# Generalizing DFL

Which is where we reap the most benefits

# Two-Stage Stochastic Optimization

**If DFL targets one-stage stochastic optimization, could we do two-stage?**

- For example, in first stage we decide what to pack in our suitcase
- ...During the trip, we may realize we have forgotten something
- ...And we need to spend money to buy the missing stuff

# Two-Stage Stochastic Optimization

**If DFL targets one-stage stochastic optimization, could we do two-stage?**

Two-stage problems are among the most interesting in stochastic optimization

- They involve making a set of decisions now
- Then observing how uncertainty unfolds
- ...And making a second set of decisions

The former are called first-stage decisions, the latter recourse actions

**Here's an example we will use for this topic**

Say we need to secure a supply of resources

- First, we make contracts with primary suppliers to minimize costs
- If there are unexpected setbacks (e.g. insufficient yields)
- ...Then we can buy what we lack from another source, but at a higher cost

# Two-Stage Stochastic Optimization

**Let's define two-stage stochastic optimization problems (2s-SOP) formally:**

$$\text{argmin}_z \left\{ f(z) + \mathbb{E}_{y \sim P(Y|x)} \left[ \min_{z''} r(z'', z, y) \right] \mid z \in F, z'' \in F''(z, y) \right\}$$

- $Y$ represents the uncertain information
- $z$ is the vector of first stage decisions
- $F$ is the feasible space for the first stage
- $z''$ is the vector of recourse actions
- $z''$ is not fixed: it can change for every sampled $y$
- The set of feasible recourse actions $F''(z, y)$ also changes for every $y$
- $f$ is the immediate cost function, $r$ is the cost of the recourse actions

# A Simple Example

## We will consider this simple problem

...Which is based on our previous supply planning example:

$$\text{argmin}_z \; c^T z + \mathbb{E}_{y \sim P(Y|x)} \left[ \min_{z''} c'' z'' \right]$$

$$\text{subject to: } y^T z + z'' \geq y_{min}$$

$$z \in \{0, 1\}^n, z'' \in \mathbb{N}_0$$

- $z_j = 1$ iff we choose then $h$-th supply contract
- $c_j$ is the cost of the $j$-th contract
- $y_j$ is the yield of the $j$-th contract, which is uncertain
- $y_{min}$ is the minimum total yield, which is known
- $z''$ is the number of units we buy at cost $c''$ to satisfy the yield requirement

## Scenario Based Approach

**Classical solution approaches for 2s-SOP are scenario based**

We start by sampling a finite set of $N$ values from $P(Y \mid x)$

$$
\begin{aligned}
\text{argmin}_z \min_{z''} \ & c^T z + \frac{1}{N} c'' z''_k \\
\text{subject to: } & y^T z + z''_k \geq y_{min} && \forall k = 1..N \\
& z \in \{0, 1\}^n \\
& z''_k \in \mathbb{N}_0 && \forall k = 1..N
\end{aligned}
$$

Then we build different recourse action variables for each scenario

- ...We define the feasible sets via constraints
- ...And we use the Sample Average Approximation to estimate the expectation

**The method is effective, but also computationally expensive**

# DFL for 2s-SOP

## Could we tackle 2s-SOP with DFL?

As a recap, our DFL training problem is:

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

With:

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

And:

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

## DFL for 2s-SOP

**With the same transformations used in the one-stage case, we get:**

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

**Now, say we had a DFL approch that could deal with any function $g(z, y)$**

- In this case $y$ would be a vector of uncertain parameters (not necessarily costs)
- The function should compute the equivalent of $y^T z^*(\hat{y})$
- ...I.e. the true cost of the solution computed for the estimate costs

**Under this conditions, at training time we could solve:**

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

It would still be DFL, just a bit more general

## DFL for 2s-SOP

**At this point, let's choose:**

$$g(z, y) = \min_{z''} \left\{ f(z) + r(z'', z, y) \mid z'' \in F''(z, y) \right\}$$

- For a given solution $z$, $g(z, y)$ computes the best possible objective
- ...Assuming that the value of the parameters is $y$

**By substituting in the training formulation we get:**

$$\text{argmin}_\theta \; f(z^*(\hat{y})) + \mathbb{E}_{y \sim P(Y|x)} \left[ \min_{z''} r(z'', z^*(\hat{y}), y) \right]$$
$$\text{subject to: } \hat{y} = h(x; \theta), z^*(\hat{y}) \in F, z'' \in F''(z, y)$$

...Which can definitely be used for 2s-SOP problems!

