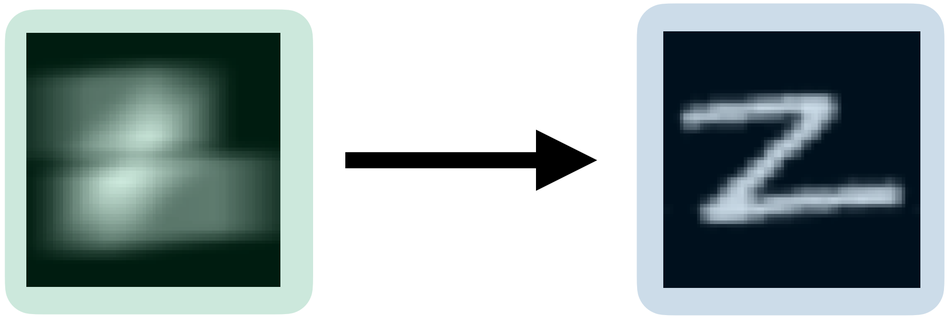
gradients

independent from iterate dimensions

Drori and Teboulle (2014), Taylor, Hendrickx, Gilneur (2017), and many others including Ryu, De Klerk, Grimmer…

Classical worst-case convergence bounds can be very loose

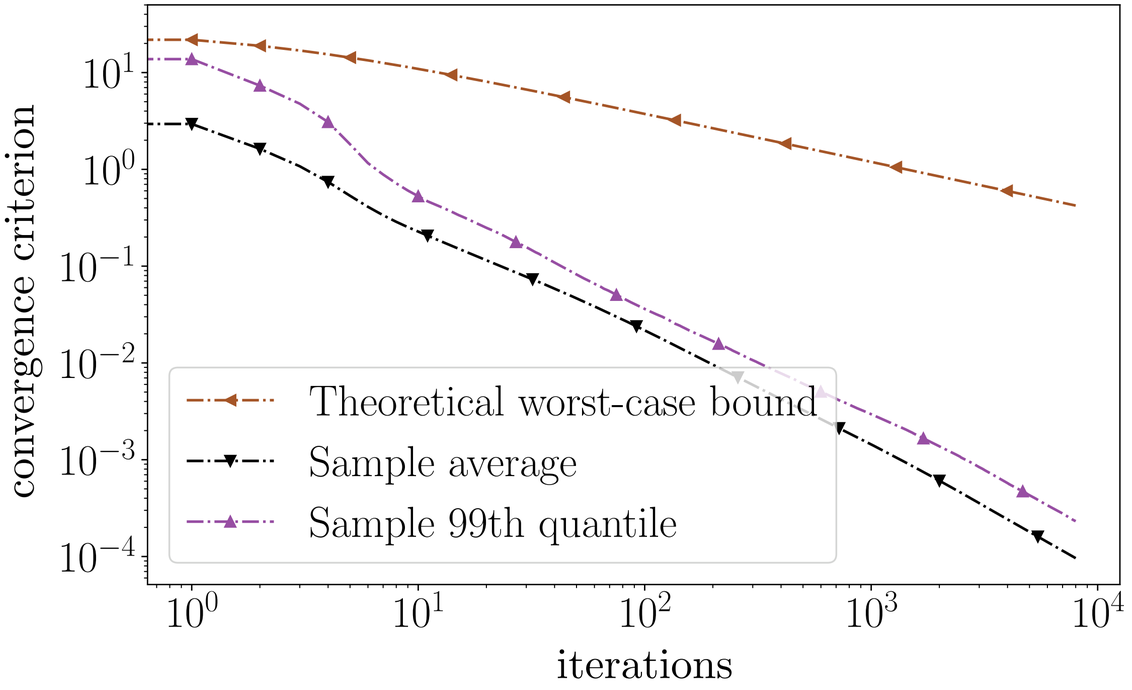
image deblurring problem
emnist dataset



$$\begin{aligned} \text{minimize} \quad & \|Az - x\|_2^2 + \lambda \|z\|_1 \\ \text{subject to} \quad & 0 \leq z \leq 1 \end{aligned}$$

blurred image

deblurred image

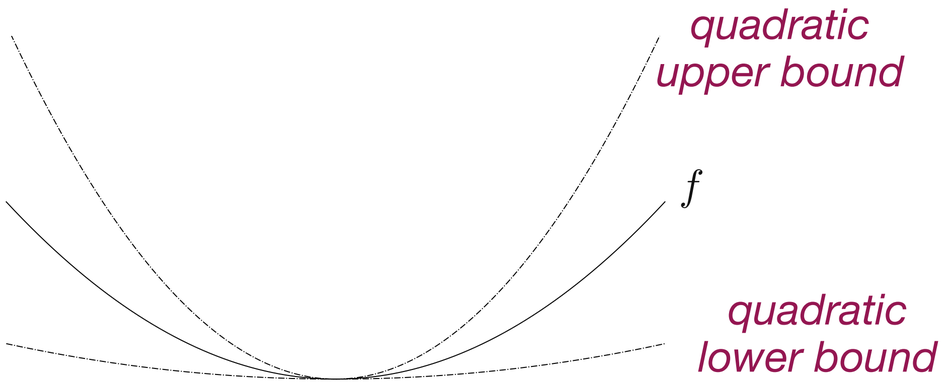


why are worst-case bounds pessimistic?

