OptNet:

Differentiable Optimization as a Layer in Neural Networks

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Big picture

What are the “atomic operations” or building blocks of modern AI systems?

View of the current situation: Matrix-vector products (dense or sparse/structured), (sub)differentiable non-linear functions, random sampling

This talk: We should consider (convex) optimization as another potential layer, to be composed with others

Note: we already use optimization in the learning procedures, but we should also consider it as an operation for inference and control

Optimization in deep learning

Recently there has been a lot of work in applying more generic optimization methods within deep learning architectures

Approach 1: *Unroll* an optimization procedure (like gradient descent) as a network itself (Domke, 2012; Goodfellow, 2013; Maclaurin et al., 2015; Belanger and McCallum, 2015; Andrychowicz et al., 2016; Metz et al., 2017; Gregor and LeCun, 2010)

Approach 2: Directly differentiate through the argmin (Bradley and Bagnell, 2009; Mairal et al., 2012; Gould et al., 2016; Johnson et al., 2016; Amos et al., 2016; Barron and Poole, 2016)

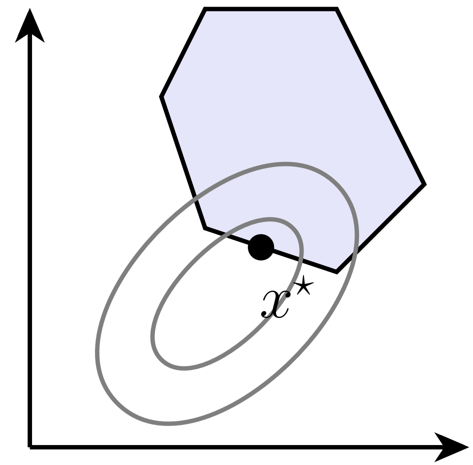
- We're going to use this approach, but consider a bit more general setting and efficient backpropagation algorithms

Optimization as a "primitive"

Optimization problems are an extremely powerful paradigm for decision-making

Example: quadratic program

$$
\begin{aligned}
\underset{x}{\text{minimize}} \quad & \frac{1}{2} x^T Q x + q^T x \\
\text{subject to} \quad & Ax = b \\
& Gx \le h
\end{aligned}
$$



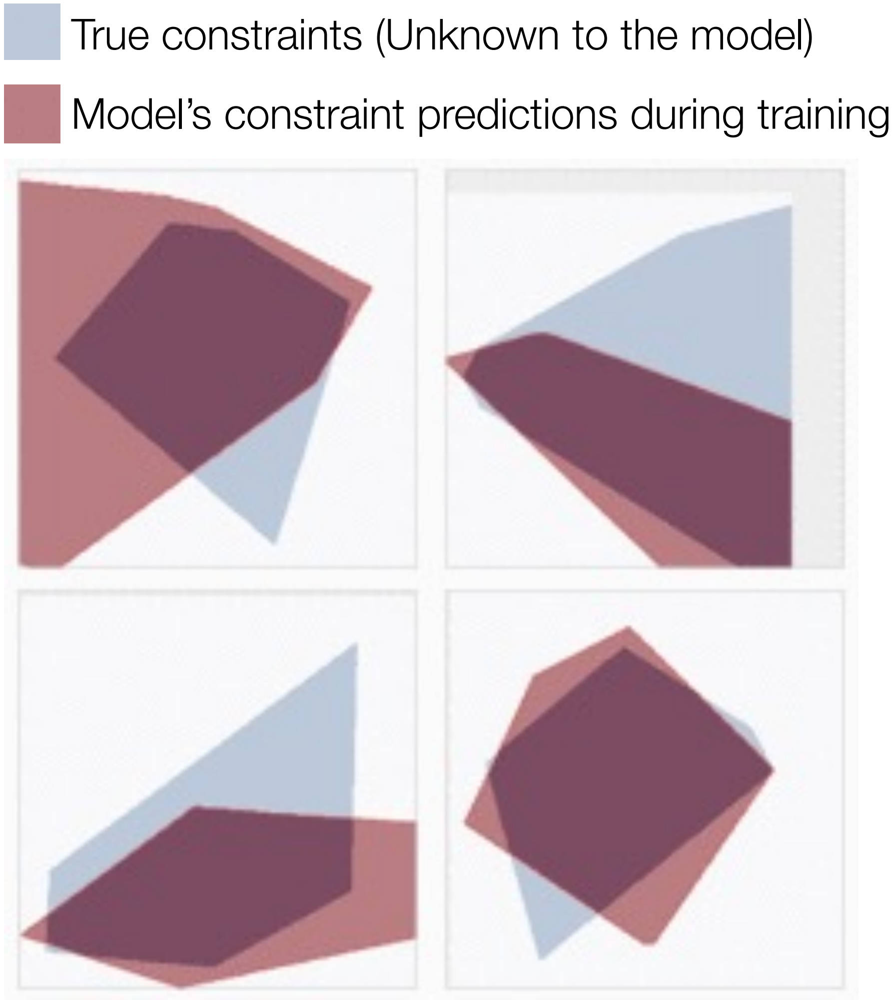
Applications in finance (Markowitz portfolio optimization), machine learning (support vector machines), control (linear-quadratic model predictive control), geometry (projections onto polyhedra)

