Explainable AI via Learning to Optimize

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Talk Overview

Setting

Problems where approximate optimization models can be hand-crafted

Learning to Optimize (L2O)

Make parameterized optimization model and use training data to tune it, *i.e.*

$$\text{(model output)} \triangleq \text{argmin (prior knowledge)} + \text{(data-driven terms)}$$

Contribution

- Demo how to build intuitive L2O models
- Provide certificates to explain whether model inferences are trustworthy

Historic Comparison of Two Approaches

Machine Learning

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

- ✔ adapt to available data
- ✘ satisfy constraints / optimality
- ✔ expressive capacity
- ✔ flexible architectures

Traditional Optimization

$$\operatorname*{argmin}_{x \in C} f(x)$$

- ✘ adapt to available data
- ✔ guaranteed optimality
- ✔ interpretable models
- ✔ scalable first-order algorithms

L2O Overview

- Originated with LISTA[1] where authors took existing algorithm (ISTA) and replaced analytic terms for affine mappings with parameters and tuned them with training data to quickly solving sparse coding problems
- Inspired by optimization (may be written via fixed points)
- Can be used in embedded form (*e.g.* optimization is one layer in model)
- Has switched emphasis (in our work) to using *many* iterations

[1] Gregor and LeCun. *Learning fast approximations of sparse coding*. 2010.

Related Work

- **Plug and Play** (parameters not tuned on data used for inferences)

  Plug externally trained model in an algorithm as a proximal/gradient update

- **Deep Unfolding** (does not run to convergence, limited guarantees)

  Apply “small” # of updates, with (possibly) different parameters in each step

- **Predict-then-Optimize** (single “layer” usage, special case of L2O)

  Learn mapping from data to apt optimization problem, and then solve

What is Explainable?

Model Design $\rightarrow$ Inference Properties[2]

A model is explainable provided a domain expert can identify the core design elements of a model and how they translate to expected inference properties

Inference Properties $\rightarrow$ Model Design $+$ Training Data

An inference is explainable provided its properties can be linked to the model's design and intended use, enabling identification of trustworthy inferences

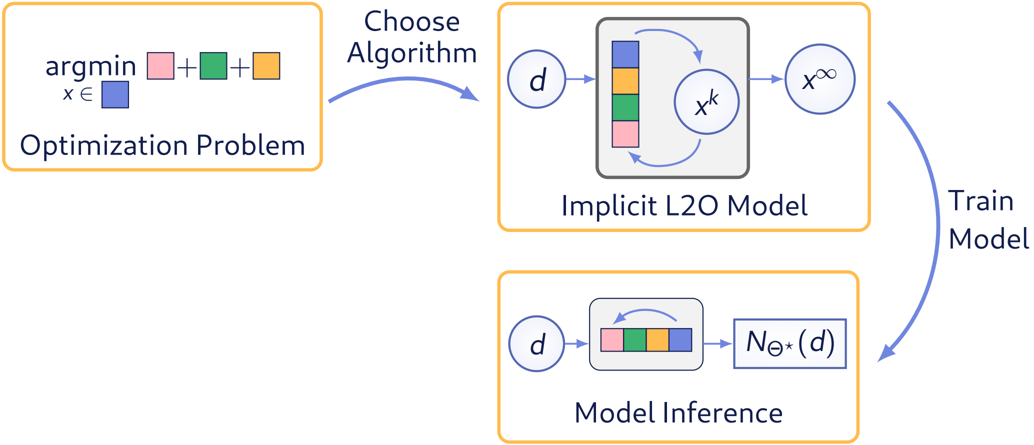
Explainable models *and* inferences are achieved via L2O with our certificates[3]

[2]These are properties for inferences on data matching the distribution of training data
[3]These certificates can be used for post-conditions in production code

Outline

1. How to Build an Explainable L2O Model
2. Trustworthiness Certificates

L2O via Building Blocks



Key L2O Steps

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

$$N_\Theta(d) = S_\Theta(x_{\Theta,d}), \quad \text{where} \quad x_{\Theta,d} \triangleq \underset{x}{\operatorname{argmin}}\, f_\Theta(x;\ d)$$

Note: We focus on case where S_Θ is identity, but this part can take many forms

(*e.g.* S_Θ can be a classifier)

Note: Constraints can be included in this formulation (via indicator functions)

2. Forward prop by applying an apt first-order algorithm until convergence

Note: For best performance, test like you train (*i.e.* use same # of iterations)