## Grouding the Approach

**We can ground the approach by relying on the scenario-based formulation**

In our example problem, we compute $z^*(y)$ by solving:

$$
\begin{aligned}
z^*(y) = \text{argmin}_z \text{min}_{z''} c^T z + c'' z''_k \\
\text{subject to: } y^T z + z''_k \geq y_{min} \\
z \in \{0, 1\}^n \\
z''_k \in \mathbb{N}_0
\end{aligned}
$$

And we define $g(z, y)$ as:

$$
\begin{aligned}
g(z, y) = \text{min}_{z''}\ c^T z + c'' z''_k \\
\text{subject to: } y^T z + z''_k \geq y_{min} \\
z''_k \in \mathbb{N}_0
\end{aligned}
$$

# Overview and Properties

**Intuitively, the approach works as follows**

- We observe $x$ and we compute $\hat{y}$
- We compute $z^*(\hat{y})$ by solving a scenario problem
- We compute $g(z^*(\hat{y}), y)$ by solving a scenario problem with fixed $z$ values

...And we end up minimizing the expected cost of the 2s-SOP

**We have 1 restriction and 3 "superpowers" w.r.t. the classical approach**

- The restriction: we control $z^*$ only through $\theta$
- Superpower 1: we are not restricted to a single $x$
- Superpower 2: works with any distribution
- Superpower 3: at inference time, we always consider a single scenario

# Scalable Two-stage Stochastic Optimization

## The last advantage is massive

The weakest point of classical 2s-SOP approach is scalability

- Multiple scenarios are required to obtain good results
- ...But they also add more variables

With NP-hard problem, the solution time can grow exponentially

## With this approach, the computational cost is all at training time

- It can even be lower, since you always deal with single scenarios
- There are alternatives, such as [1], where ML is used to estimate the recourse
- ...These have their own pros and cons

*[1] Dumouchelle, Justin, et al. "Neur2sp: Neural two-stage stochastic programming." arXiv preprint arXiv:2205.12006 (2022).*

# The Elephant in the Room

**So far, so good, but how to we make $g(z, y)$ differentiable?**

There are a few alternatives, all with limitations:

- The approach from [1] handles parameters in the problem constraints
  - It is based on the idea of differencing the recourse action
  - ...But it is (mostly) restricted to 1D packing problems
- The approach from [2] can be used for 2s-SOP with a stretch
  - It based on idea of embedding a MILP solver in ML
  - ...But it's semantic does not fully align with 2s-SOP

**Here, we will see a different technique**

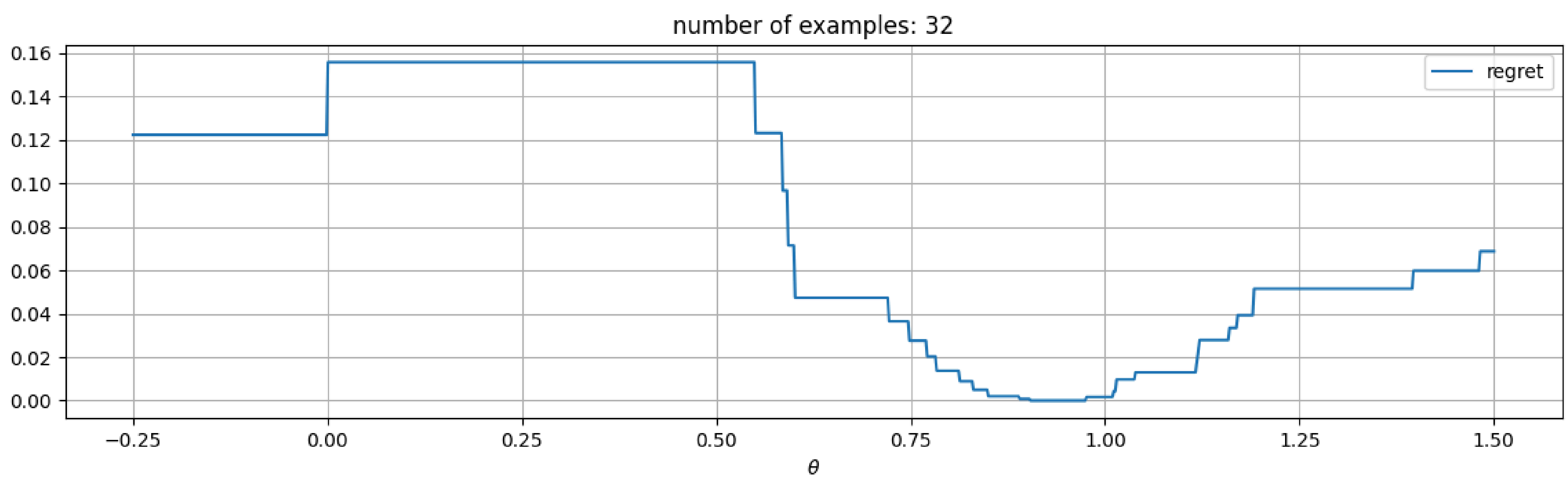
*[1] Hu, X., Lee, J. C. H., and Lee, J. H. M. Predict+optimize for packing and covering lps with unknown parameters in constraints. CoRR, abs/2209.03668, 2022. doi: 10. 48550/arXiv.2209.03668.*