Illustrative Example: Learning Hard Constraints

Given regression data (x, y) generated from a constrained optimization problem.

Idea: Randomly initialize hard constraints in an OptNet layer and learn them from data with gradients

$$\hat{y} = \underset{z}{\operatorname{argmin}} \ f(x, z)$$
$$\text{subject to } Gz \leq h$$



Talk Overview

1. Our contribution: OptNet layers
2. qpth: Our efficient and differentiable PyTorch QP solver
3. Experiments
    1. MNIST
    2. 1D Signal Denoising
    3. Mini-Sudoku

Our Contribution: The OptNet Approach

A network where the output of a single layer is the *solution* to a QP involving parameters defined by the previous layer z_i

$$
\begin{aligned}
z_{i+1} = \quad & \underset{z}{\operatorname{argmin}} \ \frac{1}{2} z^T \boxed{Q(z_i) z} + q(z_i)^T z \\
& \text{subject to } \ A(z_i) z = b(z_i) \\
& \qquad\qquad\quad G(z_i) z \leq h(z_i)
\end{aligned}
$$

The matrix $Q(z_i)$ depends on the previous layer z_i

Learnable parameters: Q, q, A, b, G, h

Can capture much more expressive functions than a single traditional feedforward layer (polytope of QP has exponential number of points)

Continuous in z_i if parameters are all continuous functions, and $Q(z_i)$ strictly positive definite

Example OptNet Layer

General Definition:

$$\begin{aligned} z_{i+1} = \quad & \underset{z}{\operatorname{argmin}} \ \frac{1}{2} z^T Q(z_i) z + q(z_i)^T z \\ & \text{subject to } \ A(z_i) z = b(z_i) \\ & \qquad\qquad G(z_i) z \le h(z_i) \end{aligned}$$

Parameterization that is **always feasible**:

- Connect the previous layer only in the linear term $q(z_i) = z_i$
- Use a Cholesky so that $Q = LL^T + \epsilon$
- Pick some feasible point $z_0 \in \mathbb{R}$ and $s_0 > 0$ and let $b = Az_0$ and $h = Gz_0 + s_0$

Learnable parameters: $L, A, G, z_0, \text{and } s_0$

Differentiating through OptNet layers

$$
\begin{aligned}
z_{i+1} = \quad & \underset{z}{\operatorname{argmin}} \ \frac{1}{2} z^T Q(z_i) z + q(z_i)^T z \\
& \text{subject to } \ A(z_i) z = b(z_i) \\
& \qquad\qquad G(z_i) z \leq h(z_i)
\end{aligned}
$$

How do we compute the Jacobians?

