# Applicability of DFL

'Cause the Devil is in the Details

# Let's Second-Guess Ourselvers

**However, let's not discount the prediction-focused approach yet**

In fact, it's easy to see that:

$$\mathbb{E}[\text{regret}(y, \hat{y})] \xrightarrow[\mathbb{E}[L(y,\hat{y})]\to 0]{} 0$$

Intuitively:

- The more accurate we can be, the lower the regret
- Eventually, perfect predictions will result in 0 regret

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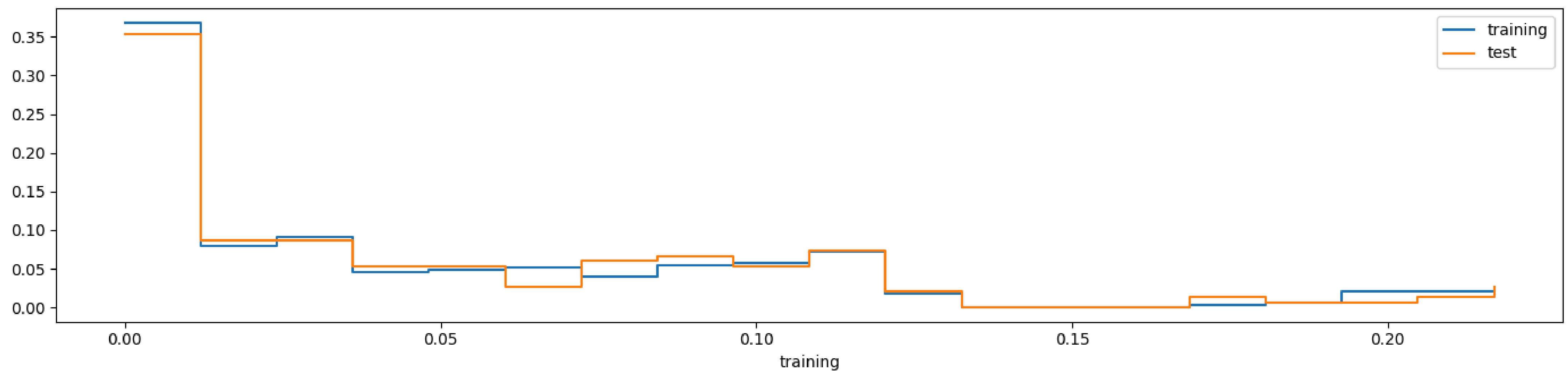
**But then... What if we make our model bigger?**

- We could get good predictions and good regret
- ...And training would be much faster

# Our Baseline

## Let's check again the results for our PFL linear regressor

In [105]:
```
pfl = util.build_ml_model(input_size=1, output_size=nitems, hidden=[], name='pfl_det', outpu
history = util.train_ml_model(pfl, data_tr.index.values, data_tr.values, epochs=1000, loss=
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', pri
```



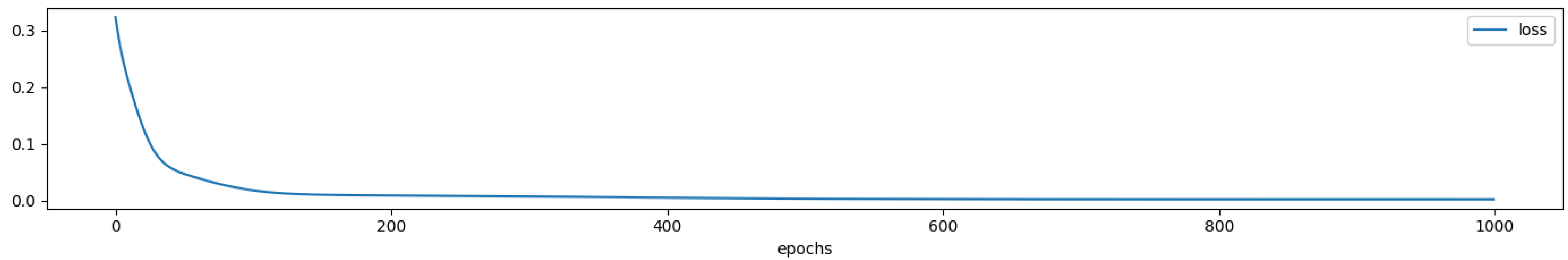

```
Mean: 0.053 (training), 0.053 (test)
```