Issues with classical convergence analysis

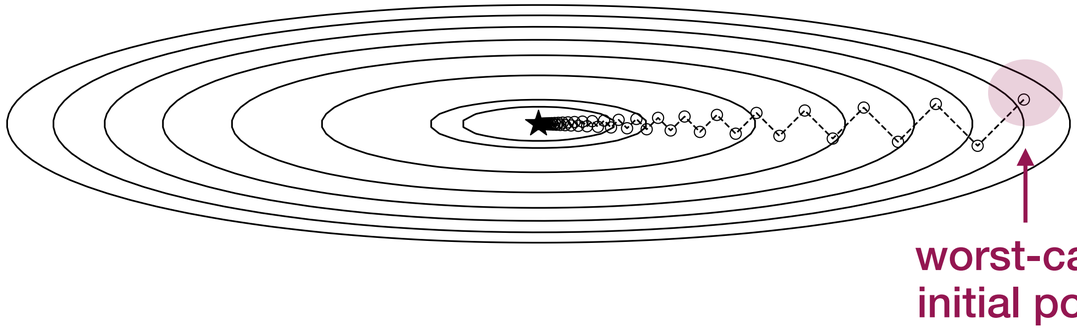
general function classes

(f is strongly convex and smooth...)



we may never encounter that function

pessimistic bounds



we may never start from that point

practical settings

minimize $f(z, x)$

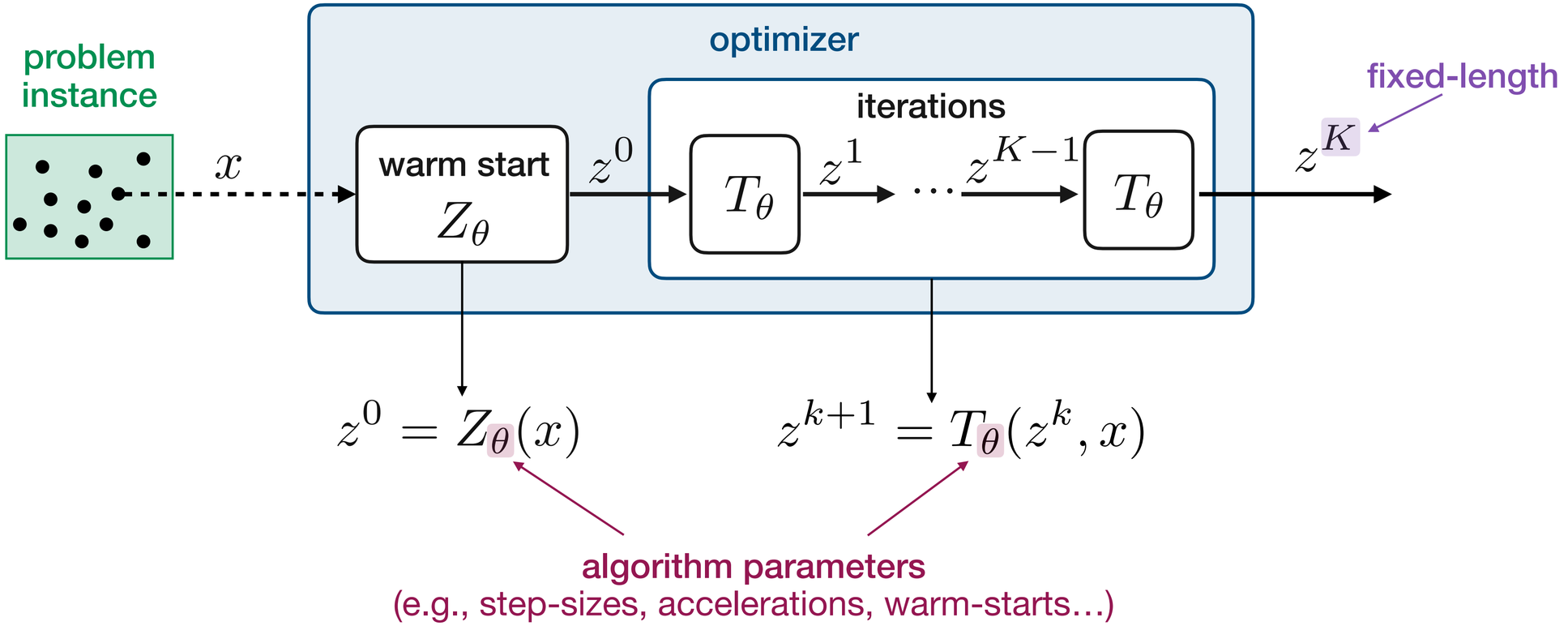
subject to $z \in C(x)$

same problem with varying parameters

$x \sim \mathbf{P}$

(unknown distribution)

Algorithms as fixed-length computational graphs



example

projected gradient descent

$$z^{k+1} = \Pi_{C(x)}(z^k - \theta \nabla_z f(z^k, x))$$

Verifying the algorithm performance after K iterations

goal

estimate norm of fixed-point residual

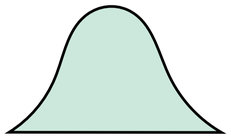
$$r^K(x) = \|z^K - z^{K-1}\|$$

worst-case

$$\max_{x \in \mathcal{X}} r^K(x) \leq \epsilon$$

problem instances

convergence tolerance



probabilistic

$$\mathbf{P}\left(r^K(x) > \epsilon\right) \leq \eta$$

probability bound

problem instances

convergence tolerance

Vinit Ranjan

Worst-case algorithm verification

Parametric quadratic optimization

performance metric

problem instances

$$\max_{x \in \mathcal{X}} r^K(x) = \quad \text{maximize} \quad \|z^K - z^{K-1}\|$$
$$\text{subject to} \quad z^{k+1} = T_\theta(z^k, x), \quad k = 0, \ldots, K-1$$
$$z^0 = Z_\theta(x), \quad x \in \mathcal{X}$$

directly encode proximal algorithms
without interpolation inequalities

	step	verification constraint
affine *(e.g., gradient, restarts, linear system solves)*	$Dz^{k+1} = Az^k + Bx$	$Dz^{k+1} = Az^k + Bx$
elementwise maximum *(e.g., separable projections, soft-thresholding,…)*	$z^{k+1} = \max\{z^k, 0\}$	$z^{k+1} \geq 0, \quad z^{k+1} \geq z^k$ $(z^{k+1})^T(z^{k+1} - z^k) = 0$

similar to ReLU

similar to neural network verification

Liu et al. (2021), Albarghouthi (2021)

