



## 03. Breaking Off



# 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:

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

- $Y$  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:

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

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  $P(Y \mid X = x)$

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

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 do something similar with DFL?**

As a recap, our DFL training problem is:

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

With:

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

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:

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

Now, say we had a DLF approach 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:

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

It would still be DFL, just a bit more general



## DFL for 2s-SOP

At this point, let's choose:

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

- 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:

$$\operatorname{argmin}_{\theta} f(z^*(\hat{y})) + \mathbb{E}_{y \sim P(Y|X=x)} \left[ \min_{z''} r(z'', z^*(\hat{y}), y) \right]$$

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:

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

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

$$\begin{aligned} g(z, y) &= \min_{z''} c^T z + c'' z''_k \\ \text{subject to: } &y^T z + z''_k \geq y_{min} \quad \forall k = 1..N \\ &z''_k \in \mathbb{N}_0 \quad \forall k = 1..N \end{aligned}$$



# 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

**Compared to the classical approach, we have 1 restriction and 3 "superpowers"**

- 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, that solution time may grow exponentially

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

- It can even be lower, since information from other  $x$  values
- ...Can be used by the ML model to improve inference
- There are alternatives with similar advantages (e.g. ML to estimate recourse)
- ...But they have their own drawbacks (e.g. using ML model encodings)



# 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] is designed for 2s-SOP
  - 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 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.

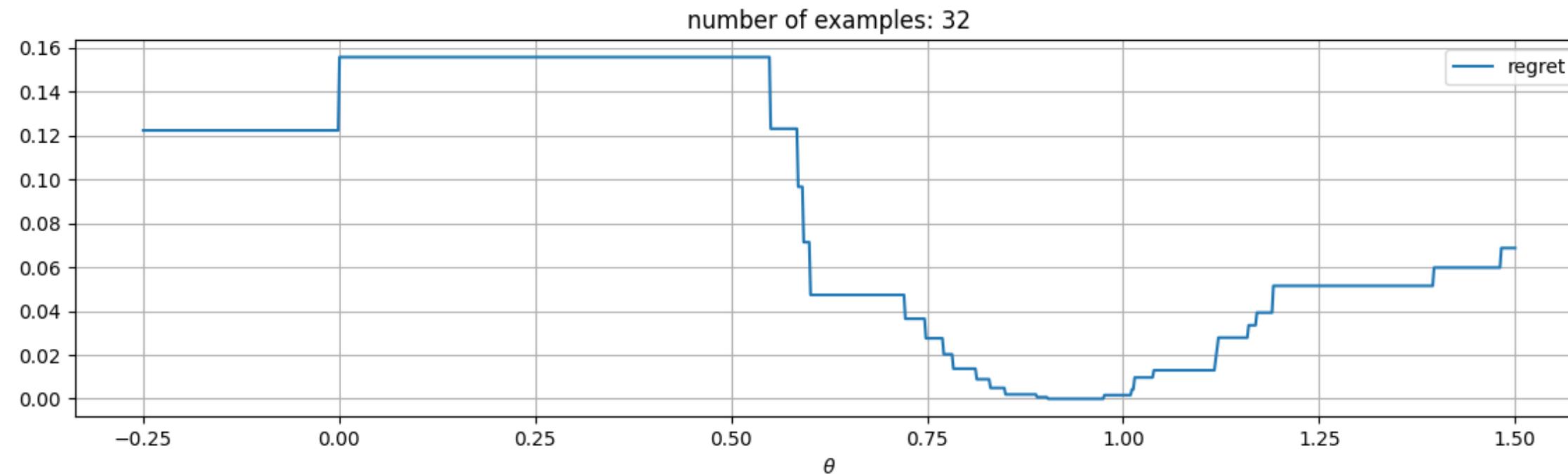
[2] Paulus, Anselm, et al. "Comboptnet: Fit the right np-hard problem by learning integer programming constraints." International Conference on Machine Learning. PMLR, 2021.