This will be our main baseline

# PFL Strikes Back

## Let's try to use a non-linear model

In [106]:
```
pfl_acc = util.build_ml_model(input_size=1, output_size=nitems, hidden=[8], name='pfl_det_ac
history = util.train_ml_model(pfl_acc, data_tr.index.values, data_tr.values, epochs=1000, lo
util.plot_training_history(history, figsize=figsize_narrow, print_scores=False, print_time=T
util.print_ml_metrics(pfl_acc, data_tr.index.values, data_tr.values, label='training')
util.print_ml_metrics(pfl_acc, data_ts.index.values, data_ts.values, label='test')
```



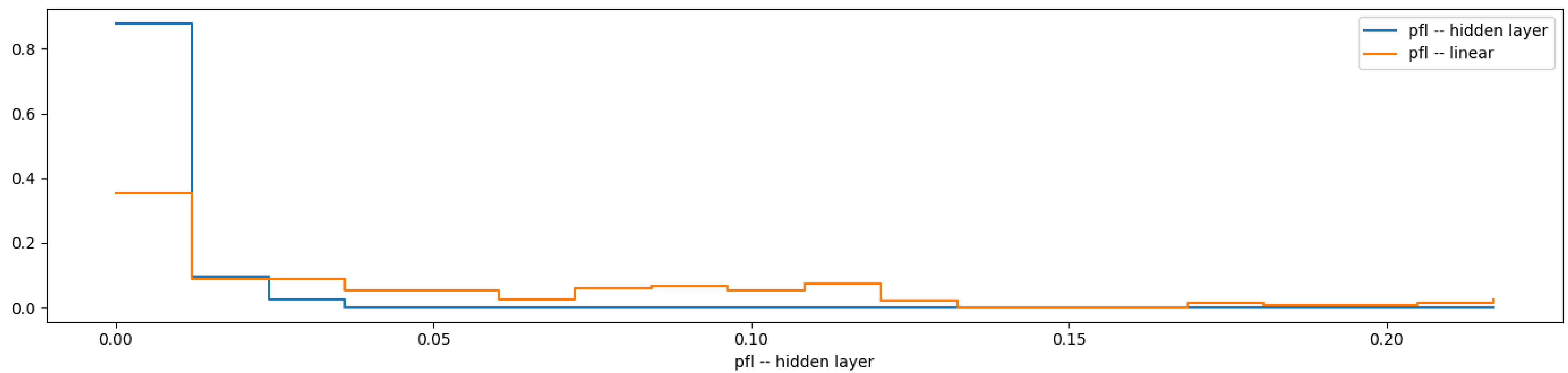

```
Training time: 7.6650 sec
R2: 0.98, MAE: 0.031, RMSE: 0.04 (training)
R2: 0.98, MAE: 0.031, RMSE: 0.04 (test)
```

More accurate, it is!

# PFL Strikes Back

## ...And the improvement in terms of regret is remarkable

In [107]:
```
r_ts_acc = util.compute_regret(prb, pfl_acc, data_ts.index.values, data_ts.values)
util.plot_histogram(r_ts_acc, figsize=figsize, label='pfl -- hidden layer', data2=r_ts, labe
```




```
Mean: 0.004 (pfl -- hidden layer), 0.053 (pfl -- linear)
```

- DFL might do better with the same model complexity
- ...But the return would be diminished

# Evening the Field

## Can't we do anything about it?

- DFL predictions will always be off (more or less)
- ...But there are ways to make the approach faster

## For example:

- You can use a problem relaxation, as in [1]
- You can limit recomputation by caching past solutions, as in [2]
- You can warm start the DFL approach with the PFL weights