Relaxing verification problem to an SDP

The verification problem is NP-hard
(by reduction from 0-1 integer programming)

→ **convex semidefinite program relaxation**

	step	verification constraint	relaxed constraint
elementwise maximum *(e.g., box projections, soft-thresholding,…)*	$z^{k+1} = \max\{z^k, 0\}$	$z^{k+1} \geq 0, \quad z^{k+1} \geq z^k$ $(z^{k+1})^T(z^{k+1} - z^k) = 0$	$z^{k+1} \geq 0, \quad z^{k+1} \geq z^k$ $\mathbf{tr}\left(\begin{bmatrix} I & -I/2 \\ -I/2 & 0 \end{bmatrix} M\right) = 0$ $M \succeq \begin{bmatrix} z^{k+1} \\ z^k \end{bmatrix} \begin{bmatrix} z^{k+1} \\ z^k \end{bmatrix}^T$

depends on iterate dimensions

Raghunathan et al. (2018), Dathathri et al. (2020),
Fazlyab et al. (2020), Chen et al. (2022), Brown et al. (2022)

Unconstrained QP

Exact SDP reformulation

minimize $(1/2)z^T P z + x^T z$ (parameters)

verification problem

maximize $\|z^K - z^{K-1}\|$

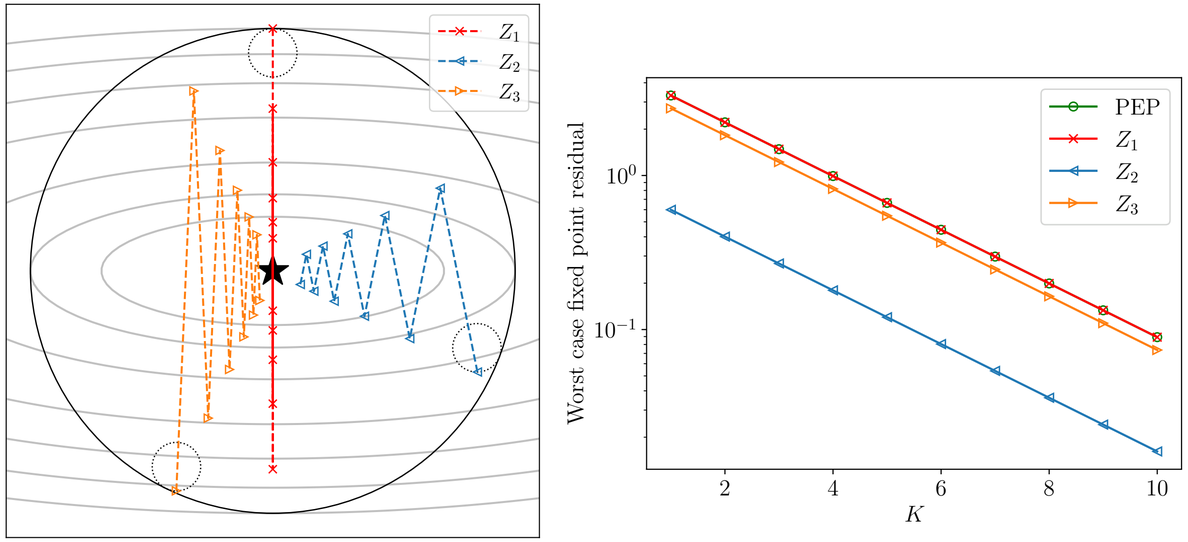
subject to $z^{k+1} = z^k - \theta(Pz^k + x), \quad k = 0, \ldots, K-1$ (gradient descent)