3. Backprop consists of using built-in autograd on *last step of forward prop*

Toy Example – Signal Recovery via Dictionary Learning

- **Task**

  Recover a signal $x_d^\star$ from linear measurements $d = Ax_d^\star$

- **Key Knowledge**

  Signal $x_d^\star$ has low dimensional structure (but is *not* sparse)

- **L2O Model**

  For a "sparsifying matrix" K, we estimate

$$x_d^\star \approx \underset{x}{\operatorname{argmin}} \|Kx\|_1 \quad \text{s.t.} \quad Ax = d$$

Toy Example – Signal Recovery via Dictionary Learning

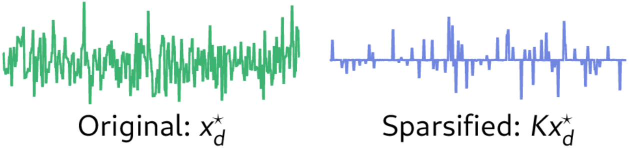


Figure 1: Applying the learned K sparsifies $x_d^\star$ (shown for test data d)

Fix weights $\Theta = K \in \mathbb{R}^{250\times 250}$, noting $x_d^\star \in \mathbb{R}^{250}$ and $d \in \mathbb{R}^{100}$, and set

$$N_\Theta(d) \triangleq \operatorname*{argmin}_x \|Kx\|_1 \ \text{ s.t. } \ Ax = d$$

For a distribution of measurement/signal pairs $(d, x_d^\star)$, train by minimizing

$$\min_\Theta \mathbb{E}_d \left[\|x_d^\star - N_\Theta(d)\|^2 \right]$$

Jacobian-free Backprop (JFB)

```
x_fxd_pt = find_fixed_point(d)
y = apply_opt_update(x_fxd_pt, d)
loss = criterion(y, labels)
loss.backward()
optimizer.step()
```

Figure 2: Sample PyTorch code for backpropagation. The `find_fixed_point` function repeatedly applies `apply_opt_update` until a fixed point is (approximately) found.

(Informal) Theorem[4]

Backpropping through the final step of a fixed point algorithm (as shown above) yields a *preconditioned* gradient

[4] Wu Fung, *et al. JFB: Jacobian-Free Backpropagation for Implicit Networks*, 2022.

Outline

1. How to Build an Explainable L2O Model
2. Trustworthiness Certificates

What Inferences are Trustworthy?

An inference is trustworthy provided its properties can satisfactorily be linked to a model's design and intended use

We make this concrete using certificates

- Each property in model design corresponds to a certificate for inferences
- Each certificate is a tuple: (property name, label)
- Labels can be "pass," "warning," or "fail"
- (All certificate labels read "pass") $\Longrightarrow$ trustworthy inference

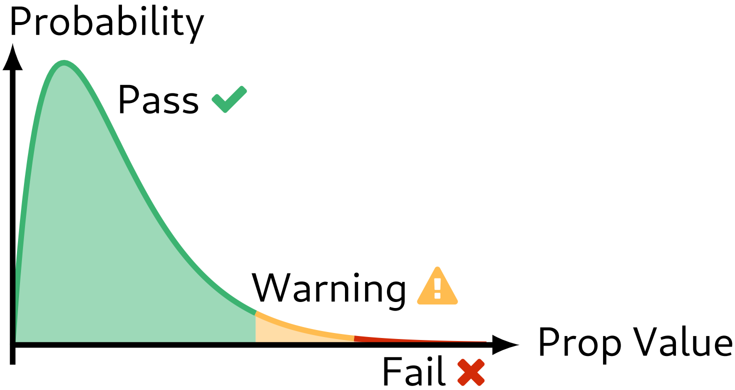


Figure 3: Probability distribution for values of a particular model property. The majority of samples drawn from this distribution pass while the outliers in the tail fail.

How to Compute Certificate Labels

Labels are derived from nonnegative inference property value (smaller is better):

$$\text{(inference)} \to \text{(property value)} \to \text{(label)}$$

Set p_p to desired probability for "pass" labels[5] (similarly for p_w and warnings) and

$$\text{label}(\alpha) \triangleq \begin{cases} \text{pass} & \text{if } \alpha \in [0, c_p] \\ \text{warning} & \text{if } \alpha \in (c_p, c_w] \\ \text{fail} & \text{otherwise} \end{cases}$$

with c_p such that $\mathbb{P}_{d \sim \mathcal{D}}\big[\text{(property value)}(N_{\Theta^\star}(d)) \leq c_p\big] = p_p$, and similarly for c_w

[5] Here $p_p = 0.95$ means 95% of inferences $N_\Theta(d)$ pass with d drawn from training distribution $\mathcal{D}$

Property Value Functions

Concept	Quantity	Formula
Sparsity	# Nonzeros	$\|x\|_0$
$\approx$ Sparsity	ℓ_1 norm	$\|x\|_1$
Measurements	Relative Error	$\|Ax - d\| / \|d\|$
Soft Constraint	Distance to Set	$d_C(x)$
Hard Constraint	Indicator Function	$\delta_C(x)$
Regularization	Proximal Residual	$\|x - \text{prox}_{f_\Theta}(x)\|$

Table 1: Example formulas for property value functions.