Let's see the last two tricks in deeper detail


*[1] Mandi, Jayanta, and Tias Guns. "Interior point solving for lp-based prediction+ optimisation." Advances in Neural Information Processing Systems 33 (2020): 7272-7282.*
*[2] Maxime Mulamba, Jayanta Mandi, Michelangelo Diligenti, Michele Lombardi, Victor Bucarey, Tias Guns: Contrastive Losses and Solution Caching for Predict-and-Optimize. IJCAI 2021: 2833-2840*

## Warm Starting and Solution Caching

**Warm starting simple consists in using the PFL weights to initialize $\theta$**

Since accuracy is correlated with regret, this might accelerate convergence

# Warm Starting and Solution Caching

**Warm starting simple consists in using the PFL weights to initialize $\theta$**

Since accuracy is correlated with regret, this might accelerate convergence

**Solution caching is applicable if the feasible space is fixed**

I.e. to problems in the form:

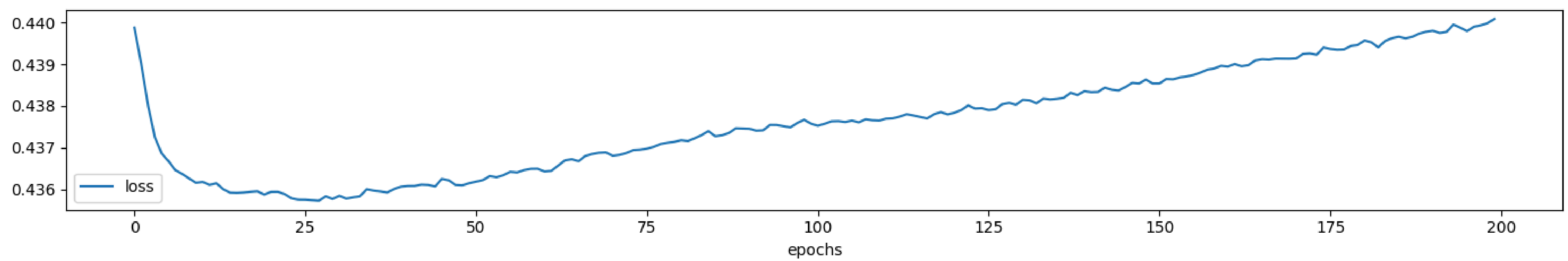
$$z^*(y) = \text{argmin}_z \{ f(z) \mid z \in F \}$$

- During training, we maintain a solution cache $S$
- Initially, we populate $S$ with the true optimal solutions $z^*(y_i)$ for all examples
- Before computing $z^*(\hat{y})$ for the current prediction we flip a coin
- With probability $p$, we run the computation (and store any new solution in $S$)
- With probability $1 - p$, we solve instead $\hat{z}^*(\hat{y}) = \text{argmin}_z \{ f(z) \mid z \in S \}$

# Speeding Up DFL

## Let's use DFL with linear regression, a warm start, and a solution cache

In [108]:
```
spo = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[], name
history = util.train_dfl_model(spo, data_tr.index.values, data_tr.values, epochs=200, verbos
util.plot_training_history(history, figsize=figsize_narrow, print_scores=False, print_time=T
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')
```



