OptNet:
Differentiable Optimization as a Layer in Neural Networks

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ICML 2017
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 problems are an extremely powerful paradigm for decision-making.

Example: quadratic program

\[
\begin{align*}
\text{minimize} & \quad \frac{1}{2} x^T Q x + q^T x \\
\text{subject to} & \quad A x = b \\
& \quad G x \leq h
\end{align*}
\]

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

\[
\hat{y} = \arg\min_z f(x, z) \quad \text{subject to } Gz \leq h
\]
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 $z_i$

$$z_{i+1} = \arg\min_z \frac{1}{2} z^T Q(z_i)z + q(z_i)^T z$$
subject to $A(z_i)z = b(z_i)$
$G(z_i)z \leq h(z_i)$

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:

\[
    z_{i+1} = \arg\min_z \frac{1}{2} z^T Q(z_i) z + q(z_i)^T z \\
    \text{subject to } A(z_i) z = b(z_i) \\
    G(z_i) z \leq h(z_i)
\]

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**: \( L, A, G, z_0, \) and \( s_0 \)
Differentiating through OptNet layers

\[ z_{i+1} = \text{argmin}_z \frac{1}{2} z^T Q(z_i) z + q(z_i)^T z \]

subject to \( A(z_i) z = b(z_i) \)
\( G(z_i) z \leq h(z_i) \)

How do we compute the Jacobians?

\[
\begin{align*}
\frac{\partial z_{i+1}}{\partial z_i} & \quad \frac{\partial z_{i+1}}{\partial Q} & \quad \frac{\partial z_{i+1}}{\partial q} & \quad \frac{\partial z_{i+1}}{\partial A} & \quad \frac{\partial z_{i+1}}{\partial b} & \quad \frac{\partial z_{i+1}}{\partial G} & \quad \frac{\partial z_{i+1}}{\partial h}
\end{align*}
\]

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

1. Our contribution: OptNet layers
2. qpth: Our efficient and differentiable PyTorch QP solver
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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](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.

$$ z^* = \arg\min_z \frac{1}{2} \|y - z\|_2^2 + \lambda \|Dz\|_1 $$

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

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>1</td>
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<td>3</td>
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<td>3</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>4</td>
</tr>
</tbody>
</table>

The OptNet Approach:
\[
\arg\min_z \epsilon \|z\|_2^2 + p^T z \\
\text{subject to } Az = b \\
z \geq 0
\]

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