Rambling Away from Decision Focused Learning

A circuitous investigatation of what DFL can do
if you keep pushing at its limits

What I'll present is the result of joint work!

Many thanks to: Senne Berden, Victor Bucarey, Allegra De Filippo, Michelangelo Diligenti, Tias Guns, Jayanta Mandi, Irfan Mahmutogullari, Michela Milano, Maxime Mulamba, Mattia Silvestri

01. Getting Started

Getting Started

As stated, our starting point is Decision Focused Learning

Specifically the SPO formulation, where we focus on problems in the form:

$$z^*(y) = \text{argmin}_z \{ y^T z \mid z \in F \}$$

- z is the set of decisions (numeric or discrete)
- F is the feasible space
- y is a cost vector, which is not directly measureable

Rather than to y, we have access to an observable x

- Based on x, we can attempt to train a parametric estimator $h(x, \theta)$
- ...Using training examples $\{(x_i, y_i)\}_{i=1}^m$

A Possible Example

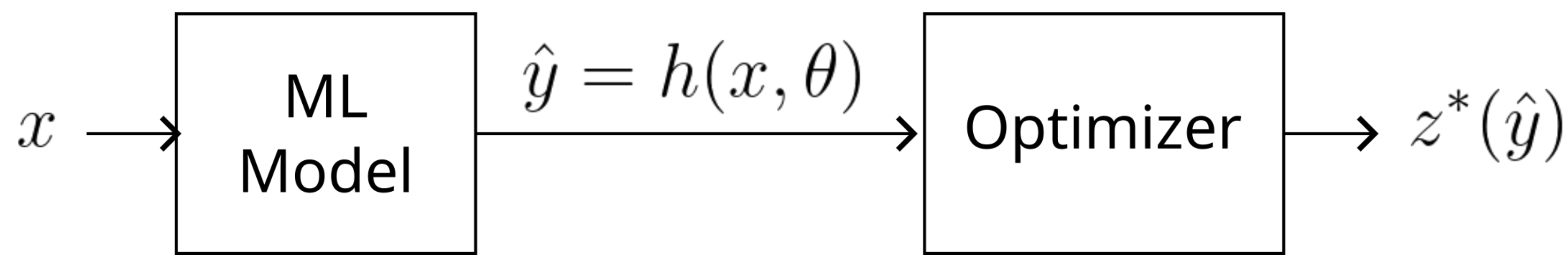
For example, we may have to deal with routing problem

We need to select the best path to reach our destination

- We don't know the current state of the traffic
- But we can guess! E.g. based on the time, weather, etc.

Inference

This setup involves using the estimator and the optimizer in sequence



At inference time:

- We observe x
- We evaluate our estimator $h(x, \theta)$ to obtain y
- We solve the problem to obtain $z^*(y)$

Overall, the process consists in evaluating:

$$z^*(h(x, \theta))$$

A Two-phase Approach

We can use supervised learning for the estimator

Formally, we obtain an optimal parameter vector by solving:

$$\theta^* = \text{argmin}_\theta \{\mathbb{E}_{(x,y)\sim P(X,Y)}[L(\hat{y}, y)] \mid \hat{y} = h(x, \theta)\}$$

- Where L is a suitable loss function (e.g. a squred error)
- We'll refer to this as a prediction-focused approach

However, using supervised learning is suboptimal

- A small mistake in terms of L
- ...May lead the optimizer to choosing a poor solution

The root of the issue is a misalignment between the cost metric at training and inference time

Spotting Trouble

Let's see this in action on a toy problem

Consider this two-variable optimization problem:

$$\text{argmin}_z \{ y_0 z_0 + y_1 z_1 \mid z_0 + z_1 = 1 \}$$

Let's assume that the true relation between x (a scalar) and y is:

$$\begin{aligned} y_0 &= 2.5x^2 \\ y_1 &= 0.3 + 0.8x \end{aligned}$$

...But that we can only learn this model with a scalar weight θ:

$$\begin{aligned} \hat{y}_0 &= \theta^2 x \\ \hat{y}_1 &= 0.5\theta \end{aligned}$$