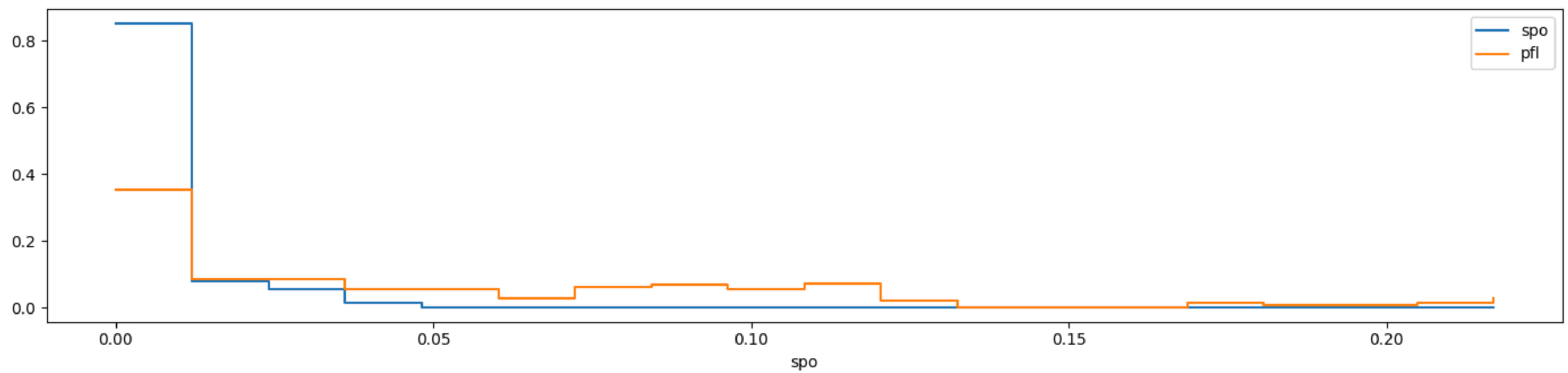

```
Training time: 30.4938 sec
R2: 0.77, MAE: 0.099, RMSE: 0.13 (training)
R2: 0.77, MAE: 0.1, RMSE: 0.13 (test)
```

The training time is still large, but much lower than our earlier DFL attempt

# Speeding Up DFL

## And the regret is even better!

```
In [109]: 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_
```




```
Mean: 0.004 (spo), 0.053 (pfl)
```

We are matching the more complex PFL model with a simple linear regressor

# Reflecting on What we Have

**Therefore, DFL gives us at least two benefits**

First, it can lead to lower regret compared to a prediction-focused appraach

- As the models become more complex we have diminishing returns
- ...But for some applications every little bit counts

Second, it may allow using simpler ML models

- Simple models are faster to evaluate
- ...But more importantly they are easier to explain
- E.g. we can easily perform feature importance analysis

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**Intuitively, DFL works best where PFL has estimation issues**
Can we exploit this fact to maximize our advantage?

# Maximizing Results

**There's a simple case where PFL cannot make perfect predictions**

You just need need to target a stochastic problem!

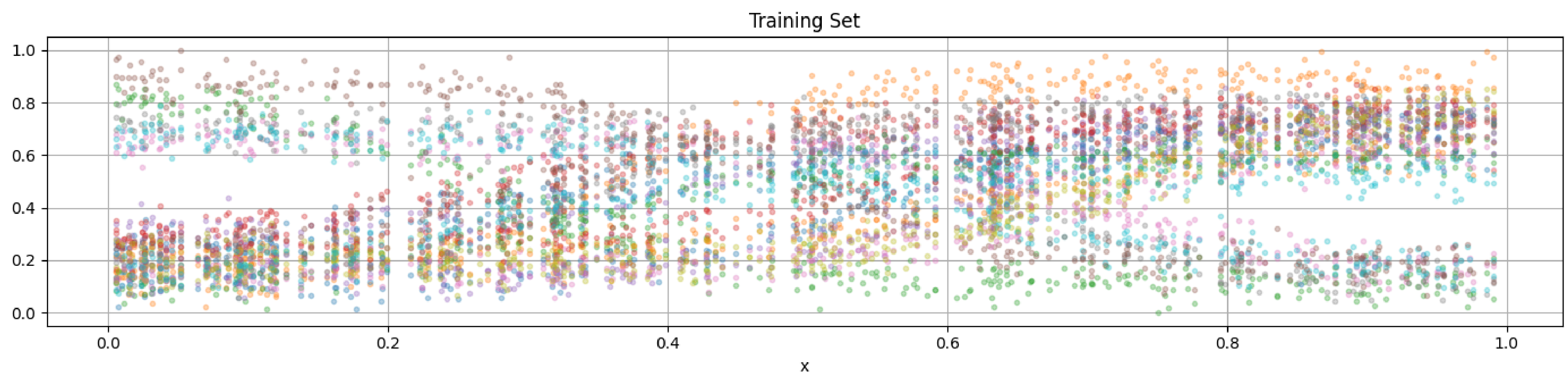
- E.g. you can usually tell the traffic situation based on (e.g.) time and weather
- ...But there still a lot of variability