*[2] Paulus, Anselm, et al. "Comboptnet: Fit the right np-hard problem by learning integer programming constraints." International Conference on Machine Learning. PMLR, 2021.*

# Looking Back at SPO

**Let's look again at the regret loss for our original toy example**

```
In [18]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=32, figsi
```

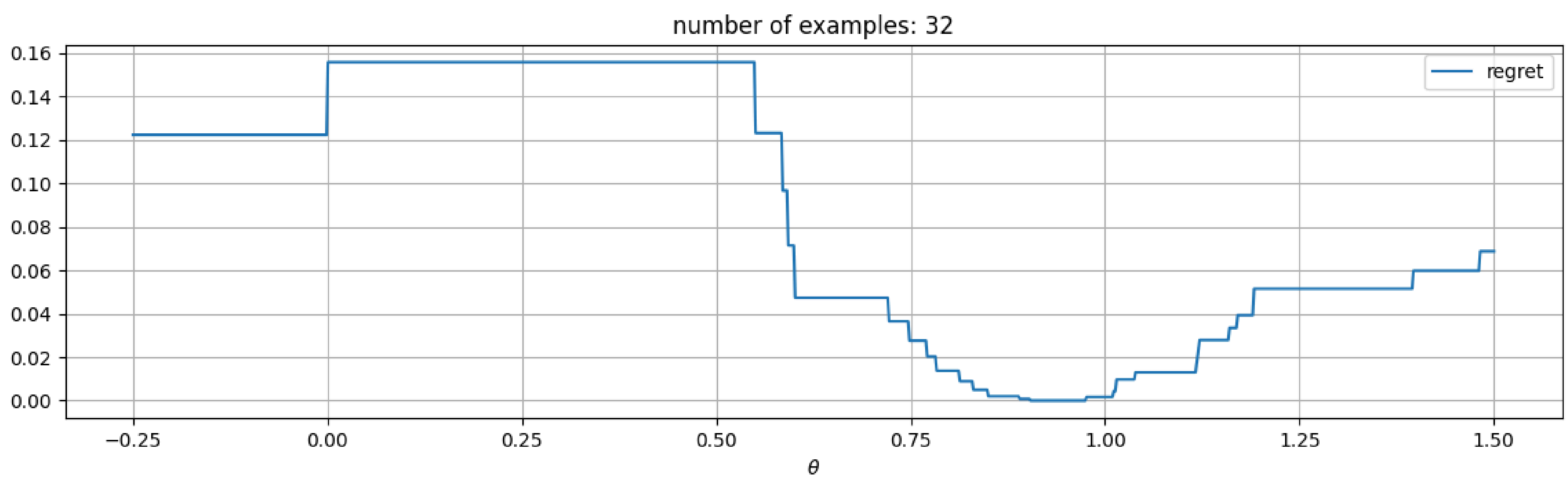



- It is non-differentiable at places, and flat almost everywhere
- Can we think of another way to address these issues?

# Looking Back at SPO

## If we could act on this function itself, a simple solution would be smoothing

```
In [19]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=32, figsi
```




- We could think of computing a convolution with a Gaussian kernel
- It would be like applying a Gaussian filter to an image

# Stochastic Smoothing

**But how can we do it through an optimization problem?**

A viable approach is using stochastic smoothing

- Rather than learning a point estimator $h(x; \theta)$
- We learn a stochastic estimator s.t. $\hat{y} \sim \mathcal{N}(h(x; \theta), \sigma)$

**Intuitively:**

- We still use a point estimator, but to predict a vector of means
- Then we sample $\hat{y}$ from a normal distribution having the specified mean
- ...And a fixed standard deviation

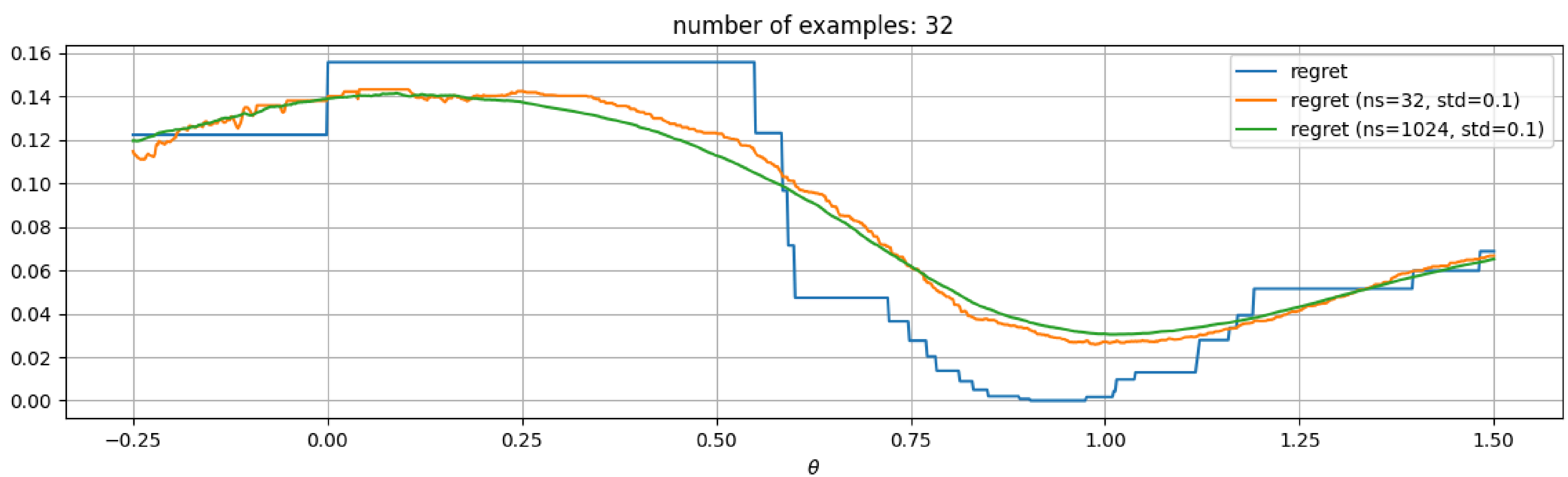
We end up smoothing over $\hat{y}$ rather than over $\theta$