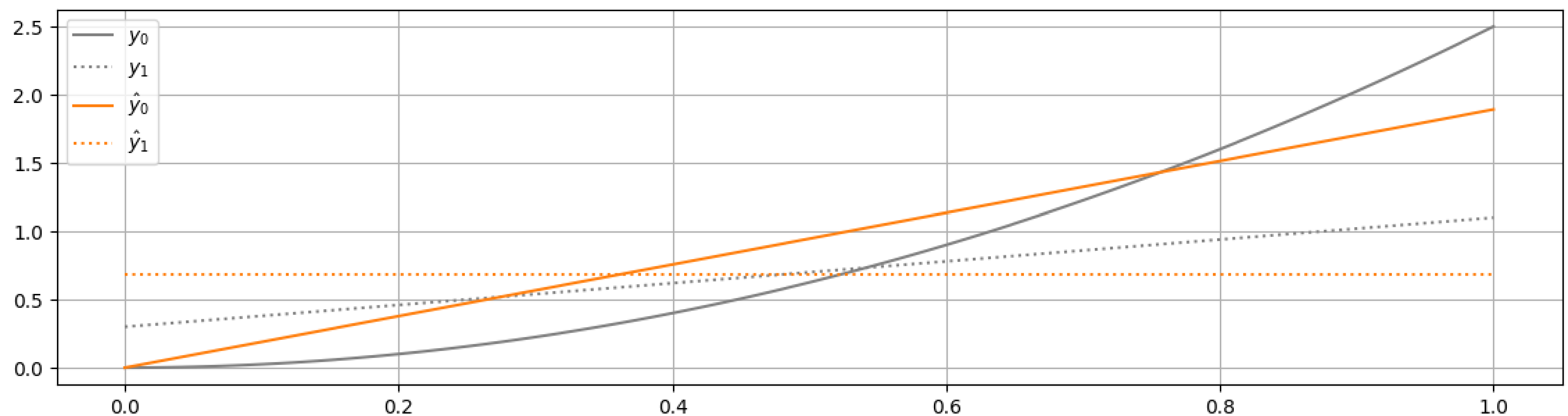
Our model cannot represent the true relation exactly

Spotting Trouble

This is what we get from supervised learning with uniformly distribute data:

```
In [15]: util.draw(w=None, figsize=figsize, model=1)
```

```
Optimized theta: 1.375
```

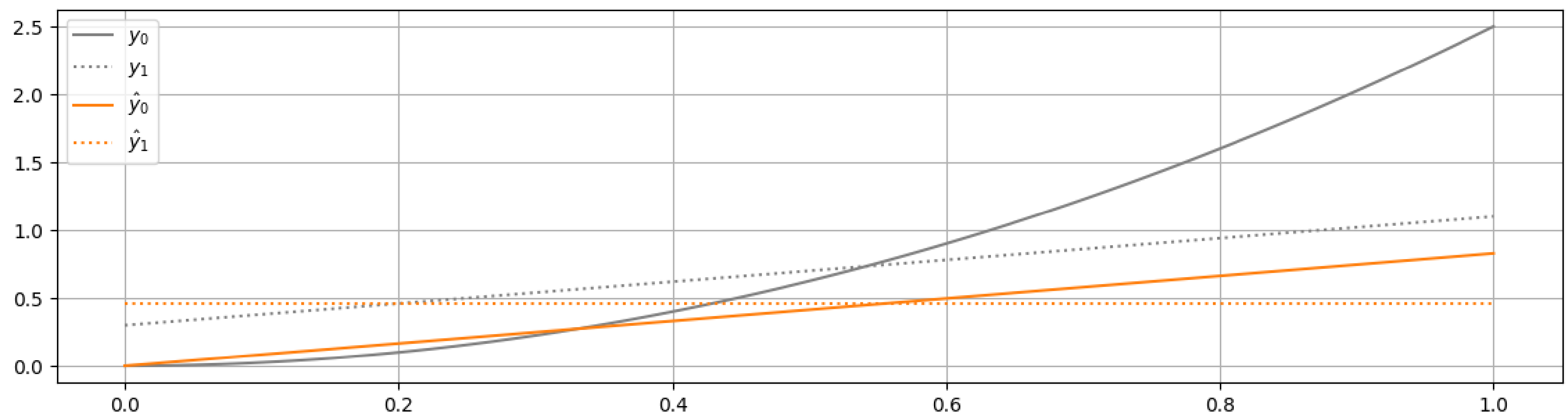


- The crossing point of the grey lines is where we should pick item 0 instead of 1
- The orange lines (trained model) miss it by a wide margin

Not All is Lost

However, we cas sidestep the issue by disergarding accuracy

```
In [16]: util.draw(w=0.91, figsize=figsize, model=1)
```



- If we focus on choosing θ to match the crossing point
- ...We lead the optimizer to consistently making the correct choice

The Main DFL Idea

DFL attempts to achieve this by using a task-based loss at training time

There's some consensus on this "holy grail" training problem:

$$\theta^* = \text{argmin}_\theta \{ \mathbb{E}_{(x,y)\sim P(X,Y)} [\text{regret}(\hat{y}, y)] \mid \hat{y} = h(x, \theta) \}$$

Where in our setting we have:

$$\text{regret}(\hat{y}, y) = y^T z^*(\hat{y}) - y^T z^*(y)$$

- $z^*(\hat{y})$ is the best solution with the estimated costs
- $z^*(y)$ is the best solution with the true costs