$$
\frac{\partial z_{i+1}}{\partial z_i} \quad \frac{\partial z_{i+1}}{\partial Q} \quad \frac{\partial z_{i+1}}{\partial q} \quad \frac{\partial z_{i+1}}{\partial A} \quad \frac{\partial z_{i+1}}{\partial b} \quad \frac{\partial z_{i+1}}{\partial G} \quad \frac{\partial z_{i+1}}{\partial h}
$$

We show how to compute these by using implicit differentiation of the KKT conditions with matrix differentials. (The details are in our paper)

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qpth: Our efficient and differentiable PyTorch QP solver

OptNet formulation is slow compared to Linear+ReLU layers, even with highly optimized solvers

We implemented our own primal-dual interior point algorithm for QPs, specialized for minibatch processing of multiple same-sized problems using batch GPU factorization, plus some additional tricks

Nice property: We can backprop through the solver effectively "for free"

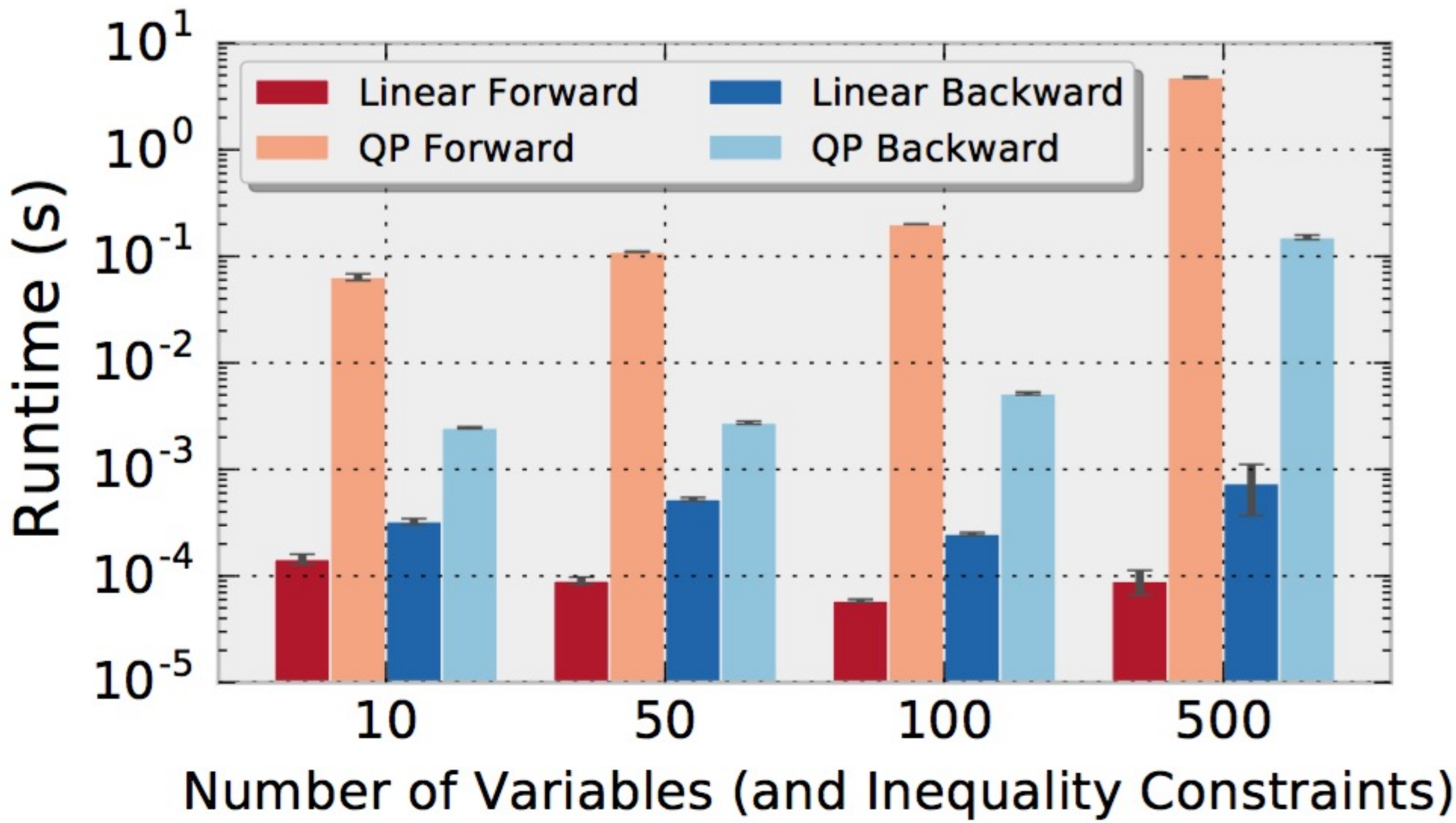
Our open source PyTorch library is available at http://locuslab.github.io/qpth