# Looking Back at SPO

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

```
In [2]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=32, figsize=f)
```



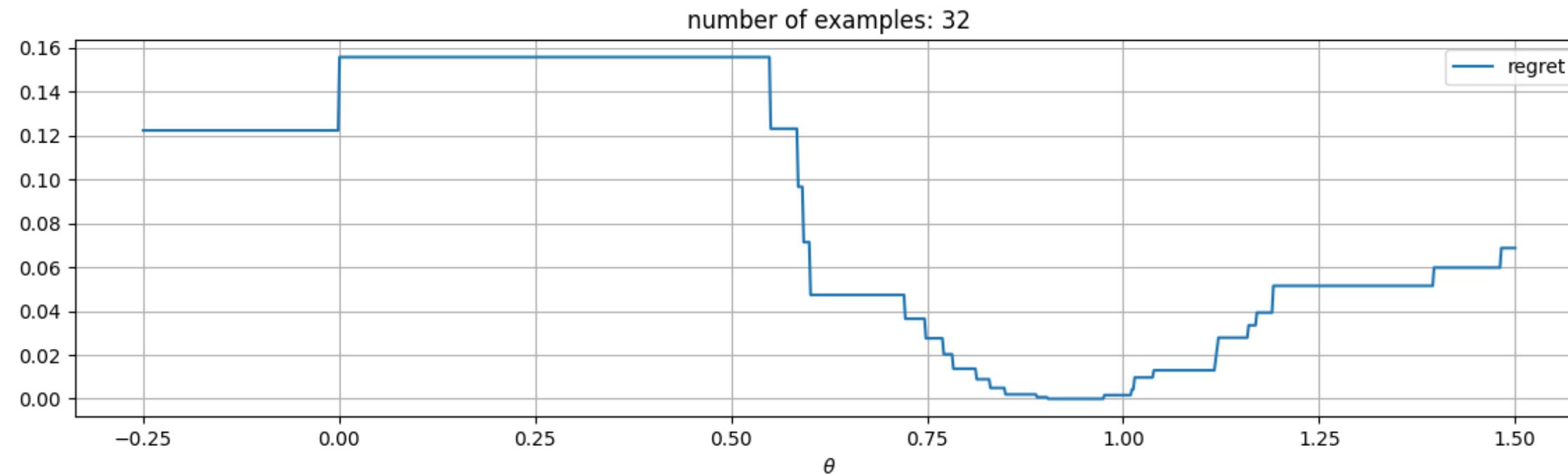
- It is non-differentiable at places, and flat almost everywhere
- Can we think of another way to address these issues?



# Looking Back at SPO

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

```
In [3]: util.draw_loss_landscape(losses=[util.RegretLoss()], model=1, seed=42, batch_size=32, figsize=f)
```



- 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  $\theta$

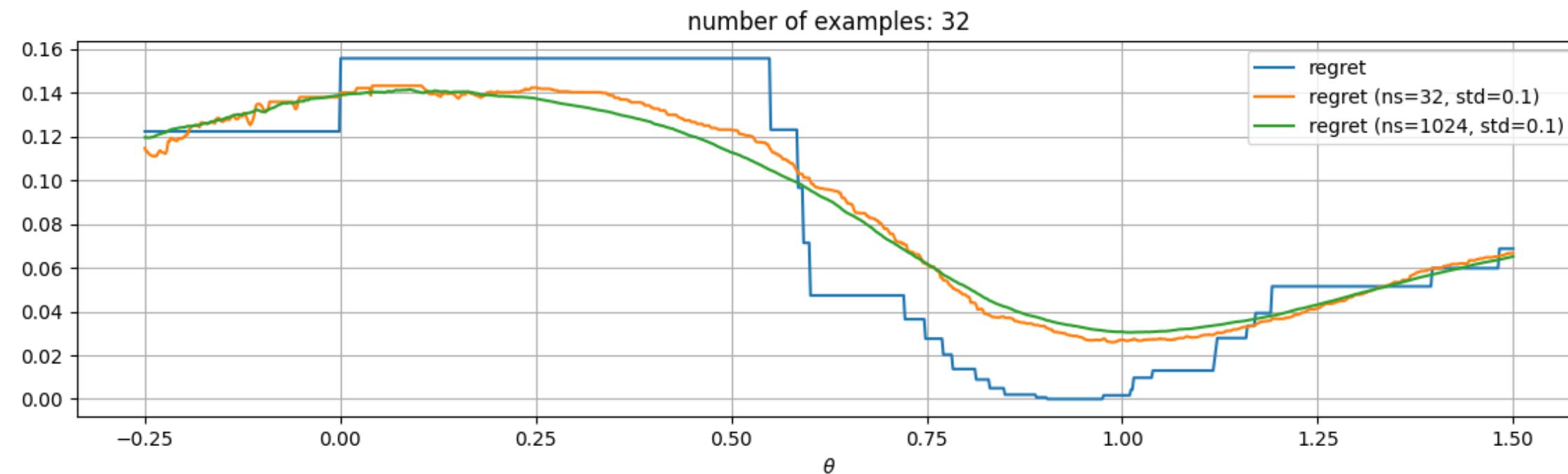
**But it's very close to what we wanted to do!**