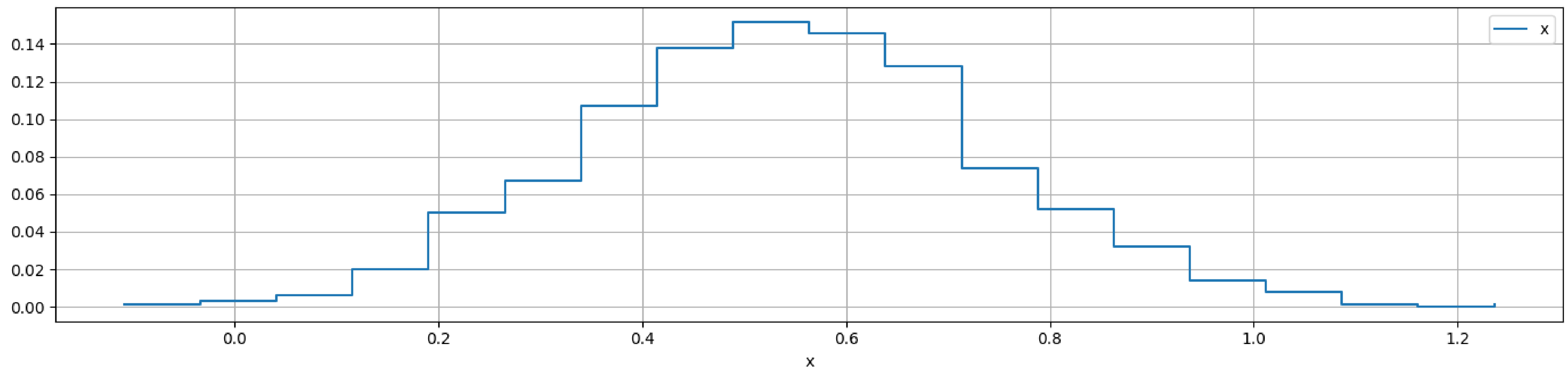
Intuitively, we want to loose as little as possible w.r.t. the best we could do

One of the main challenges in DFL is dealing with this loss

Knowing Regret

To see this, let's push our example a little further

In [17]:
```
x = util.normal_sample_(mean=0.54, std=0.2, size=1000)
util.plot_histogram(x, figsize=figsize, label='x')
```

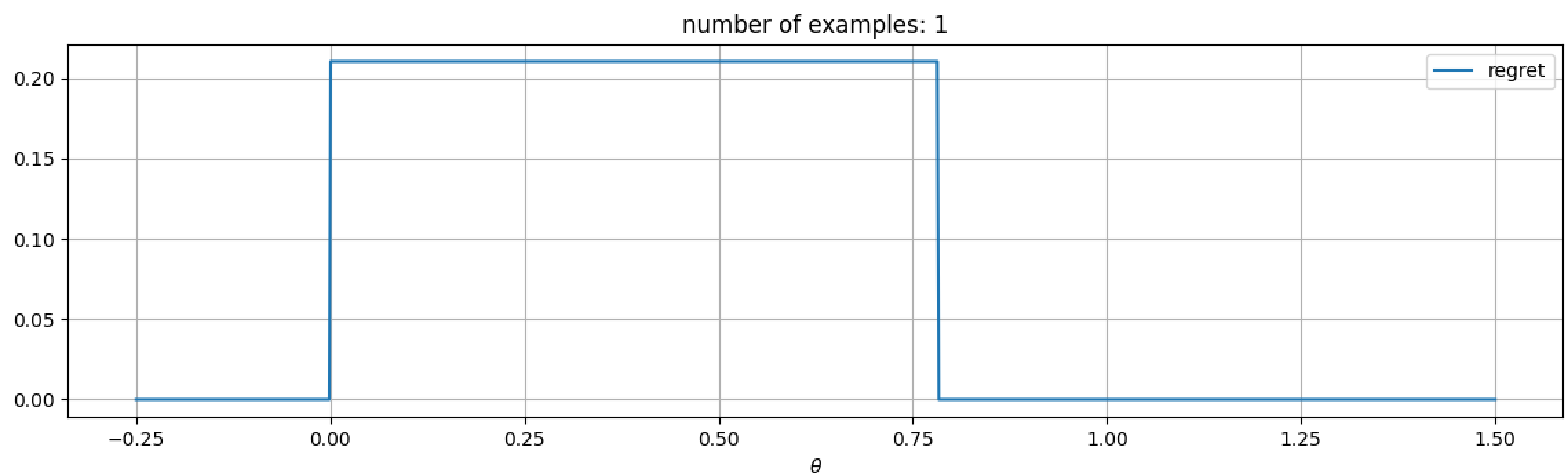


- Say we have access to a normally distributed collection of x values
- ...And to the corresponding true values y

Knowing Regret

This is how the regret looks like for a single example

```
In [18]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=1, figsize=fig
```