# Maximizing Results

## Formally, we need a stochastic process, i.e. a stochastic function

We can generate data for a stochastic variant of our problem

In [110]:
```
data_tr = util.generate_costs(nsamples=350, nitems=nitems, seed=seed, noise_scale=.15, noise
util.plot_df_cols(data_tr, figsize=figsize, title='Training Set', scatter=True)
```




We treat boh $X$ and $Y$ as random variables, with distribution $P(X, Y)$

## Adjusting Goals

**But with a stochastic process, what is our real objective?**

For a given $x$ (i.e. a given context), we can formalize it like this:

$$\text{argmin}_z \left\{ \mathbb{E}_{y \sim P(Y|x)} \left[ y^T z \right] \mid z \in F \right\}$$

- Given a value for the observable $x$
- We want to find a single decision vector $z$
- Such that $z$ is feasible
- ...And $z$ minimizes the expected cost over the distribution $P(Y \mid x)$

**This is called a one-stage stochastic optimization problem**

# ...And Keeping the Setup

**Let's look again at the DFL training problem**

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

With:

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

**Since $y^T z^*(y)$ is independent on $\theta$, this is equivalent to:**

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

Which can be rewritten as:

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

# ...And Keeping the Setup

**Now, let's restrict to the case where $x$ is fixed**

$$\theta^* = \text{argmin}_\theta \{\mathbb{E}_{y \sim P(Y|x)}[y^T z^*(\hat{y})] \mid \hat{y} = h(x;\theta)\}$$

Finally, by definition of $z^*(\cdot)$ we have:

$$\theta^* = \text{argmin}_\theta \{\mathbb{E}_{y \sim P(Y|x)}[y^T z^*(\hat{y})] \mid \hat{y} = h(x;\theta), z^*(\hat{y}) \in F\}$$

In other words:

- We are choosing $\theta$
- So that $z^*(\hat{y})$ minimizes $\mathbb{E}_{y \sim P(Y|x)}[y^T z^*(\hat{y})]$

**This is almost identical to one-stage stochastic optimization!**

# DFL For One-Stage Stochastic Optimization

**DFL can address 1s-SOPs, with one restriction and two "superpowers":**

The restriction is that we control $z$ only through $\theta$

- Therefore, depending on the chosen ML model architecture
- ...Obtaining some solutions might be impossible
- This issue can be sidestepped with a careful model choice

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**The first superpower is that we are not restricted to a single $x$ value**

- Given a new value for $x$, we just need to evaluate $h(x, \theta^*)$
- ...And then solve the usual optimization problem
- Many approaches do not deal with the estimation of the $y$ distribution

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**For the second superpower, we need to investigate a bit more**

# Classical Solution Approach

**What would be the classical solution approach?**

Starting from:

$$\operatorname{argmin}_z \left\{ \mathbb{E}_{y \sim P(Y|x)} [y^T z] \mid z \in F \right\}$$

We can use linearity to obtain:

$$\operatorname{argmin}_z \left\{ \mathbb{E}_{y \sim P(Y|x)} [y]^T z \mid z \in F \right\}$$

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- ...Then we could solve a deterministic problem

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- ...Then we could solve a deterministic problem

**But isn't this what PFL is doing?**

# Regression and Expectation

**(Stochastic) Regression is often presented as learning an expectation**

...But it's trickier than that

- Using an MSE loss is equivalent to trying to learn $\mathbb{E}_{y \sim P(Y|x)}[y]$
- ...But only assuming that $P(Y \mid x)$ is Normally distributed
- ...And that it has the same variance everywhere