**But it's very close to what we wanted to do!**

# Stochastic Smoothing

## Let's see how it works on our toy example

```
In [20]: util.draw_loss_landscape(losses=[util.RegretLoss(), util.RegretLoss(smoothing_samples=32, sı
```

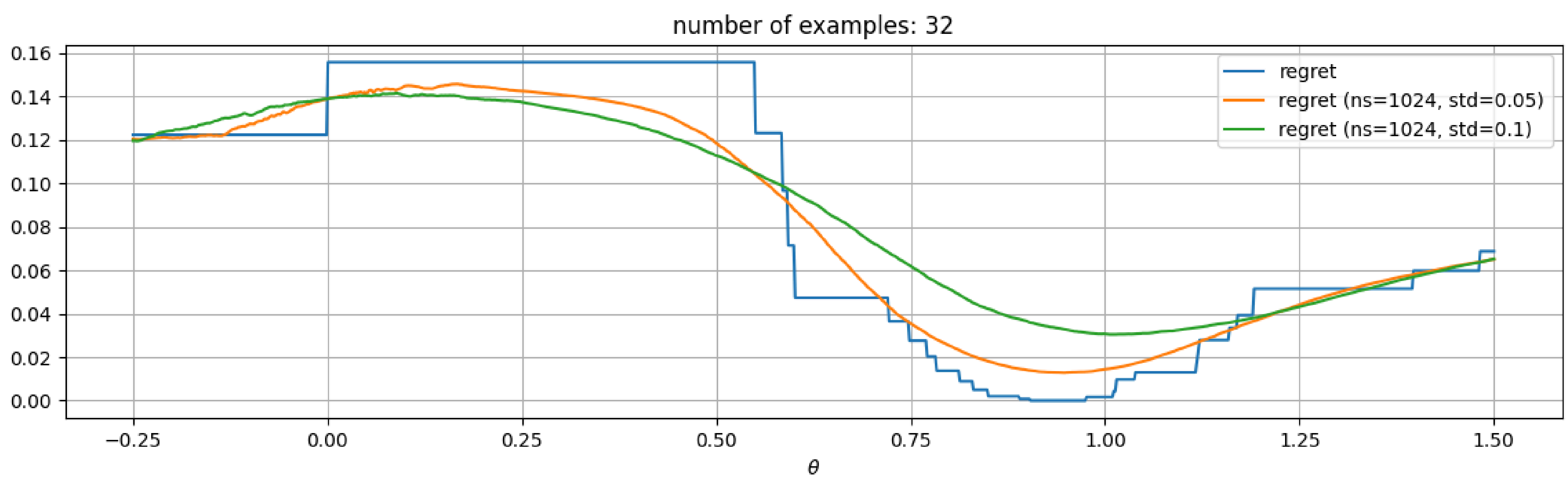



- It's a stochastic approach, some some noise is to be expected
- Using more samples leads to better smoothing

# Stochastic Smoothing

## We can control the smoothing level by adjusting $\sigma$

```
In [21]: util.draw_loss_landscape(losses=[util.RegretLoss(), util.RegretLoss(smoothing_samples=1024,
```




- Larger $\boldsymbol{\sigma}$ value remove flat sections better
- ...But also cause a shift in the position of the optimum

# Score Function Gradient Estimation

## How does that help us?

Normally, the DFL loss looks like this:

$$L_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y)}\left[\text{regret}(y, \hat{y})\right]$$

When we apply stochastic smoothing, it turns into:

$$\tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y),\hat{y}\sim\mathcal{N}(h(x,\theta))}\left[\text{regret}(y, \hat{y})\right]$$