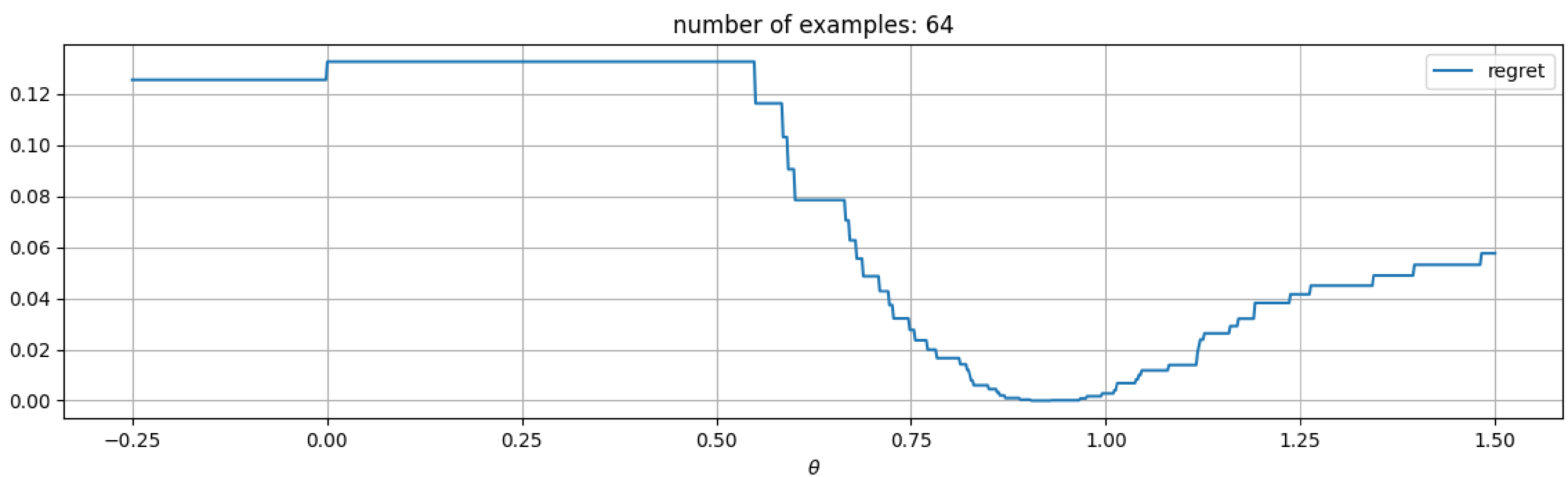


- If $f(x, \theta)$ leads to the correct decision, the regret is 0
- Otherwise we have some non-null value

Knowing Regret

...And this is the same for a larger sample

```
In [19]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=64, figsize=fi
```



- For linear problems and finite samples the regret function is piecewise constant
- ...Which makes a direct use of gradient descent impossible

SPO+ Loss

A lot of research in the DFL field is about addressing this problem

We will just recap the SPO+ loss from [1], which is (roughly) defined as:

$$\text{spo}^+(\hat{y}, y) = \hat{y}_{spo}^T z^*(y) - \hat{y}_{spo}^T z^*(\hat{y}_{spo}) \qquad \text{with:} \qquad \hat{y}_{spo} = 2\hat{y} - y$$

There are two main ideas here:

The first it to see what happens with the predicted (not the true) costs

- We know $z^*(\hat{y}_{spo})$ is the optimal solution for $\hat{y}_{spo}$
- But we wish for $z^*(y)$ to be optimal instead
- Therefore if $\hat{y}_{spo}^T z^*(y) > \hat{y}_{spo}^T z^*(\hat{y}_{spo})$ we give a penalty

With this trick, a differentiable term (i.e. $\hat{y}_{spo}$) appears in the loss

[1] Elmachtoub, Adam N., and Paul Grigas. "Smart "predict, then optimize"." Management Science 68.1 (2022): 9-26.

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There are two main ideas here:

The second is to avoid using the estimates y directly

- We rely instead on an altered cost vector, i.e. $\hat{y}_{spo}$
- Using $\hat{y}_{spo}$ directly would result in a local minimum for $\hat{y} = 0$
- With $\hat{y}_{spo}$, the local minimum is in a location _that depends on $\hat{y}$