**It is possible to do the same under more general conditions**

...But it is much more complex

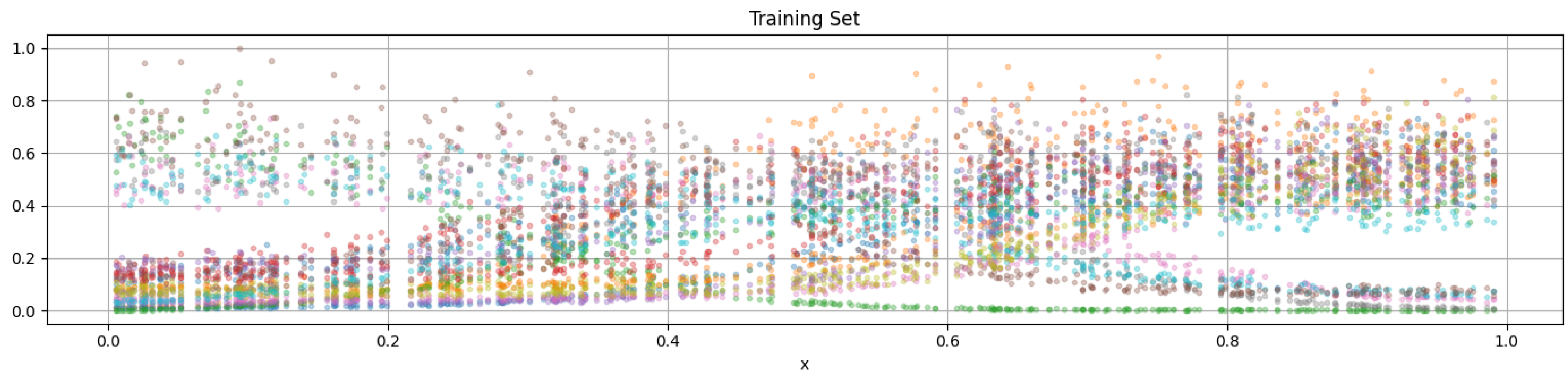
- If we know the distribution type, we can use a neuro-probabilistic model
- Otherwise, we need a fully fledged contextual generative model

In DFL, we can address this problem with 0 added effort!

# A Simple Stress Test

## We can test this idea by generating a stochastic dataset

```
In [111]: data_tr = util.generate_costs(nsamples=350, nitems=nitems, seed=seed, noise_scale=.2, noise_
          data_ts = util.generate_costs(nsamples=150, nitems=nitems, seed=seed, sampling_seed=seed+1,
          util.plot_df_cols(data_tr, figsize=figsize, title='Training Set', scatter=True)
```

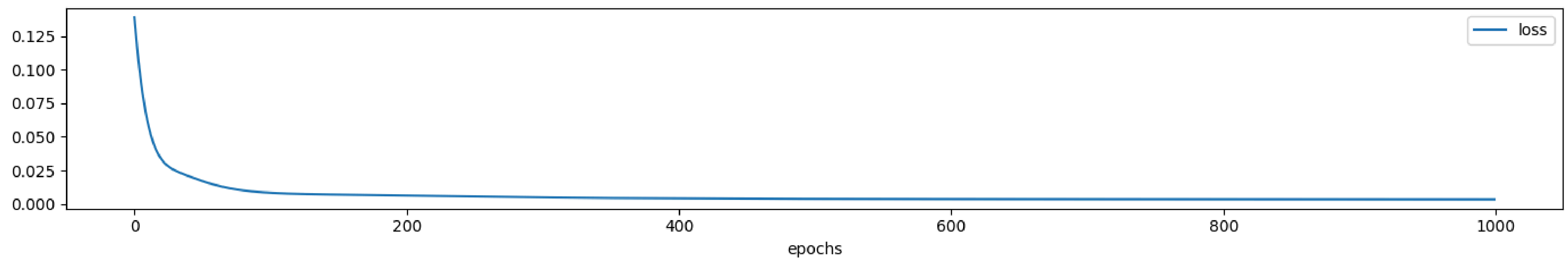



- ...And scaling the variance with $y$
- Which is also a very common setting in practice

# Training a PFL Approach

## We will train again a non-linear prediction focused approach

In [112]:
```
pfl_1s = util.build_ml_model(input_size=1, output_size=nitems, hidden=[8], name='pfl_1s', ou
history = util.train_ml_model(pfl_1s, data_tr.index.values, data_tr.values, epochs=1000, los
util.plot_training_history(history, figsize=figsize_narrow, print_scores=False, print_time=T
util.print_ml_metrics(pfl_1s, data_tr.index.values, data_tr.values, label='training')
util.print_ml_metrics(pfl_1s, data_ts.index.values, data_ts.values, label='test')
```