Add a differentiable QP OptNet layer to your PyTorch models with one line of code with our PyTorch `Function` after defining the parameters:

```
z = QPFunction()(Q, p, G, h, A, b)
```

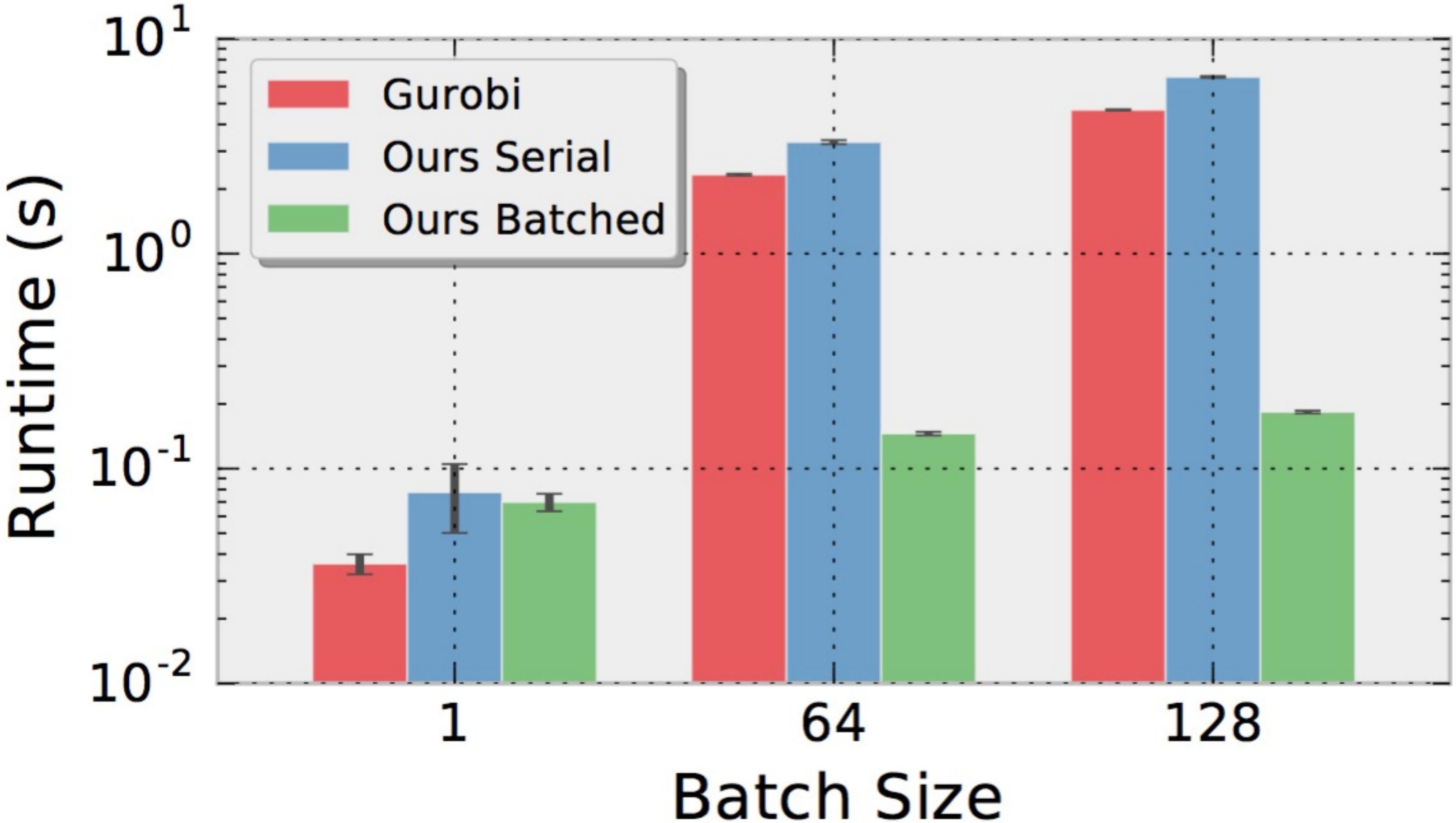
Timing Results: Comparison to a linear layer