**The expectation is now computed on $x$, $y$, and $\hat{y}$**

- We can use a sample average to handle the expectation on $\boldsymbol{x}$ and $\boldsymbol{y}$
- ...But if we do it on $\hat{\boldsymbol{y}}$ we are left with nothing differentiable

# Score Function Gradient Estimation

**So we expand the last expectation on $\hat{y}$:**

$$\tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y)}\left[\int_{\hat{y}} \text{regret}(y, \hat{y}) p(\hat{y}, \theta) d\hat{y}\right]$$

- $\text{regret}(y, \hat{y})$ cannot be differentiated, since $\hat{y}$ is a fixed sample in this setup
- However, the probability $p(\hat{y}, \theta)$ can! It's just a Normal PDF

Now, we just need a way to handle the integral

**We do it by focusing on the gradient**

Due to linearity of expectation and integration, this is given by:

$$\nabla \tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y)}\left[\int_{\hat{y}} \text{regret}(y, \hat{y}) \nabla_\theta p(\hat{y}, \theta) d\hat{y}\right]$$

## Score Function Gradient Estimation

**Let's consider again the expression we have obtained**

$$\nabla \tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y)} \left[ \int_{\hat{y}} \text{regret}(y, \hat{y}) \nabla_\theta p(\hat{y}, \theta) d\hat{y} \right]$$

Since that $\log'(f(x)) = 1/x f'(x)$, we can rewrite the formula as:

$$\nabla \tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y)} \left[ \int_{\hat{y}} \text{regret}(y, \hat{y}) p(\hat{y}, \theta) \nabla_\theta \log p(\hat{y}, \theta) d\hat{y} \right]$$

Now, the integral is again an expectation, so we have:

$$\nabla \tilde{L}_{DFL}(\theta) = \mathbb{E}_{(x,y)\sim P(X,Y), \hat{y}\sim \mathcal{N}(h(x,\theta),\sigma)} \left[ \text{regret}(y, \hat{y}) \nabla_\theta \log p(\hat{y}, \theta) \right]$$

# Score Function Gradient Estimation

**Finally, we can use a sample average to approximate both expectations:**

$$\nabla \tilde{L}_{DFL}(\theta) \simeq \frac{1}{m} \sum_{i=1}^{m} \frac{1}{N} \sum_{k=1}^{N} \text{regret}(y, \hat{y}) \nabla_\theta \log p(\hat{y}, \theta)$$

- For every training example we sample $\hat{y}$ from the stochastic estimator
- We compute $\text{regret}(y, \hat{y})$ as usual
- ...And we obtain a gradient since $p(\hat{y}, \theta)$ is easily differentiable in $\theta$

**We can trick a tensor engine into doing the calculation by using this loss:**

$$\tilde{L}_{DFL}(\theta) \simeq \frac{1}{m} \sum_{i=1}^{m} \frac{1}{N} \sum_{k=1}^{N} \text{regret}(y, \hat{y}) \log p(\hat{y}, \theta)$$

# Score Function Gradient Estimation

**This approach is also know as Score Function Gradient Estimation (SFGE)**

- It is a known approach (similar to [3]), but it has not been used in DFL
- We applied it to 2s-SOP in [4] (accepted, not yet published)

**It works with any function, not just regret**

...And in practice it can be improved by standardizing the gradient terms:

$$\nabla \tilde{L}_{DFL}(\theta) \simeq \frac{1}{m} \sum_{i=1}^{m} \frac{1}{N} \sum_{k=1}^{N} \frac{g(\hat{y}, y) - \text{mean}(g(\hat{\mathbf{y}}, \mathbf{y}))}{\text{std}(g(\hat{\mathbf{y}}, \mathbf{y}))} \nabla \log p(\hat{y}, \theta)$$

- Standardization helps in particular with small numbers of samples


*[3] Berthet, Quentin, et al. "Learning with differentiable pertubed optimizers." Advances in neural information processing systems 33 (2020): 9508-9519.*