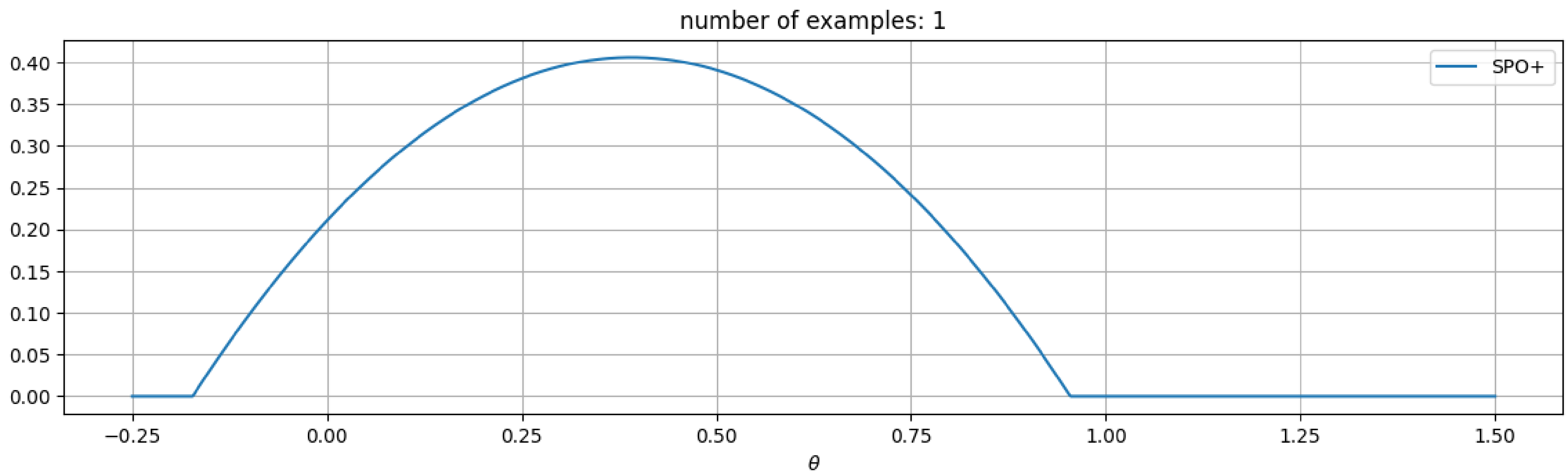
We'll try to visualize this phenomenon

[1] Elmachtoub, Adam N., and Paul Grigas. "Smart "predict, then optimize"." Management Science 68.1 (2022): 9-26.

SPO+ Loss

This is the SPO+ loss for a single example on our toy problem

In [20]:
```
util.draw_loss_landscape(losses=[util.SPOPlusLoss()], model=1, seed=42, batch_size=1, figsize=fi
```

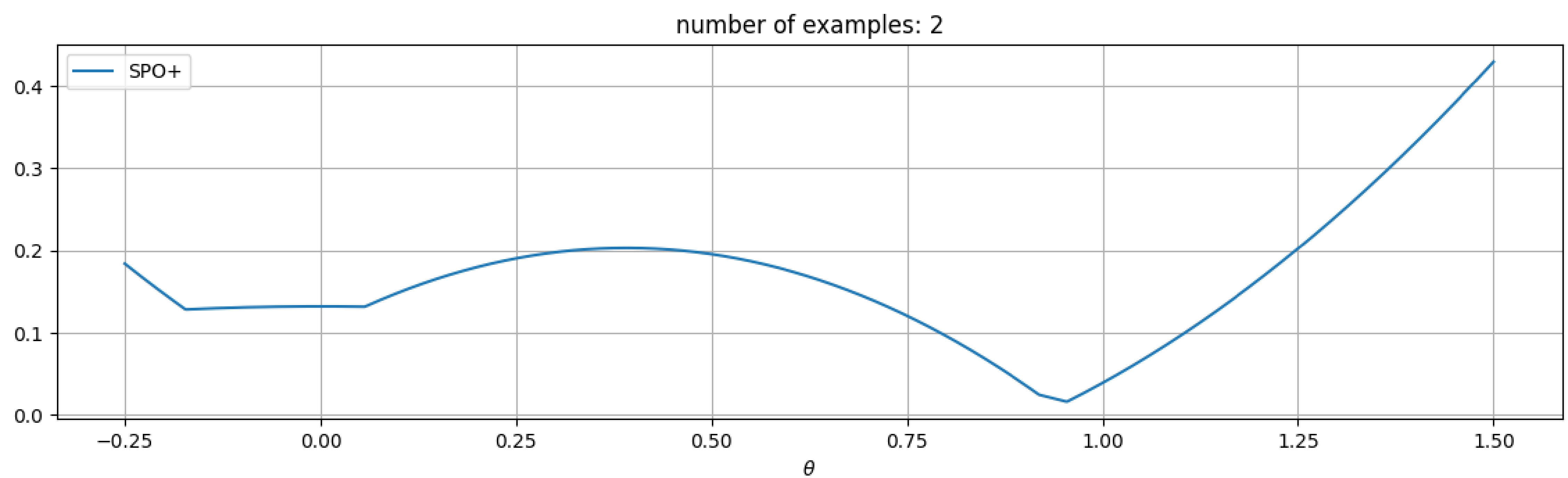


- As expected, there are two local minima

SPO+ Loss

This is the SPO+ loss for a two examples

```
In [21]: util.draw_loss_landscape(losses=[util.SPOPlusLoss()], model=1, seed=42, batch_size=2, figsize=fi
```