OptNet layers are more expensive but still tractable



Timing Results: Comparison to Gurobi

Batched QP solvers are crucial for tractability



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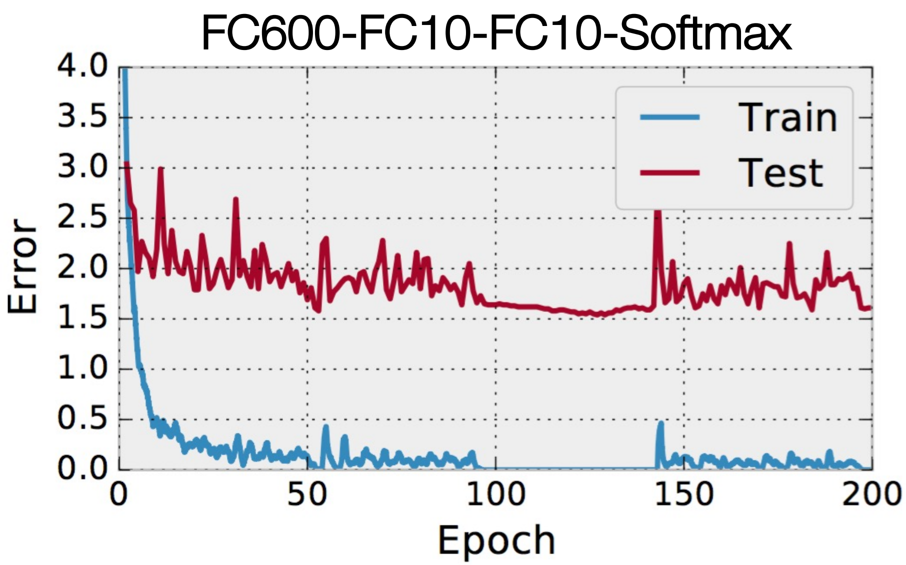
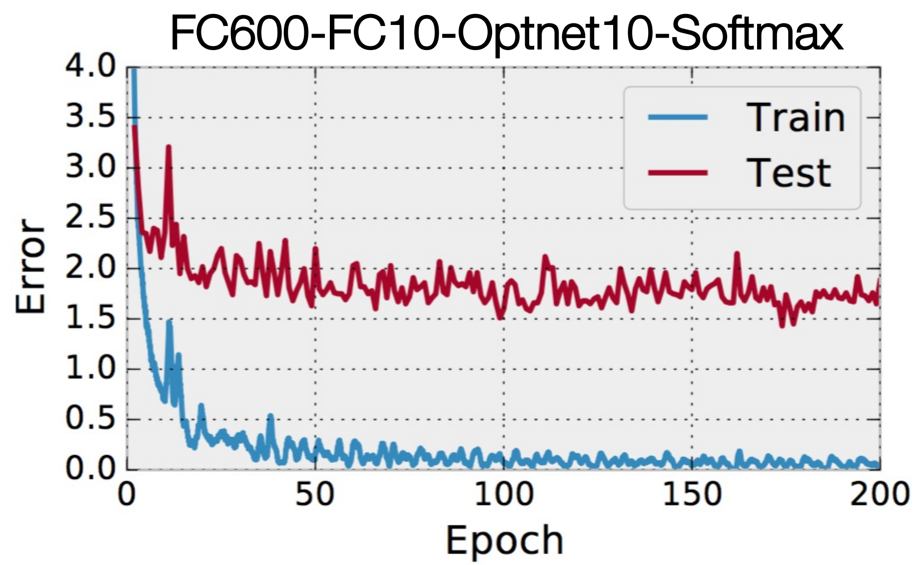
Results: MNIST