$z^0 = Z_\theta(x), \quad x \in \mathcal{X}$

warm-starts

case I $Z_\theta(x) = Z_1, Z_2,$ or Z_3

$x \in \mathcal{X} = \{0\}$



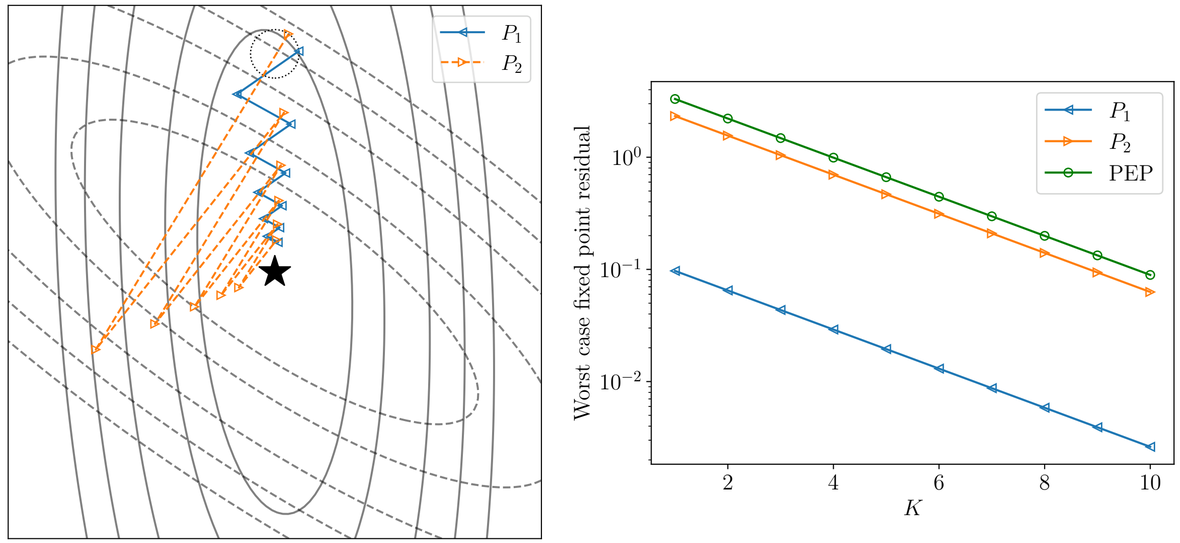
PEP cannot distinguish warm-starts

rotated functions

case II $Z_\theta(x) = \{z \mid \|z - 0.9 \cdot \mathbf{1}\| \leq 0.1\}$

$x \in \mathcal{X} = \{0\}$

P_1, P_2 rotations of P



PEP cannot distinguish quadratic functions

Nonnegative least-squares verification

nonnegative least squares

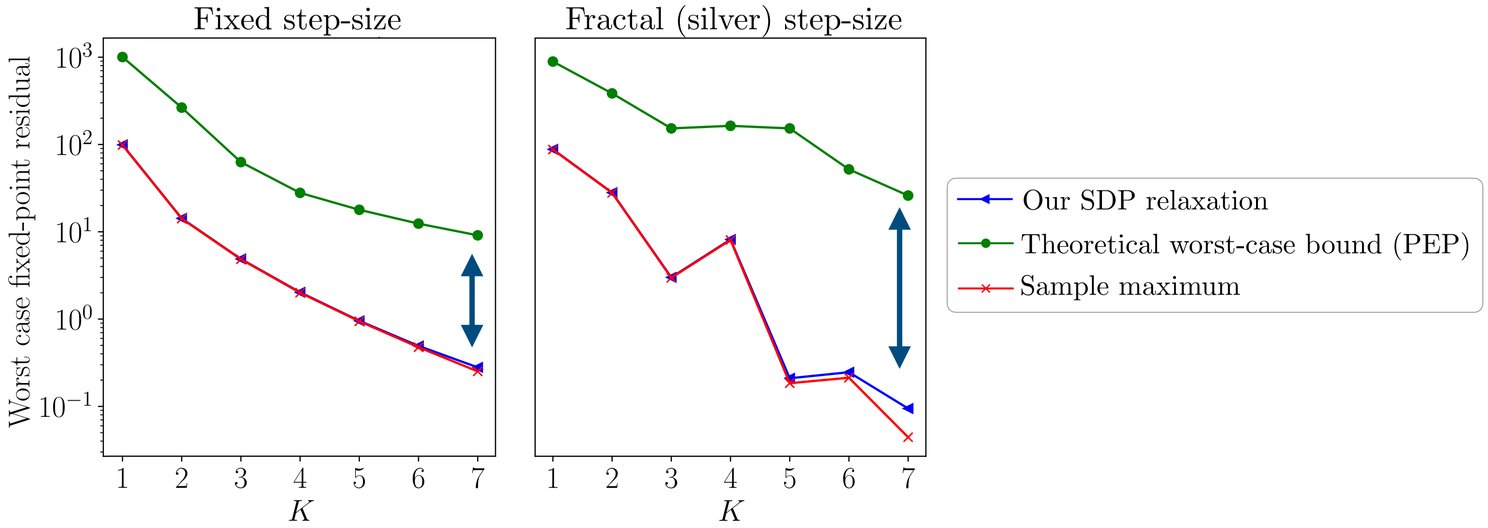
$$\begin{array}{ll} \text{minimize} & (1/2)\|Az - x\|_2^2 \\ \text{subject to} & z \geq 0 \end{array}$$

parameters

verification problem

projected gradient descent

$$\begin{array}{ll} \text{maximize} & \|z^K - z^{K-1}\| \\ \text{subject to} & z^{k+1} = \max\{(I - \theta A^T A)z^k + \theta(A^T x), 0\}, \quad k = 0, \ldots, K-1 \\ & z^0 = \{0\}, \quad x \in \mathcal{X} = \{x \mid \|x - 30 \cdot \mathbf{1}\| \leq 0.5\} \end{array}$$



10x-1000x reduction *(exploiting parametric structure)*

computationally more expensive than PEP *(up to 1000 seconds for these instances)*

Verification of First-Order Methods for Parametric Quadratic Optimization
V. Ranjan and B. Stellato
arXiv e-prints:2403.03331 (2024)
github.com/stellatogrp/algorithm_verification

Verifying the algorithm performance after K iterations

goal

estimate norm of fixed-point residual

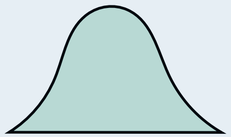
$$r^K(x) = \|z^K - z^{K-1}\|$$

worst-case

$$\max_{x \in \mathcal{X}} r^K(x) \leq \epsilon$$

problem instances

convergence tolerance



probabilistic

$$\mathbf{P}\left(r^K(x) > \epsilon\right) \leq \eta$$

probability bound

problem instances

convergence tolerance

Probabilistic analysis

goal

estimate probability of computing bad-quality solutions

$$\mathbf{P}(r^K(x) > \epsilon)$$

any metric
(e.g., fixed-point residual)

issue

we don't know P!

data

$$D = \{x^i\}_{i=1}^N$$

how can we bound the true probability?

Our recipe to bound performance

goal

estimate probability of computing bad-quality solutions

$$\mathbf{P}(r^K(x) > \epsilon) = \mathop{\mathbf{E}}_{x\sim P}(e(x))$$

$r^K(x)$: any metric (e.g., fixed-point residual)

$e(x)$: error $\mathbf{1}(r^K(x) > \epsilon)$

step 1

run K steps for N parametric instances

instances x_i → candidate solutions $z^K(x_i)$

step 2

compute empirical risk

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

step 3

bound true risk *(next slide)*

$$\mathop{\mathbf{E}}_{x\sim P}(e(x)) \leq \text{bound}$$

Statistical learning gives us probabilistic guarantees

sample convergence bound

with probability $1 - \delta$

$$\mathbf{P}(r^K(x) > \epsilon) = \underbrace{\mathop{\mathbf{E}}_{x \sim P}(e(x))}_{\text{true risk}} \leq \underbrace{\mathrm{kl}^{-1}}_{\substack{\text{inverse kl} \\ \text{divergence} \\ \textit{(1D convex} \\ \textit{problem)}}} \left(\underbrace{\frac{1}{N} \sum_{i=1}^{N} e(x_i)}_{\text{empirical risk}} \middle| \underbrace{\frac{\log(2/\delta)}{N}}_{\substack{\text{regularizer} \\ \text{number of} \\ \text{instances}}} \right)$$

interpretation of bound equal to B

With probability $1 - \delta$, the fixed-point residual is above ϵ after K steps

B fraction of times

Langford (2001)