# Stochastic Smoothing

Let's see how it works on our toy example

```
In [4]: util.draw_loss_landscape(losses=[util.RegretLoss(), util.RegretLoss(smoothing_samples=32, smoothing_std=0.1), util.RegretLoss(smoothing_samples=1024, smoothing_std=0.1)], n_examples=32)
```



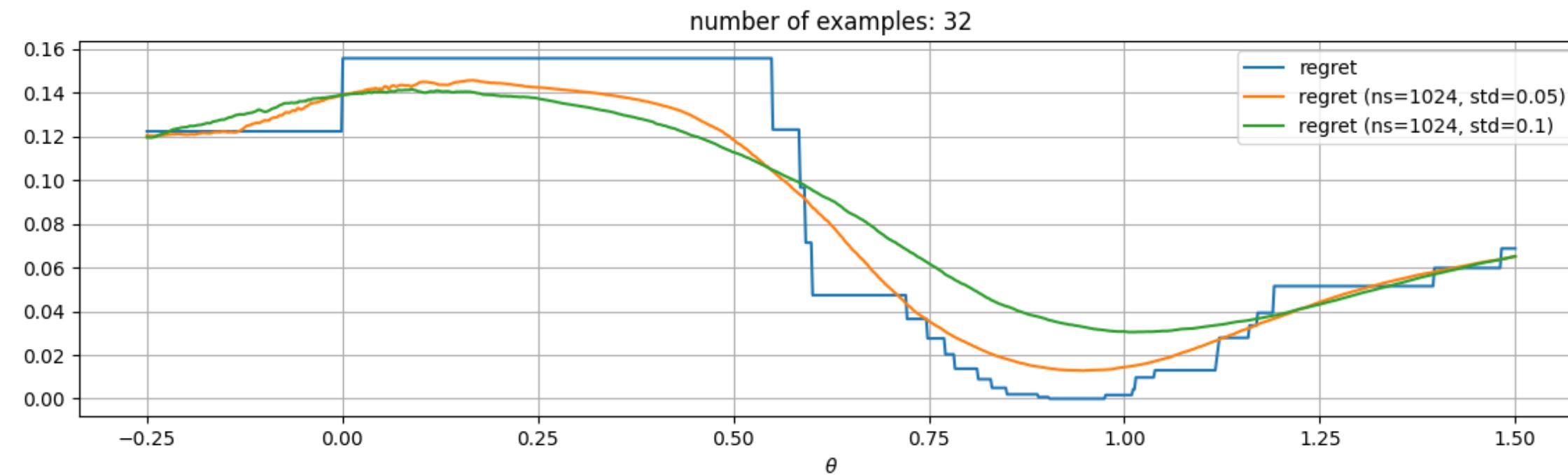
- It's a stochastic approach, some noise is to be expected
- Using **more samples** leads to better smoothing