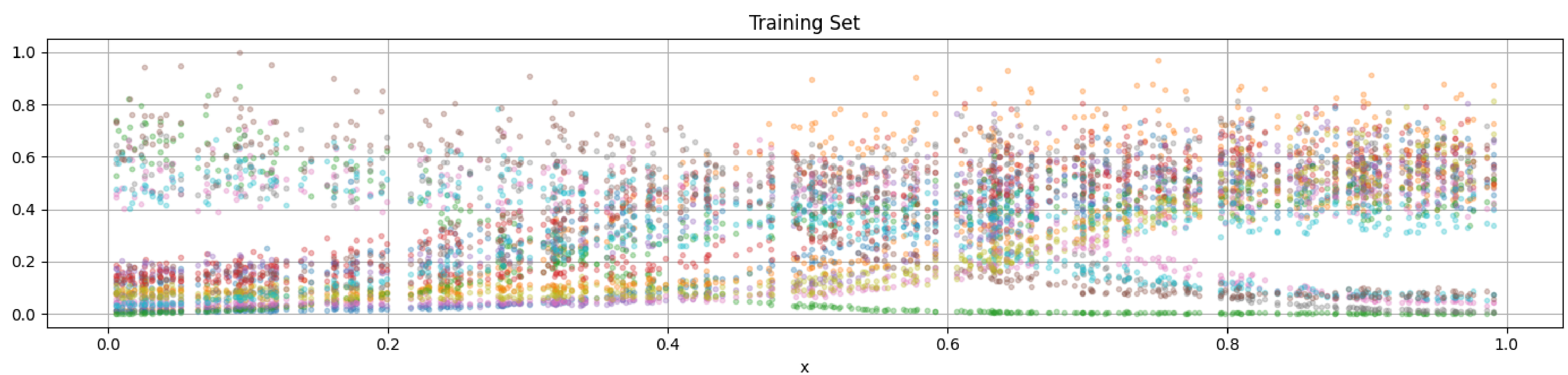
*[4] Silvestri, Mattia et al. "Score Function Gradient Estimation to Widen the Applicability ofDecision-focused Learning", Differetiable Almost Everywhere workshop at ICML 2023*

# A Practical Example

## We test this on our supply planning problem

We start by generaring a dataset of contract values (the costs are fixed)

In [22]:
```
seed, nitems = 42, 20
data_tr = util.generate_costs(nsamples=350, nitems=nitems, seed=seed, noise_scale=.2, noise_
util.plot_df_cols(data_tr, figsize=figsize, title='Training Set', scatter=True)
```




The distribution is the same we used for the one-stage problem

# A Practical Example

## Then we generate the remaining problem parameters

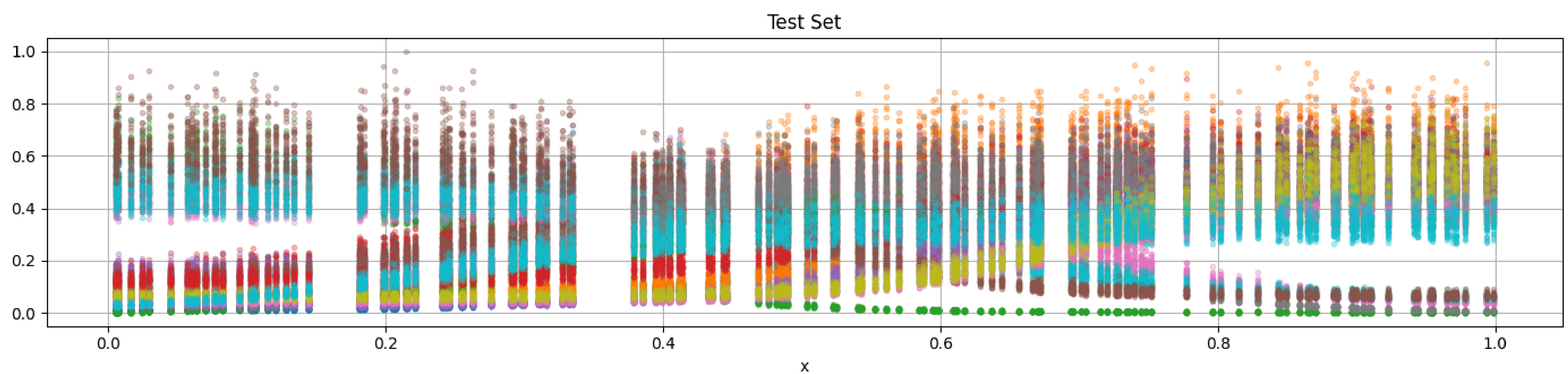
```
In [23]: # Generate the problem
         rel_req = 0.6
         rel_buffer_cost = 10
         prb = util.generate_2s_problem(nitems, requirement=rel_req * data_tr.mean().sum(), rel_buffe
         prb

Out[23]: ProductionProblem2Stage(costs=[1.14981605 1.38028572 1.29279758 1.23946339 1.06240746 1.06
         239781
          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=3.886210116908654, buffer_cost=11.830809153591137)
```

- The minimum value if 60% of the sum of average values on the training data
- Buying in the second stage is 10 times more expensive then the average cost

# A Practical Example

## For testing, we generate multiple samples per instance

```
In [24]: data_ts = util.generate_costs(nsamples=150, nitems=nitems, seed=seed, sampling_seed=seed+1,
         util.plot_df_cols(data_ts, figsize=figsize, title='Test Set', scatter=True)
```