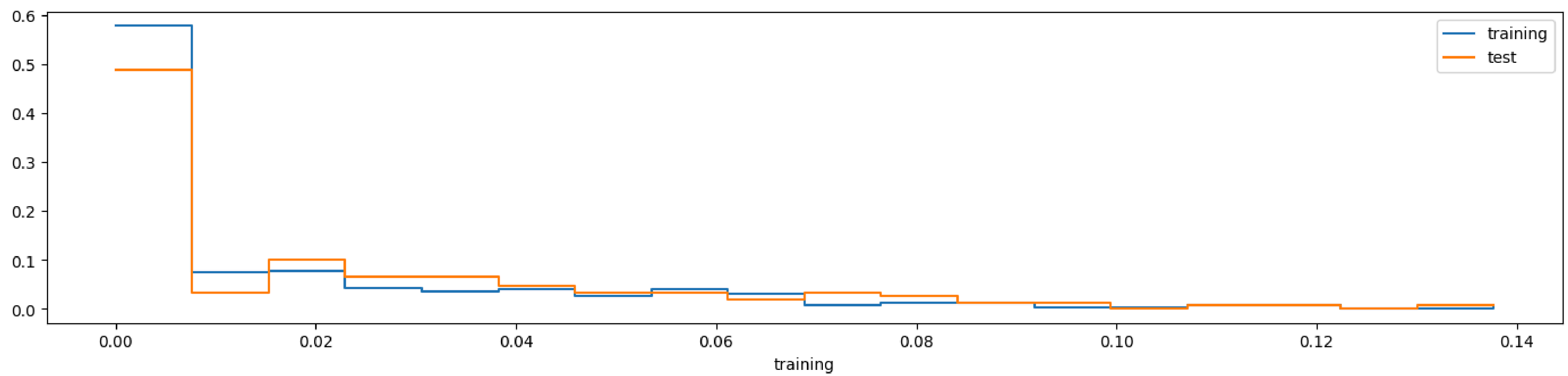

```
Training time: 7.8414 sec
R2: 0.91, MAE: 0.042, RMSE: 0.06 (training)
R2: 0.91, MAE: 0.042, RMSE: 0.06 (test)
```

The accuracy is (inevitably) worse, but still pretty good

# PFL Regret

## Let's evaluate the regret of the PFL approach

In [113]:
```
r_tr_1s = util.compute_regret(prb, pfl_1s, data_tr.index.values, data_tr.values)
r_ts_1s = util.compute_regret(prb, pfl_1s, data_ts.index.values, data_ts.values)
util.plot_histogram(r_tr_1s, figsize=figsize, label='training', data2=r_ts_1s, label2='test
```



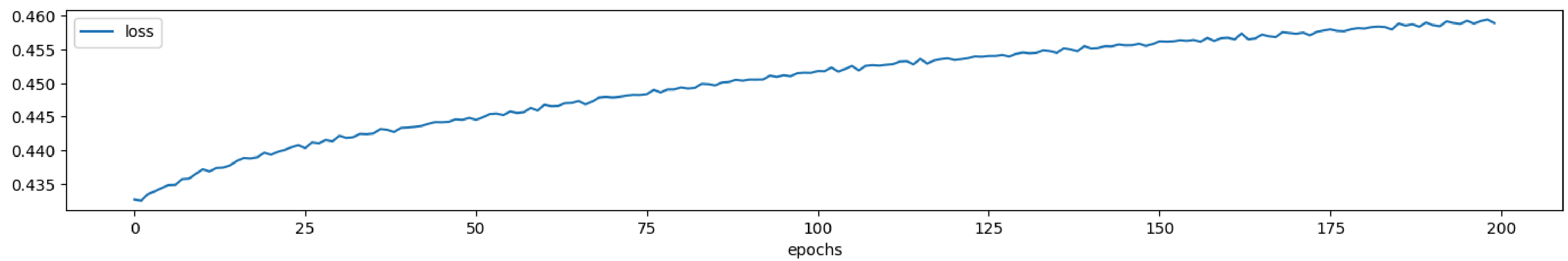

```
Mean: 0.018 (training), 0.024 (test)
```