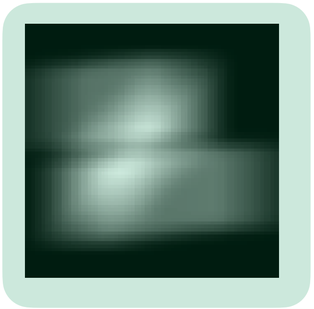
Success rates for OSQP in image deblurring

minimize $\|Az - x\|_2^2 + \lambda\|z\|_1$

subject to $0 \le z \le 1$

blurred image

deblurred image



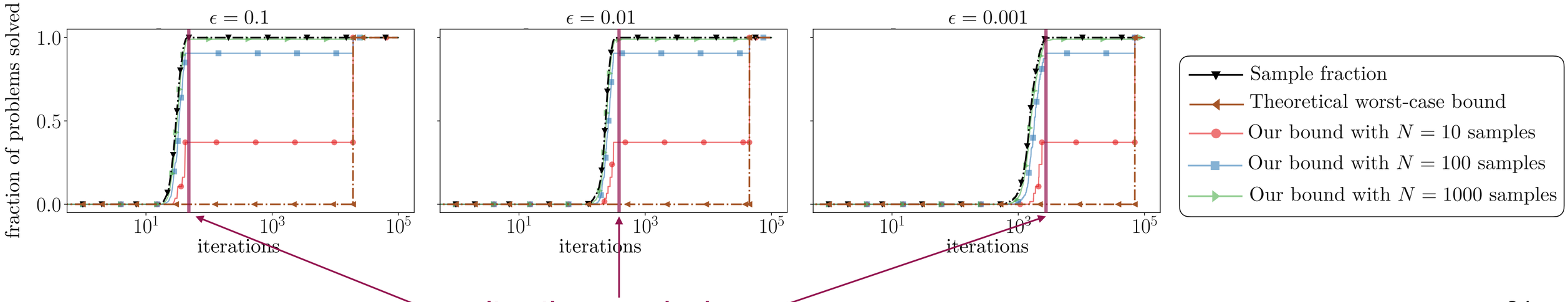
Solve with OSQP solver

fraction of problems solved

$$1 - \mathop{\mathbf{E}}_{x \sim P}(e(x))$$

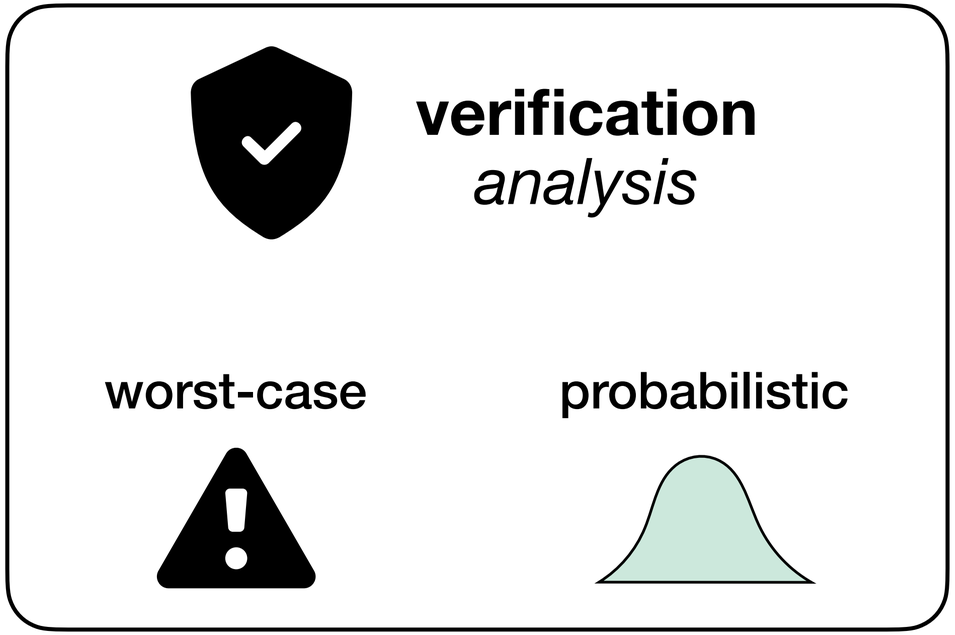
error

$$\mathbf{1}(r^K(x) > \epsilon)$$



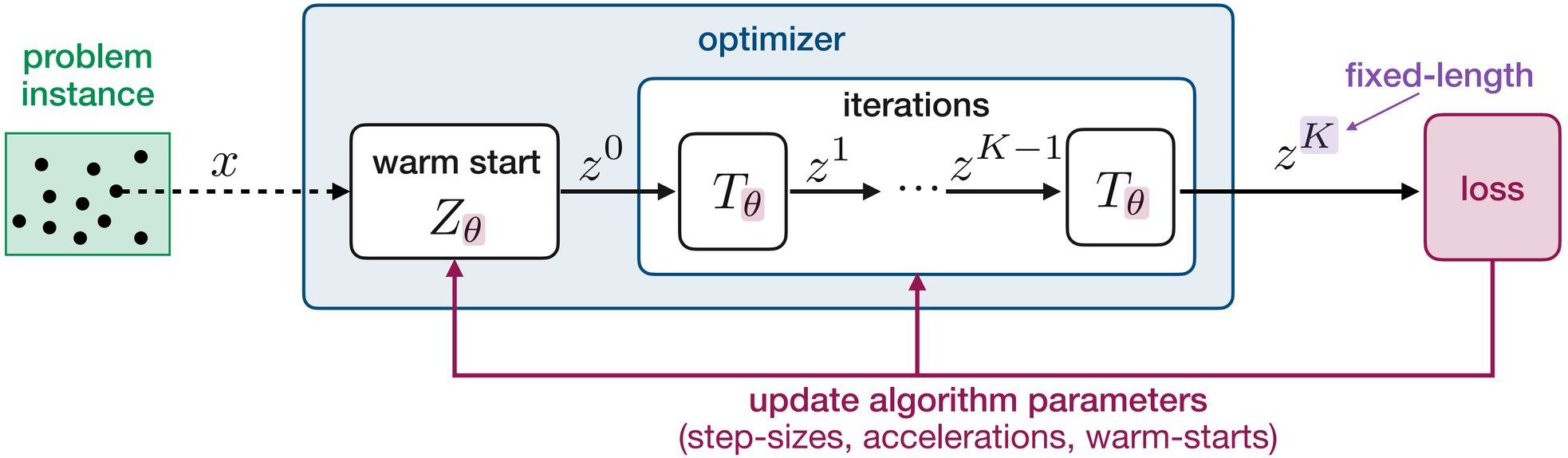
iterations required to solve all test instances