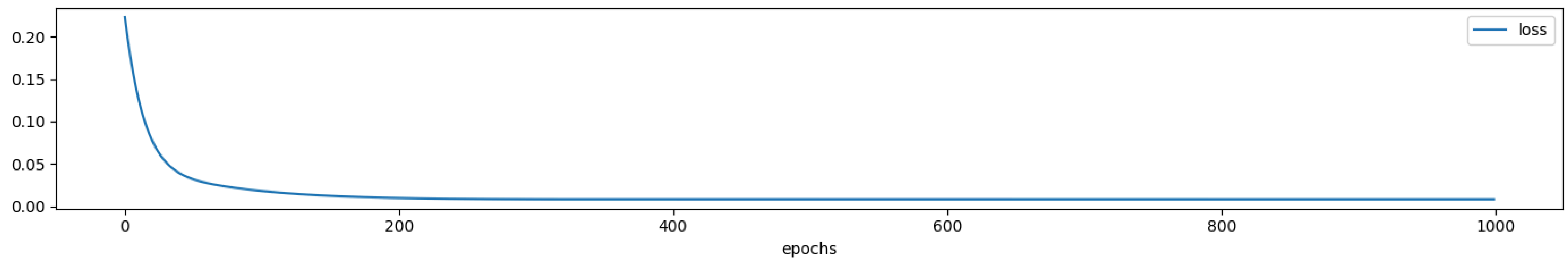



By doing this, we get a more reliable evaluation of uncertainty

# A PFL Approach

## We start by training a prediction focused approach

```
In [25]: pfl_2s = util.build_ml_model(input_size=1, output_size=nitems, hidden=[], name='pfl_2s', ou
         history = util.train_ml_model(pfl_2s, 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_2s, data_tr.index.values, data_tr.values, label='training')
         util.print_ml_metrics(pfl_2s, data_ts.index.values, data_ts.values, label='training')
```




```
Training time: 6.9677 sec
R2: 0.80, MAE: 0.071, RMSE: 0.09 (training)
R2: 0.75, MAE: 0.071, RMSE: 0.09 (training)
```

This is as fast at inference time as DFL, and can be used for warm-starting

# Evaluating Two-Stage Approaches

**Two-state stochastic approaches can be evaluated in two ways**

We can compare then with the best we could do

- The cost different is the proper regret
- Its computation requires solving a 2s-SOP with high accuracy
- ...Making it a very computationally expensive metric

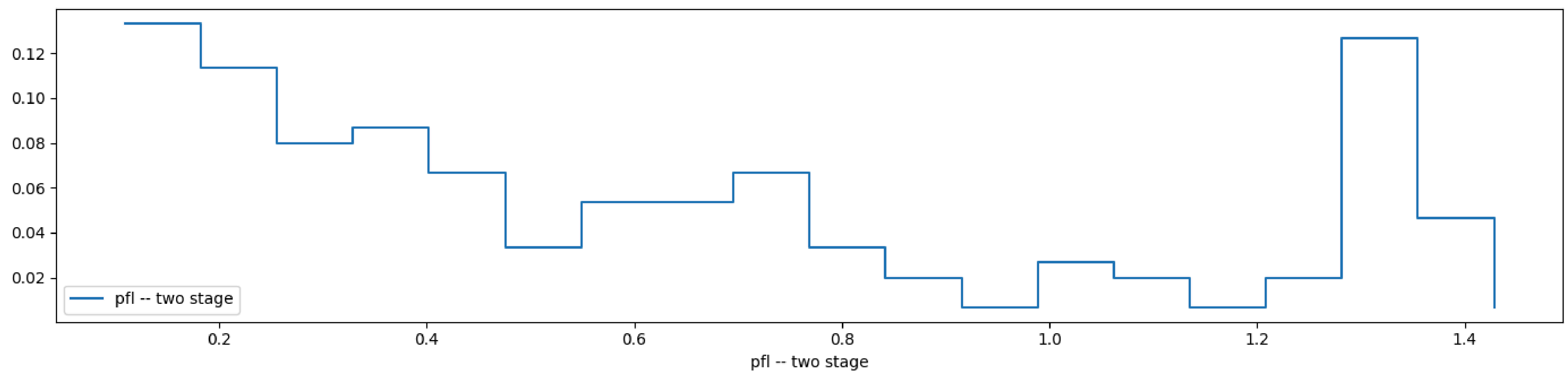
We can compare them with the expected cost of a clairvoyant approach

- The cost difference is called Expected Value of Perfect Information
- ...Or sometimes Post-hoc regret
- Its computation requires solving a 2s-SOP with just a single scenario
- ...So it's much faster, but only provide an upper bound on true regret

# Evaluating the PFL Approach

## Let's check the EVPF/Post-hoc regret for the PFL Approach

In [26]:
```
pfl_2s_evpf = util.compute_evpf_2s(prb, pfl_2s, data_ts, tlim=10)
util.plot_histogram(pfl_2s_evpf, figsize=figsize, label='pfl -- two stage', print_mean=True
```




```
Mean: 0.632 (pfl -- two stage)
```