# Stochastic Smoothing

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

```
In [5]: util.draw_loss_landscape(losses=[util.RegretLoss(), util.RegretLoss(smoothing_samples=1024, smoo
```



- Larger  $\sigma$  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:

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

When we apply stochastic smoothing, it turns into:

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

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

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



# Score Function Gradient Estimation

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

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

- $\text{regret}(\hat{y}, y)$  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:

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



## Score Function Gradient Estimation

Let's consider again the expression we have obtained

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

By taking advantage of the fact that  $\log'(f(x)) = 1/x f'(x)$ , we can rewrite it as:

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

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

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



## Score Function Gradient Estimation

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

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

- For every training example we sample  $\hat{y}$  from the stochastic estimator
- We compute  $\text{regret}(\hat{y}, y)$  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:

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



# Score Function Gradient Estimation

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

- It is a known approach (see e.g. [3]), but it has never been used in DFL
- At least not until [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:

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

- Standardization helps in particular with small numbers of samples

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

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

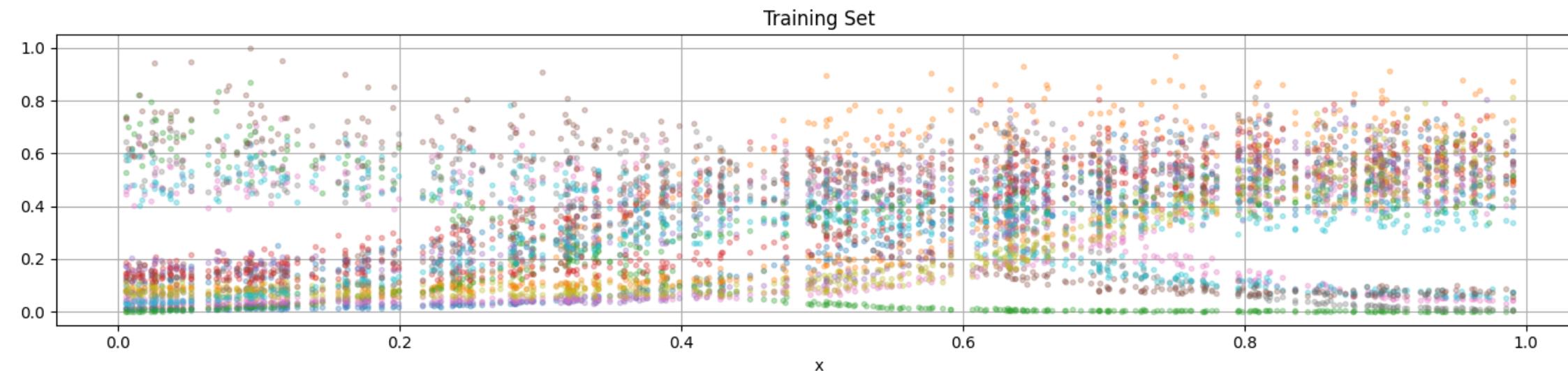


# A Practical Example

## We test this on our supply planning problem

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

```
In [21]: seed, nitems = 42, 20  
data_tr = util.generate_costs(nsamples=350, nitems=nitems, seed=seed, noise_scale=.2, noise_type='uniform')  
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 [22]: # 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_buffer_cost=rel_buffer_cost)
prb
```

```
Out[22]: ProductionProblem2Stage(costs=[1.14981605 1.38028572 1.29279758 1.23946339 1.06240746 1.062397
81
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=3.8862101169088654, buffer_cost=11.830809153591137)
```