First-order methods in parametric convex optimization



Algorithm design

Training algorithms as fixed-length computational graphs



example

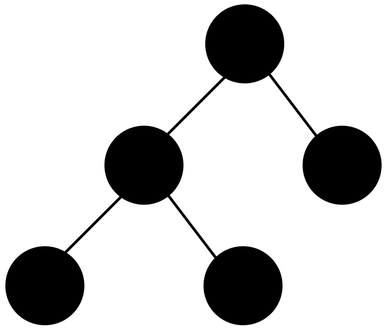
projected gradient descent

$$z^{k+1} = \Pi_{C(x)}(z^k - \theta \nabla_z f(z^k, x))$$

Learning can accelerate optimizers

Combinatorial optimization

B. Dilkina, E. Khalil, A. Lodi, P. Van Hentenryck, P. Bonami, S. Jegelka, …



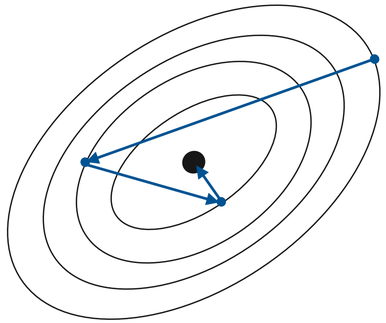
our previous contributions

The voice of optimization
D. Bertsimas, B. Stellato
Machine Learning (2021)

Online mixed-integer optimization in milliseconds
D. Bertsimas, B. Stellato
INFORMS Journal on Computing (2022)

Continuous optimization

W. Yin, B. Amos, Z. Kolter, M. Andrychowicz, C. Finn, P. Van Hentenryck …



our previous contributions

Accelerating quadratic optimization with reinforcement learning
J. Ichnowski, P. Jain, B. Stellato, … et al.
NeurIPS (2021)

No performance guarantees

↓

Can we build *rigorous* and *data-driven* performance guarantees?

Statistical learning theory for optimization algorithms

	supervised learning	learning to optimize
input		problem instance *(with parameter x)*
hypothesis	cat	residual $r_\theta^K(x)$
error	0 (1 if wrong)	$e_\theta(x) = \mathbf{1}(r_\theta^K(x) > \epsilon)$
guarantees	expected loss on new data	expected loss on new problem instances

algorithm parameters (step-sizes, accelerations, warm-starts)

PAC-Bayes generalization bounds

learning task

$$\underset{\Theta}{\text{minimize}} \; \underset{\theta\sim\Theta}{\mathbf{E}} \; \underset{x\sim P}{\mathbf{E}} \left(e_\theta(x)\right)$$

distribution of algorithm parameters
(step-sizes, accelerations, warm-starts)

can be anything

1. Pick *prior* Θ_0 before observing data
2. Observe data $D = \{x^i\}_{i=1}^N$
3. Learn *posterior* Θ: $\theta \sim \Theta$
4. Bound performance $\mathbf{P}^N \left(\underset{\theta\sim\Theta}{\mathbf{E}} \; \underset{x\sim P}{\mathbf{E}} \left(e_\theta(x)\right) \leq \hat{t}_N \right) \geq 1-\delta$

McAllester (1999), Maurer (2004)

data-driven bound

$$\hat{t}_N = \mathrm{kl}^{-1}\left(\frac{1}{N}\sum_{i=1}^N \underset{\theta\sim\Theta}{\mathbf{E}} \left(e_\theta(x_i)\right) \;\middle|\; \frac{\mathrm{KL}(\Theta||\Theta_0) + \log(2\sqrt{N}/\delta)}{2N} \right)$$

empirical risk

regularizer

Rajiv Sambharya

Learning optimizers with guarantees

minimize data-driven upper bound

with stochastic gradient methods

$$\underset{\Theta}{\text{minimize}} \quad \text{kl}^{-1}\left(\frac{1}{N}\sum_{i=1}^{N} \underset{\theta\sim\Theta}{\mathbf{E}} \left(e_\theta(x_i)\right) \;\middle|\; \frac{\text{KL}(\Theta||\Theta_0) + \log(2\sqrt{N}/\delta)}{2N} \right)$$

empirical risk

regularizer

derivative through convex optimization problem

Reeb et al. (2018)

results

distribution over algorithm parameters

$$\theta \sim \Theta = \mathcal{N}(\mu, \lambda I)$$

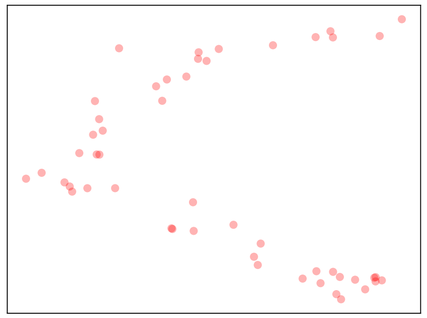
(e.g., sequence of step-sizes)

numerical performance bounds

Dziugaite et al (2017), Bartlett et al (2017, 2018), Jiang (2020), Majumdar et al (2021)