Only interesting as a sanity check and to show that an OptNet layer can be added as a layer without harming the training process.





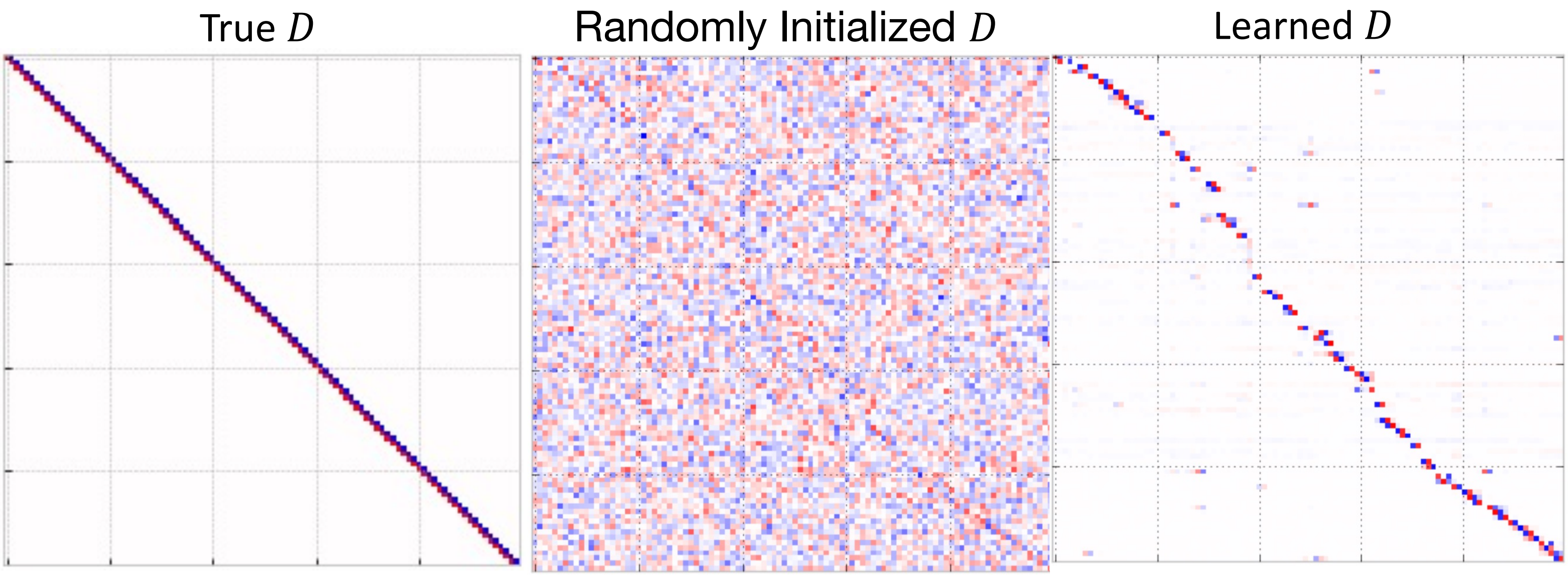
Results: 1D Signal Denoising

Task: Learn a model from data that maps from a noisy signal to a denoised signal.