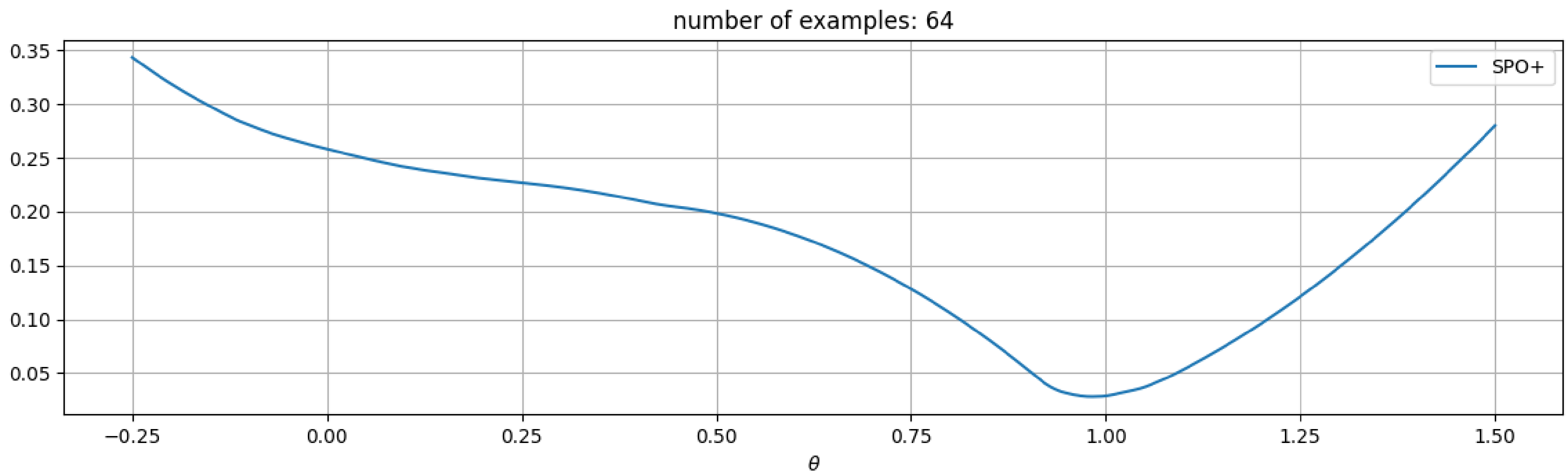


- The "good" local minima for both examples are roughly in the same place
- The "spurious" local minima fall in different position

SPO+ Loss

Over many example, the spurious local minima tend to cancel out

```
In [22]: util.draw_loss_landscape(losses=[util.SPOPlusLoss()], model=1, seed=42, batch_size=64, figsize=
```



- This effect is invaluable when training with gradient descent

A (Sligthly) More Complex Example

Let's see the approach in action on a second example

We will consider this simple optimization problem:

$$z^*(y) = \text{argmin}\{y^T z \mid v^T z \geq r, z \in \{0, 1\}^n\}$$

- We need to decide which of a set of jobs to accept
- Accepting a job ($z_j = 1$) provides immediate value v_j
- The cost y_j of the job is not known
- ...But it can be estimated based on available data

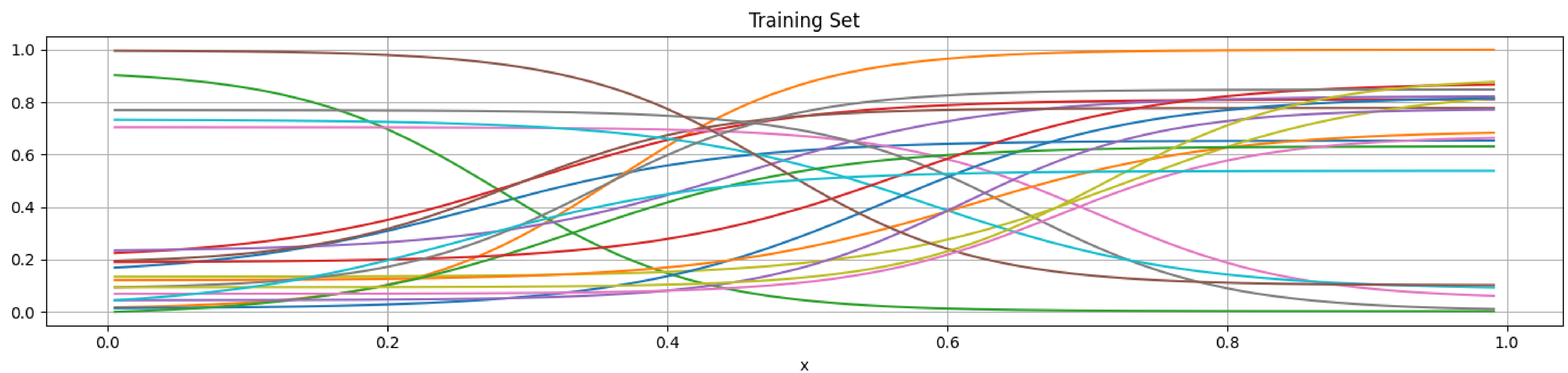
In [23]:
```
nitems, rel_req, seed = 20, 0.5, 42
prb = util.generate_problem(nitems=nitems, rel_req=rel_req, seed=seed)
display(prb)
```

```
ProductionProblem(values=[1.14981605 1.38028572 1.29279758 1.23946339 1.06240746 1.06239781
 1.02323344 1.34647046 1.240446   1.28322903 1.0082338  1.38796394
 1.33297706 1.08493564 1.07272999 1.0733618  1.1216969  1.20990257
 1.17277801 1.11649166], requirement=11.830809153591138)
```