Robust Kalman Filtering with learned warm starts

noisy trajectory



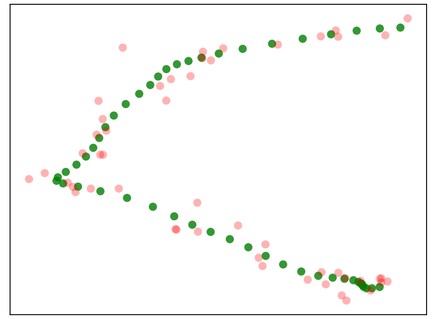
$x = \{y_t\}_{t=0}^{T-1}$

second-order cone program solver (SCS)

Huber loss

$$\begin{array}{ll} \text{minimize} & \sum_{t=0}^{T} \|w_t\|_2^2 + \psi(v_t) \\ \text{subject to} & s_{t+1} = As_t + Bw_t, \quad t = 0, \ldots, T-1 \\ & y_t = Cs_t + v_t, \qquad t = 0, \ldots, T \end{array}$$

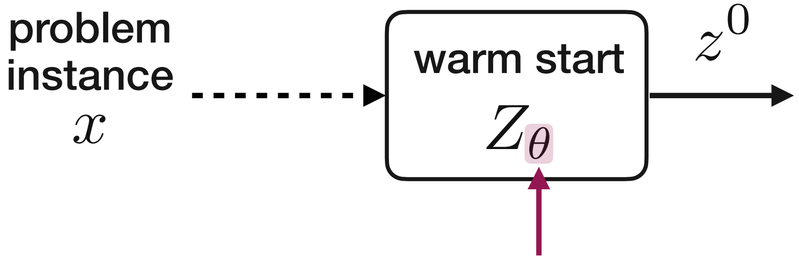
recovered trajectory



$z^\star = \{s_t^\star, w_t^\star, v_t^\star\}_{t=0}^{T-1}$

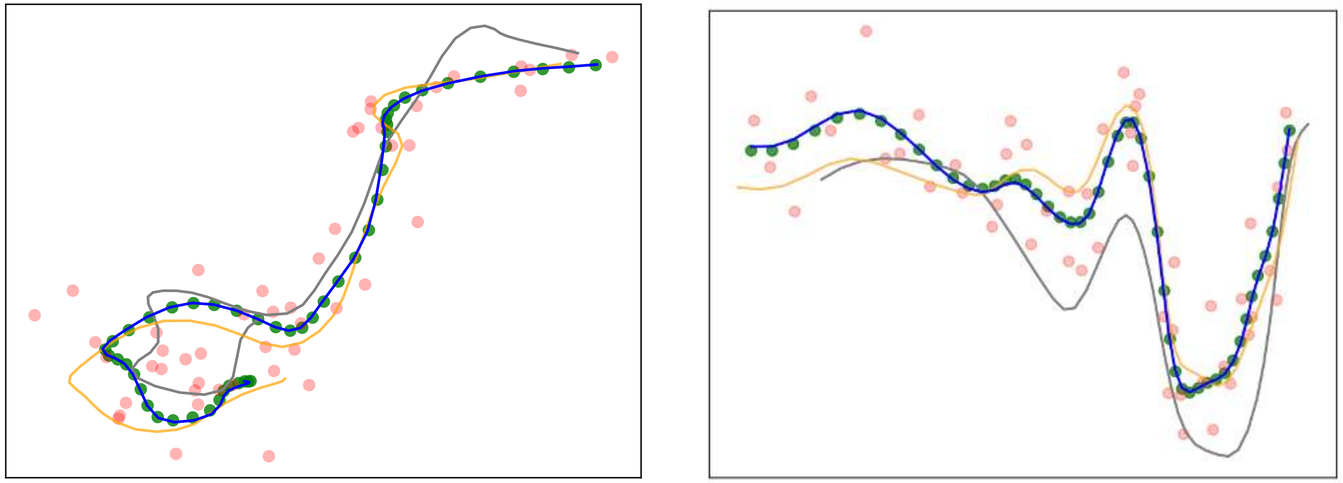
goal

learn warm-start mapping



Robust Kalman Filtering with learned warm starts

two example trajectories



points
- noisy trajectory
- optimal solution

Solution after 5 fixed-point iterations with different warm-starts
- nearest neighbor
- previous solution
- learned $K = 5$

with learning, we can estimate the state well

we also showed *warm-start specific* PAC Bayes generalization guarantees

Learning to Warm-Start Fixed-Point Optimization Algorithms
R. Sambharya, G. Hall, B. Amos, and B. Stellato
Journal of Machine Learning Research (2024)
github.com/stellatogrp/l2ws

Signal reconstruction with learned optimizer

reconstructed signal

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

known dictionary

noisy signal

performance metric
normalized mean squared error

$$\mathrm{NMSE}_{\mathrm{dB}}(z) = 10 \log_{10} \left(\|z - \bar{z}\|^2 / \|\bar{z}\|^2 \right)$$

ground truth

classical algorithm (ISTA)

$$z^{k+1} = \phi_{\lambda t} \left(z^k - t 2 D^T (D z^k - x) \right)$$

shrinkage operator

$$\phi_{\lambda t}(v) = \max\{v, \lambda t\} - \max\{-v, \lambda t\}$$

learned variants (e.g., ALISTA)

$$z^{k+1} = \phi_{\gamma^k} \left(z^k - \psi^k W^T (D z^k - x) \right)$$

algorithm parameters

$$\theta = \{\gamma^k, \psi^k\}_{k=0}^{K-1}$$

Gregor and LeCun (2010), Liu et al. (2019)

