Learning to Optimize via Implicit Networks

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Joint work with Howard Heaton[2], Daniel McKenzie[1], Qiuwei Li[3] Wotao Yin[3], Stanley Osher[4]

Colorado School of Mines[1], Typal Academy[2], Alibaba Group[3], UCLA[4]

Deep Learning

$$x^\star_d = \sigma(W^m \cdot + b^m) \circ \cdots \circ \sigma(W^1 d + b^1)$$

[1] Heaton and Wu Fung (2023). "Explainable AI via Learning to Optimize." Scientific Reports

Motivation: ML vs. Optimization Models

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✓ flexible architectures

✓ expressive capacity

satisfy constraints / optimality

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Today:

- Design and efficiently train network architectures that benefit from optimization theory. $\Longrightarrow$ NN outputs *satisfy optimality/feasibility* conditions.[1]

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Make a model by parameterizing an optimization problem via Θ to get

$$x_{\Theta,d} = \arg\min_{x \in C} f_\Theta(x; d) \tag{1}$$

Note: Constraints/analytic cost functions can be included by domain experts.

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L2O Description and Forward Propagation

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- Fixed number of iterations, e.g., $K = 10 \implies$ unrolled network
- Iterate until convergence $(K \gg 1) \implies$ **Implicit Networks**[2] [3] (outputs satisfy optimality/feasibility guarantees!)

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Assumption 1: Contractiveness of T_Θ

For fixed d, there exists $\gamma \in [0, 1)$ such that

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Banach Fixed Point Theorem

For any $x^1 \in \mathcal{U}$, if Assumption 1 holds, then the sequence $\{x^k\}$ generated by

$$x^{k+1} = T_\Theta(x^k;\ d), \quad \text{for all } k \in \mathbb{N}, \tag{3}$$

converges linearly to the unique fixed point $x_d^\star$.

Well-Defined Implicit Network

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Remark: If T_Θ is a contraction in x, we have well-defined implicit network

Training Implicit Networks

Implicit L2O: The Learning Problem

- Given data $\{(d^i, x^\star_{d^i})\}$ the training problem is given by

$$\min_{\Theta} \quad {}_{i} \quad \ell \quad x_{\Theta,d^i}, x^\star_{d^i} \tag{4}$$

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- $\dfrac{d\ell}{d\Theta} = \dfrac{d\ell}{dx_\Theta}\dfrac{dx_\Theta}{d\Theta}$. How to compute $\dfrac{dx_\Theta}{d\Theta}$?

Backpropagating Through Implicit Networks

Standard Backpropagation

To train the implicit L2O network, we need to compute the gradient of the loss function

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- memory requirements grow linearly in depth ($\mathcal{O}(K)$) $\implies$ intractable for implicit networks

Recalling the output of an implicit network is the fixed point of T_Θ:

$$x_{\Theta,d} = T_\Theta(x_{\Theta,d}; d),$$

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- Memory required to compute $\frac{dx_{\Theta,d}}{\mathrm{d}\Theta}$ is *constant* in depth! ✓
- Unfortunately, solving for $\mathcal{J}_\Theta^{-1}\frac{\partial T}{\partial \Theta}$ is often very expensive

Jacobian-free Backpropagation (JFB)

Proposed: Jacobian-free Backprop (JFB)

Goal: Avoid solving Jacobian-based equation and memory issues when training implicit networks.

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That is, approximate true gradient

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Remark: cost equivalent to computing the gradient of *one layer*!

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Jacobian-free Backprop (JFB)

Assumption 1

T_Θ is continuously diff'ble w.r.t Θ

Assumption 2

$M = \frac{\partial T}{\partial \Theta}$ has full column rank and is well-conditioned s.t. $\kappa(M^\top M) \leq \frac{1}{\gamma}$

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Main Theorem: Descent of JFB

If Assumptions 1 and 2 hold for given Θ and d, then

$$-p_\Theta = -\frac{d\ell}{dx_{\Theta,d}} \frac{\partial T}{\partial \Theta}$$

forms a descent direction for $\ell(x_{\Theta,d}, x_d)$ with respect to Θ.

Implementation of JFB

Implicit Forward + Proposed Backprop

```
x_fxd_pt = find_fixed_point(d)
x_star = apply_T(x_fxd_pt, d)
loss = criterion(x_star, labels)
loss.backward()
optimizer.step()
```

Figure 1: Sample PyTorch code for backpropagation

Remark: backpropagation is simple in PyTorch framework!