A (Sligthly) More Complex Example

Next, we generate some training (and test) data

In [24]:
```
data_tr = util.generate_costs(nsamples=350, nitems=nitems, seed=seed, noise_scale=0, noise_type=
data_ts = util.generate_costs(nsamples=150, nitems=nitems, seed=seed, sampling_seed=seed+1, nois
util.plot_df_cols(data_tr, figsize=figsize, title='Training Set')
```



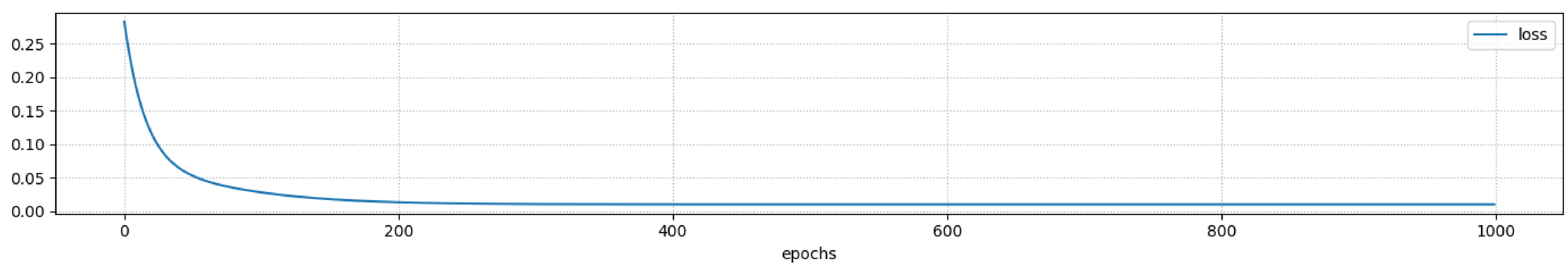
- We assume that costs can be estimated based on an scalar observable x
- The set of least expensive jobs changes considerably with x

Prediction Focused Approach

As a baseline, we'll consider a basic prediction-focused approach

```
In [25]: pfl = util.build_nn_model(input_shape=1, output_shape=nitems, hidden=[], name='pfl_det', output_
         %time history = util.train_nn_model(pfl, data_tr.index.values, data_tr.values, epochs=1000, loss
         util.plot_training_history(history, figsize=figsize_narrow, print_final_scores=False)
         util.print_ml_metrics(pfl, data_tr.index.values, data_tr.values, label='training')
         util.print_ml_metrics(pfl, data_ts.index.values, data_ts.values, label='test')
```

```
CPU times: user 8.94 s, sys: 330 ms, total: 9.27 s
Wall time: 7.36 s
```



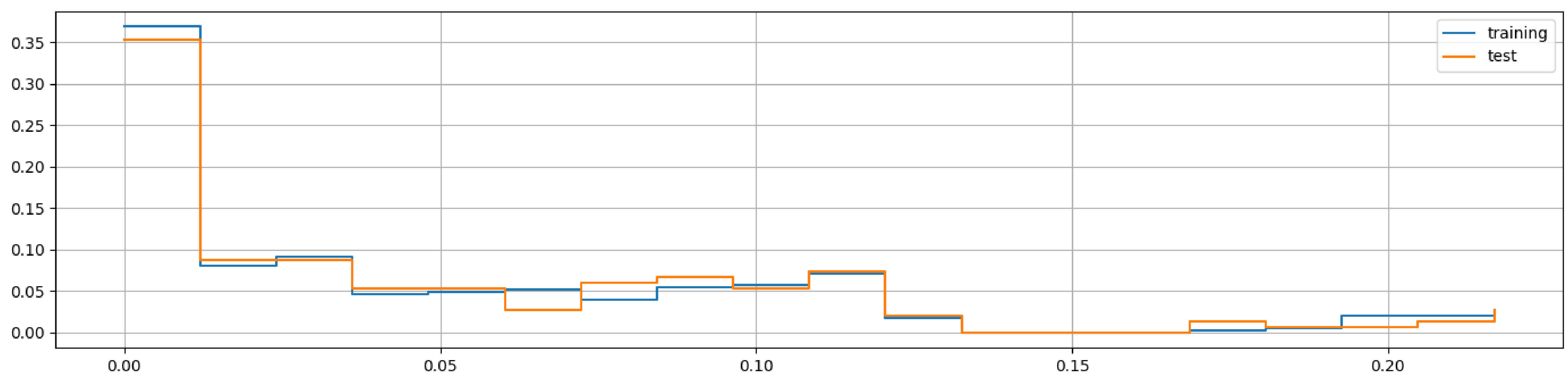

```
R2: 0.86, MAE: 0.086, RMSE: 0.10 (training)
R2: 0.86, MAE: 0.087, RMSE: 0.10 (test)
```

- The ML model is just a linear regressor, but it is decently accurate

Prediction Focused Approach

...But our true evaluation should be in terms of regret

In [26]:
```
r_tr = util.compute_regret(prb, pfl, data_tr.index.values, data_tr.values)
r_ts = util.compute_regret(prb, pfl, data_ts.index.values, data_ts.values)
util.plot_histogram(r_tr, figsize=figsize, label='training', data2=r_ts, label2='test', print_me
```