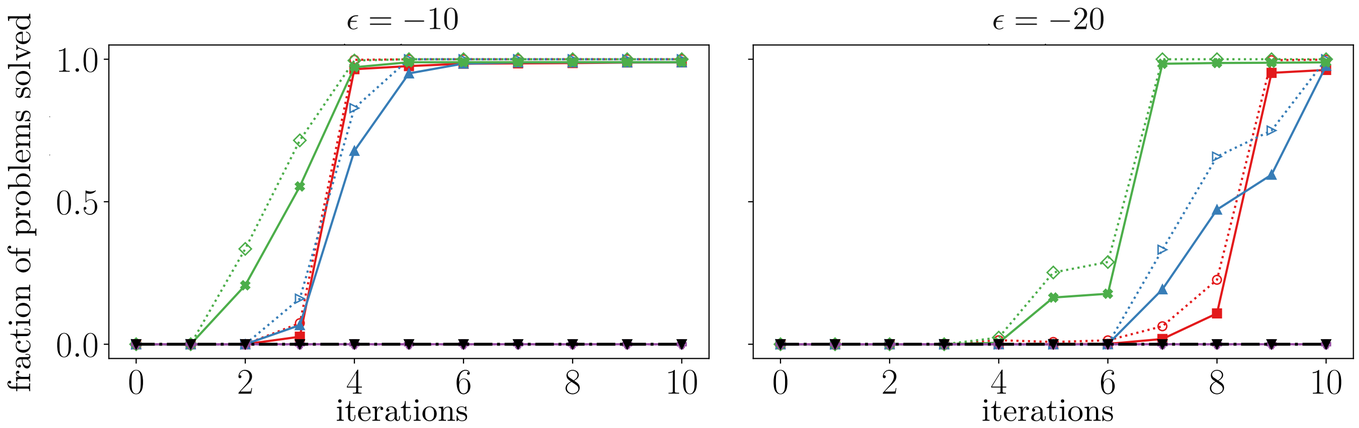
Success rates for learned optimizers in signal reconstruction

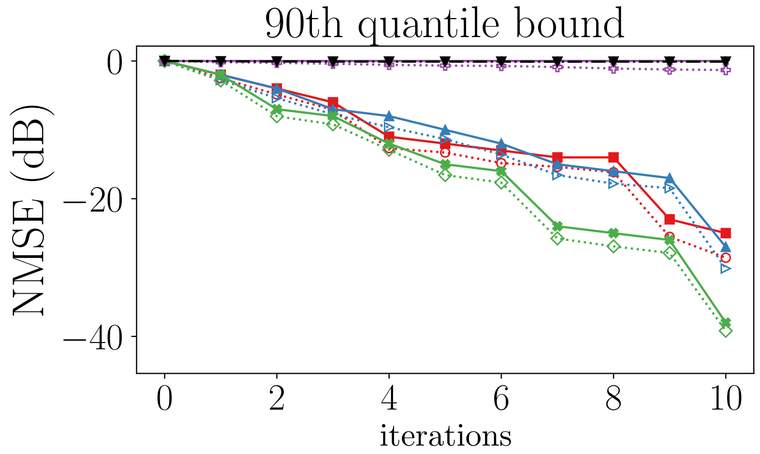
fraction of problems solved

$$1 - \mathop{\mathbf{E}}_{\theta\sim\Theta}\mathop{\mathbf{E}}_{x\sim P}(e_\theta(x))$$

error

$$e_\theta(x) = \mathbf{1}(\mathrm{NMSE}_{\mathrm{dB}}(z^K(x)) > \epsilon)$$





our bound are close to the empirical performance

learned optimizers provably perform well in just 10 iterations

Data-Driven Performance Guarantees for Classical and Learned Optimizers
R. Sambharya and B. Stellato
arxiv.org: 2404.13831 (2024)
github.com/stellatogrp/data_driven_optimizer_guarantees

Conclusions

Algorithm Design and Verification for Parametric Convex Optimization

1. **parametric** structure matters

2. **data** can help us
   - **design** optimization algorithms
   - **verify** their performance

3. we should **rethink optimization algorithms**

traditional view

- general-purpose
- one-size-fits all

→

new view

- task-specific
- trainable
- deployable anywhere

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Backup

PAC-Bayes generalization guarantees for learned warm starts

β-contractive case

$$\|Tx - Ty\|_2 \leq \beta \|x - y\|_2 \quad \forall x, y$$

$$\beta \in (0, 1)$$

Theorem: for any $\gamma > 0$ with probability at least $1 - \delta$

$$\underbrace{\mathop{\mathbf{E}}_{x \sim \mathcal{X}} \ell_\theta^k(x)}_{\text{risk}} \leq \underbrace{\frac{1}{N} \sum_{i=1}^{N} \ell_\theta^k(x_i)}_{\text{empirical risk}} + 2\beta^k \gamma + \mathcal{O}\left(\frac{\beta^k}{\gamma} (2D + 1) \sqrt{\frac{c_2(\theta) + \log(\frac{LN}{\delta})}{N}} \right)$$

penalty term

bound on $\|z^\star(x)\|_2$

As the number of iterations $k \to \infty$ the penalty term goes to zero

The contractive factor β directly affects the penalty term

We combine operator theory with PAC-Bayes theory to get the bound

Computing the KL Inverse with Convex Optimization

KL divergence between Bernoulli distributions

$$\mathrm{kl}(q \,||\, p) := \mathrm{KL}(\mathrm{Bernoulli}(q), \mathrm{Bernoulli}(p))$$

Many PAC-Bayes-type bounds bound the risk implicitly

$$\mathrm{kl}(q \,||\, p) \leq c$$

empirical risk risk regularizer

Inverting the KL divergence

$$p^\star = \mathrm{kl}^{-1}(q \mid c) = \begin{array}{ll} \text{maximize} & p \\ \text{subject to} & q \log(\frac{q}{p}) + (1-q) \log(\frac{1-q}{1-p}) \leq c \\ & 0 \leq p \leq 1 \end{array}$$

Solved within a millisecond on my laptop