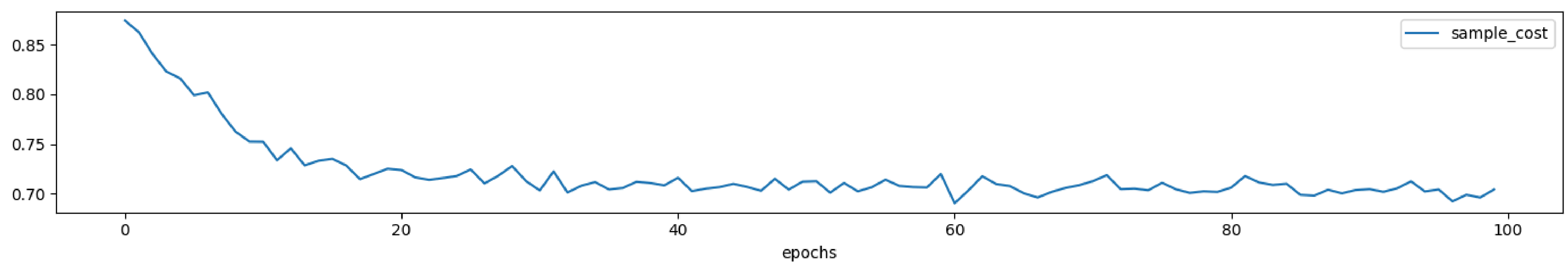
This will be our baseline

# Training a DFL Approach

## We train a DFL model with warm starting, but no solution cache

...Since the feasible space for the recourse actions is not fixed

```
In [27]: sfge_2s = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[],
         history = util.train_dfl_model(sfge_2s, data_tr.index.values, data_tr.values, epochs=100, ve
         util.plot_training_history(history, figsize=figsize_narrow, print_scores=False, print_time=T
         util.print_ml_metrics(sfge_2s, data_tr.index.values, data_tr.values, label='training')
         util.print_ml_metrics(sfge_2s, data_ts.index.values, data_ts.values, label='test')
```

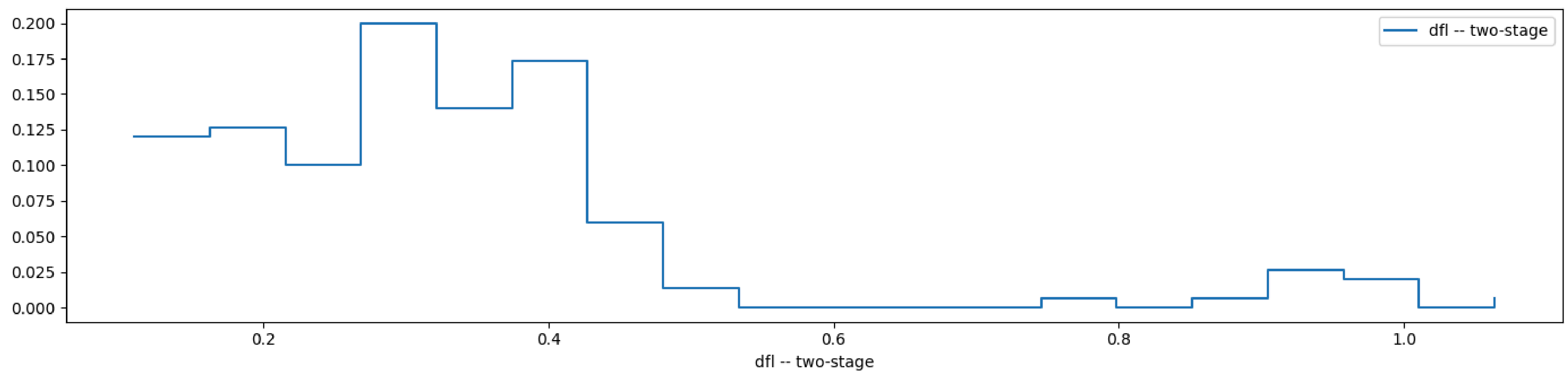



```
Training time: 131.5764 sec
R2: 0.56, MAE: 0.1, RMSE: 0.13 (training)
R2: 0.64, MAE: 0.082, RMSE: 0.10 (test)
```

# Evaluating the DFL Approach

## We can now inspect the EVPF/Post-hoc regret for the DLF approach, as well

```
In [28]: sfge_2s_evpf = util.compute_evpf_2s(prb, sfge_2s, data_ts, tlim=10)
         util.plot_histogram(sfge_2s_evpf, figsize=figsize, label='dfl -- two-stage', print_mean=Tru
```




```
Mean: 0.338 (dfl -- two-stage)
```

# A More In-depth Comparison

**A more extensive experimentation can be found in this paper**

The method has been tested on:

- Some "normal" DFL benchmarks
- Several two-stage stochastic problems

The baselines are represented by:

- Specialize methods (e.g. SPO, the one from [1]), when applicable
- A neuro-probabilistic model + a scenario based approach

Specialized method tend to work better

- ...But SFGE is much more versatile
- The best results are obtained on 2s-SOPs

# A More In-depth Comparison

## This is how the approach fares again the scenario based method

...On a problem somewhat similar to our supply planning one