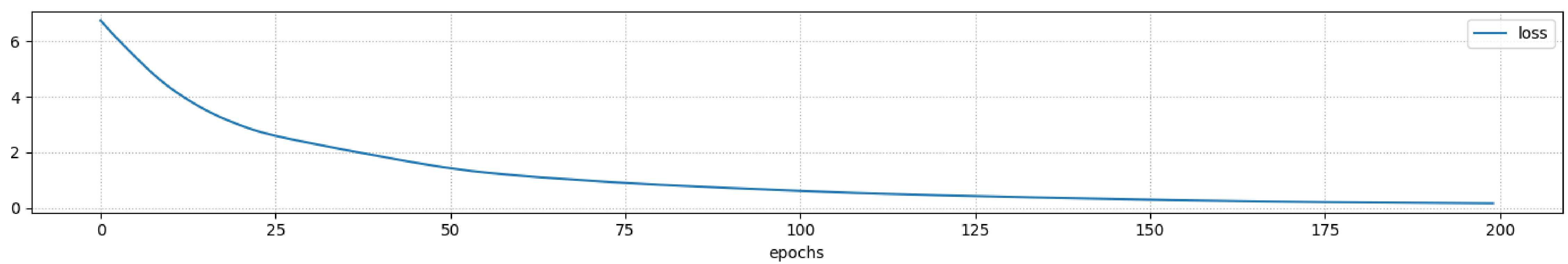

```
Mean: 0.052 (training), 0.053 (test)
```

- In this case, the average relative regret is ~5%

A Decision Focused Learning Approach

In [27]:
```
spo = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[], name='sp
%time history = util.train_dfl_model(spo, data_tr.index.values, data_tr.values, epochs=200, verb
util.plot_training_history(history, figsize=figsize_narrow, print_final_scores=False)
util.print_ml_metrics(spo, data_tr.index.values, data_tr.values, label='training')
util.print_ml_metrics(spo, data_ts.index.values, data_ts.values, label='test')
```

```
CPU times: user 4min 31s, sys: 20.3 s, total: 4min 51s
Wall time: 4min 51s
```



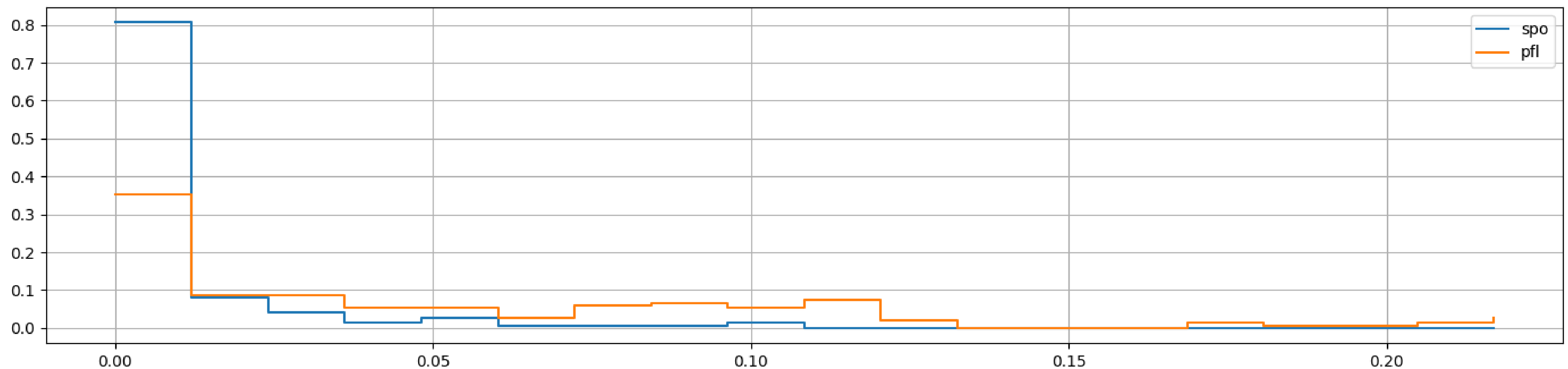

```
R2: -0.14, MAE: 0.22, RMSE: 0.27 (training)
R2: -0.14, MAE: 0.22, RMSE: 0.27 (test)
```

In terms of accuracy, this is considerably worse

Comparing Regrets

But the regret is so much better!

In [28]:
```
r_ts_spo = util.compute_regret(prb, spo, data_ts.index.values, data_ts.values)
util.plot_histogram(r_ts_spo, figsize=figsize, label='spo', data2=r_ts, label2='pfl', print_mear
```




```
Mean: 0.008 (spo), 0.053 (pfl)
```

This is the kind of result that attracted so much attention since [2]

[2] Donti, Priya, Brandon Amos, and J. Zico Kolter. "Task-based end-to-end model learning in stochastic optimization." Advances in neural information processing systems 30 (2017).