JFB works!

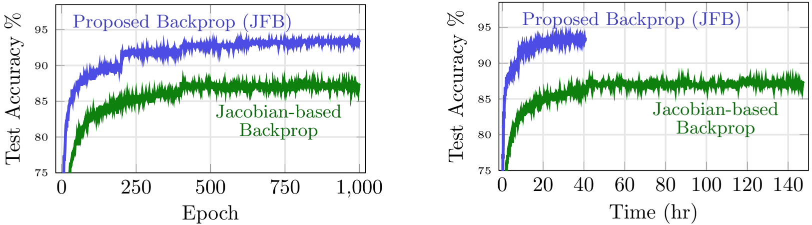
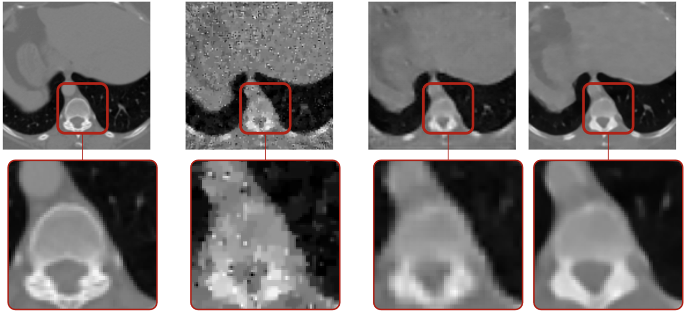


Figure 2: Training an implicit neural network on CIFAR10. JFB is faster and yields higher test accuracy than Jacobian-based backprop.

L2O Experiment: Computed Tomography



Ground truth	TV Min	U-Net	Implicit L2O
SSIM: 1.000	SSIM: 0.379	SSIM: 0.806	SSIM: 0.891
PSNR: ∞	PSNR: 21.17	PSNR: 27.83	PSNR: 31.87
	Fail ✖ – Data Regularization	Fail ✖ – Fidelity	Trustworthy ✔

Comparison of techniques, ranging from traditional to fully data-driven

$$\text{(L2O Model)} = N_\Theta(d) = \operatorname*{arg\,min}_{x\in[0,1]^n} \ f_\Theta(Kx) \quad \text{s.t.} \quad Ax = b \tag{5}$$

Shortest Path Problem: given a graph and origin/destination nodes, find the path that incurs minimal cost.

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Problem Formulation:

$$x_\Theta(d) \triangleq \underset{x \in \mathcal{C}}{\arg\min}\, w_\Theta(d)^\top x \tag{6}$$

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Remedy: Define implicit network using three-operator splitting:

$$T(x;d) = x - P_{\mathcal{C}_1}(x) + P_{\mathcal{C}_2}\left(2P_{\mathcal{C}_1}(x) - x - \nabla f_\Theta(P_{\mathcal{C}_1}(x);d)\right), \tag{7}$$

where note that $P_{\mathcal{C}_1}$ and $P_{\mathcal{C}_2}$ are trivial to compute.

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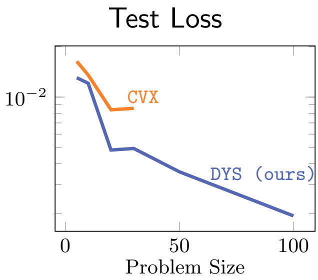

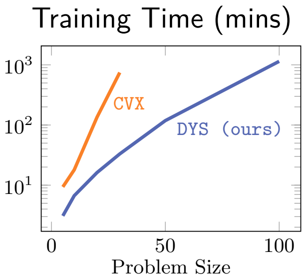

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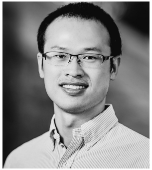
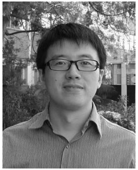
- Implicit L2O models can be efficiently trained using Jacobian-Free Backpropagation
- Implicit L2O + JFB have found success in traffic flow, computed tomography, and knapsack problem
- More details can be found in papers:
  - *Explainable AI via Learning to Optimize*, Scientific Reports, 2023
  - *JFB: Jacobian-Free Backpropagation for Implicit Networks*, AAAI, 2022
  - Three Operator Splitting for Learning to Predict Equilibria in Convex Games, SIMODS, 2024
  - Learning to Solve Integer Linear Programs with Davis-Yin Splitting, TMLR, 2024

Collaborators and Acknowledgments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