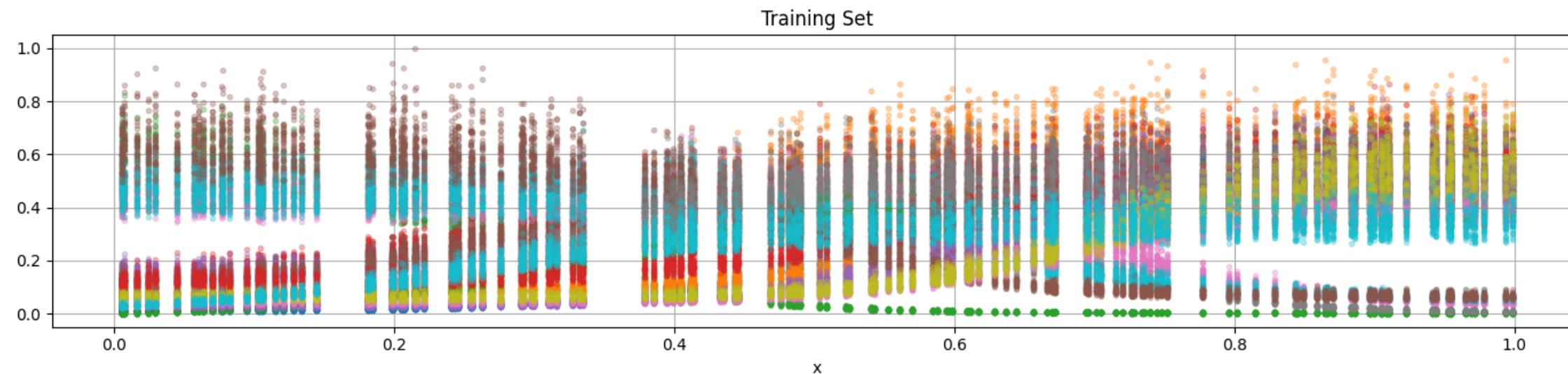
- The minimum value if 60% of the sum of average values on the training data
- Buying in the second stage is 10 times more expensive then the average cost



# A Practical Example

For testing, we generate multiple samples per instance

```
In [23]: data_ts = util.generate_costs(nsamples=150, nitems=nitems, seed=seed, sampling_seed=seed+1, noise=noise)
util.plot_df_cols(data_ts, figsize=figsize, title='Training Set', scatter=True)
```



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



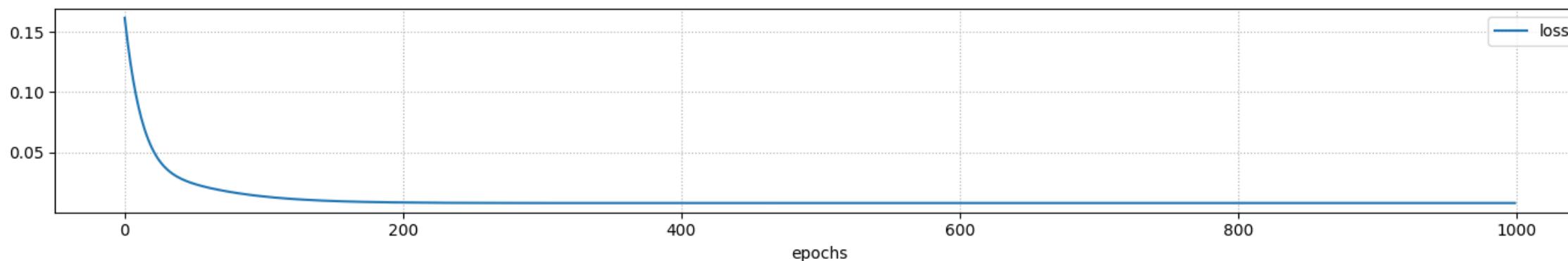
# A PFL Approach

## We start by training a prediction focused approach

```
In [24]: pfl_2s = util.build_nn_model(input_shape=1, output_shape=nitems, hidden=[], name='pfl_2s', output_activation='softmax')
@time history = util.train_nn_model(pfl_2s, data_tr.index.values, data_tr.values, epochs=1000, verbose=False)
util.plot_training_history(history, figsize=figsize_narrow, print_final_scores=False)
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')
```

CPU times: user 8.21 s, sys: 352 ms, total: 8.56 s

Wall time: 6.83 s



R2: 0.80, MAE: 0.071, RMSE: 0.09 (training)