Total Variation Denoising Approach: Solve the following optimization problem where D is the differencing operator.

$$z^\star = \operatorname*{argmin}_z \frac{1}{2}||y - z||_2^2 + \lambda||Dz||_1$$

OptNet Application: Randomly initialize the differencing operator D and learn it from data with gradients $\partial z^\star / \partial D$



Results: Mini-Sudoku

Sudoku can be posed as a constraint-satisfaction optimization problem

- Every row should contain the digits 1-4
- Every column should contain the digits 1-4
- Every partitioned sub-block should contain the digits 1-4

Task: Learn a model from data that maps from unsolved boards to solved boards.

Example input/output pair:

			3
1			
		4	
4			1

2	4	1	3
1	3	2	4
3	1	4	2
4	2	3	1

The OptNet Approach:

$$\begin{aligned} \operatorname*{argmin}_{z} \quad & \epsilon \|z\|_2^2 + p^T z \\ \text{subject to} \quad & Az = b \\ & z \geq 0 \end{aligned}$$

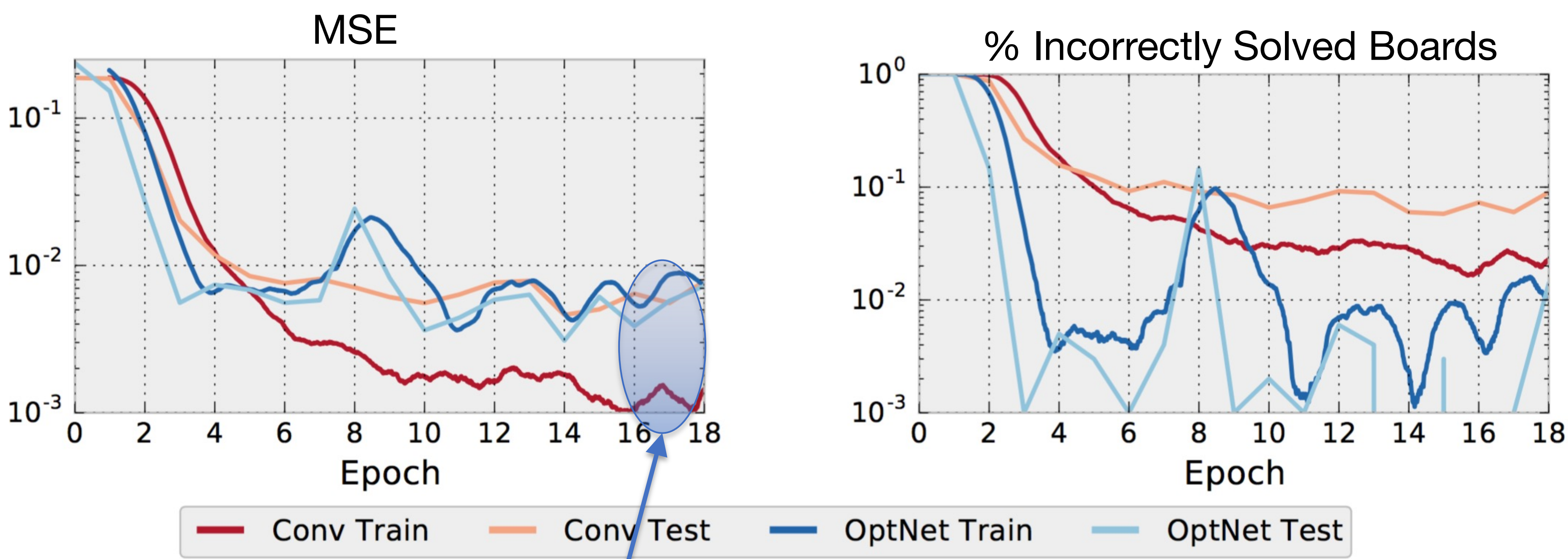
Arbitrary parameters

One-hot encoding of unsolved puzzle

Results: Mini-Sudoku

The OptNet layer exactly learns the mini-Sudoku constraints from data!

Baseline: A deep convolutional feed-forward network



Convolutional network: Significant train/test gap
OptNet: Small gap, generalizes well

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The full PyTorch source code to reproduce all of our experiments is available online at https://github.com/locuslab/optnet

Our PyTorch QP solver is freely available online at https://locuslab.github.io/qpth