The regret has slighly worsened, due to the effect of uncertainty

# Training a DFL Approach

## We also a DFL approach with the same non-linear model

In [114]:
```
spo_1s = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[8],
history = util.train_dfl_model(spo_1s, data_tr.index.values, data_tr.values, epochs=200, ve
util.plot_training_history(history, figsize=figsize_narrow, print_scores=False, print_time=T
util.print_ml_metrics(spo_1s, data_tr.index.values, data_tr.values, label='training')
util.print_ml_metrics(spo_1s, data_ts.index.values, data_ts.values, label='test')
```

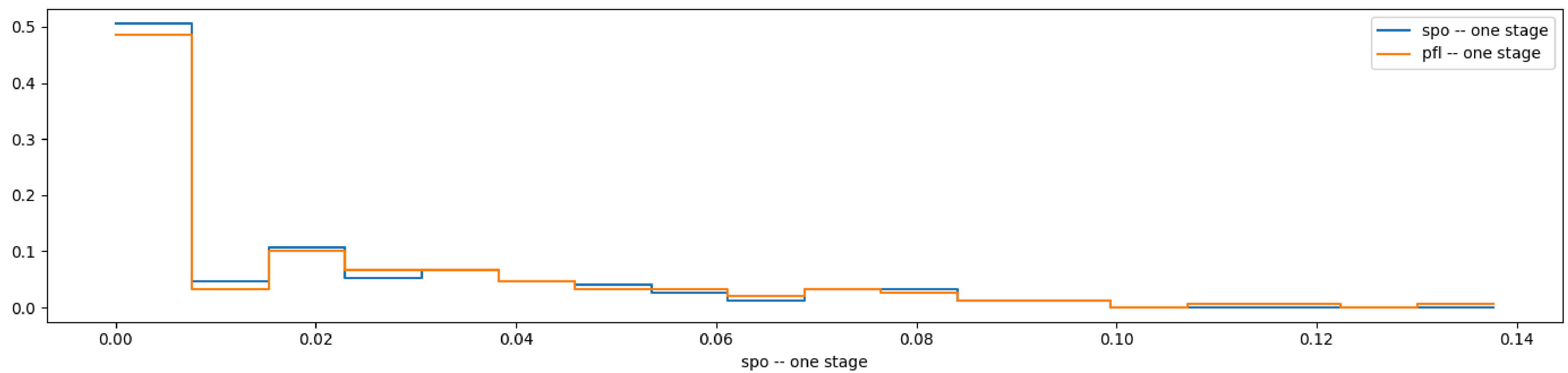



```
Training time: 22.6284 sec
R2: 0.82, MAE: 0.062, RMSE: 0.09 (training)
R2: 0.82, MAE: 0.063, RMSE: 0.09 (test)
```

# DFL Regret

## Now we can compare the regret for both approaches

In [115]:
```
r_ts_spo_1s = util.compute_regret(prb, spo_1s, data_ts.index.values, data_ts.values)
util.plot_histogram(r_ts_spo_1s, figsize=figsize, label='spo -- one stage', data2=r_ts_1s,
```




```
Mean: 0.020 (spo -- one stage), 0.024 (pfl -- one stage)
```

- There is a significant gap again
- Since the PFL approach is operating on an incorrect semantic

## Considerations

**DFL can be thought of as a one-stage stochastic optimization approach**

In this setting:

- In particular, using a more accurate PFL model might still have poor regret
- ...Unless we know a lot about the distribution
- ...or we use a very complex estimator
- Conversely, DFL has not such issues

**The gap becomes wider in case of non-linear cost functions:**

- In this case the expected cost would not be equivalent to a sum of expectations
- But a DFL approach would have no such issues
- ...Provided it could deal with with non-linear functions