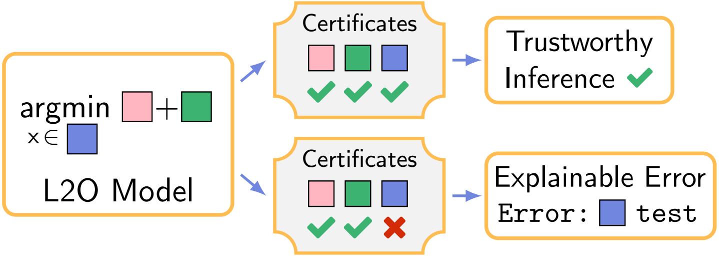


Figure 4: Two example inferences, one with passing labels and one with a fail label.

Toy Example (Continued)

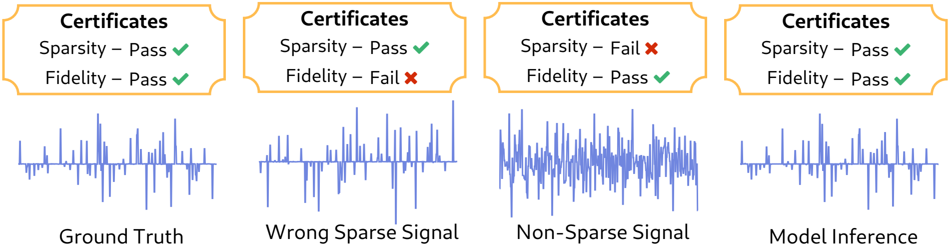
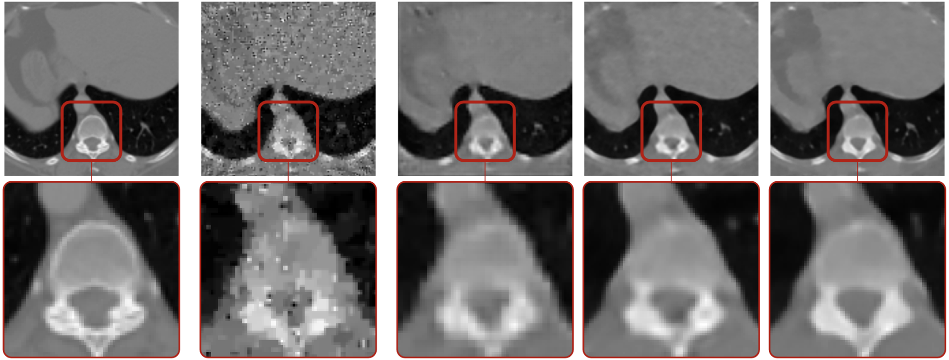


Figure 5: For sample d from test data, sparsified $KN_{\Theta}(d)$ of each inference $N_{\Theta}(d)$ is shown

CT Image Reconstruction



Ground truth	TV Min	U-Net	F-FPN	Implicit L2O
SSIM: 1.000	SSIM: 0.379	SSIM: 0.806	SSIM: 0.853	SSIM: 0.891
PSNR: ∞	PSNR: 21.17	PSNR: 27.83	PSNR: 30.32	PSNR: 31.87

Figure 6: Comparison of techniques, ranging from analytic to fully data-driven

$$\text{(L2O Model)} = N_\Theta(d) \triangleq \underset{x\in[0,1]^n}{\operatorname{argmin}} f_\Theta(Kx) \ \text{ s.t. } \ \|Ax - d\| \leq \delta$$

Summary

- Models with optimization layers that have tunable parameters can be readily designed and explained by domain experts
- With a well-chosen algorithm, implicit L2O models can be trained using JFB
- Certificates can be used to identify whether properties of each inference are consistent with training data (*i.e.* via post-conditions in software)

docs site	xai-l2o.research.typal.academy
preprint	arXiv.org/abs/2204.14174
reprint	Nature Scientific Reports (*accepted, coming soon*)