R2: 0.75, MAE: 0.072, RMSE: 0.09 (training)



This is as fast as the DFL approach, and can be used for warm-starting

# Evaluating Two-Stage Approaches

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

We can compare them with **the best we could do**

- The cost difference 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**

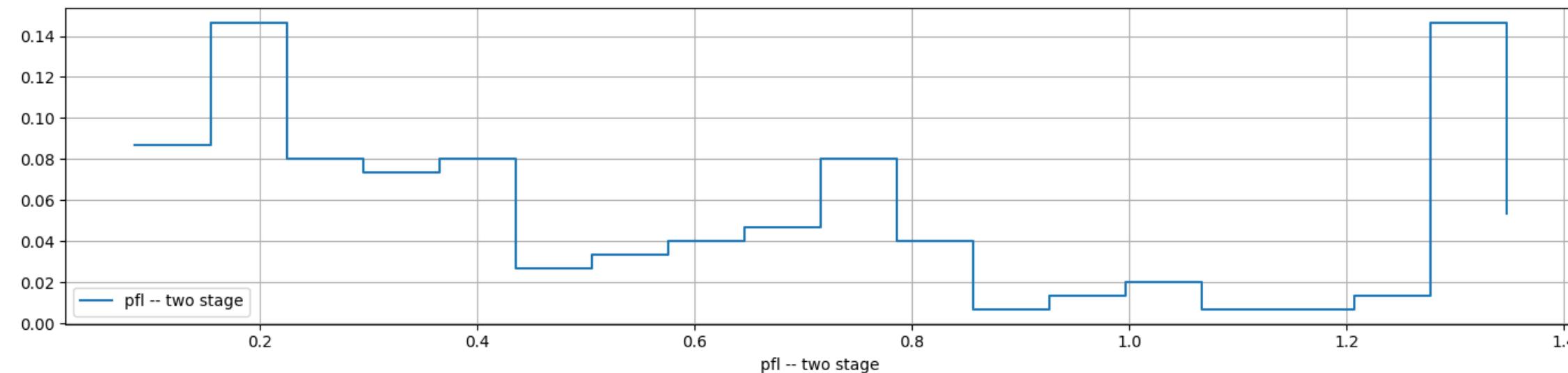
- The cost difference is called Expected Value of Perfect Information
- ...Or sometimes Post-hoc regret
- Its computation requires solving a 2s-SOP **with just a single scenario**
- ...So it's much faster, but only provide an upper bound on true regret



# Evaluating the PFL Approach

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

```
In [25]: 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: 0.634 (pfl -- two stage)

This will be our baseline



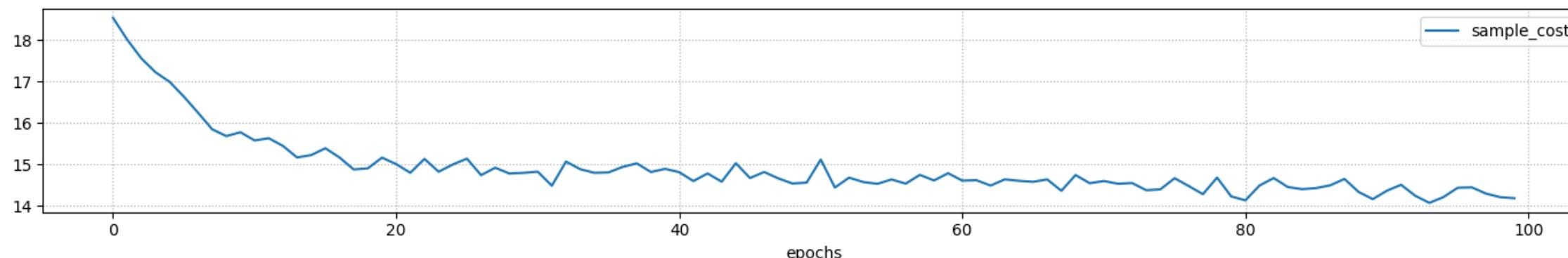
# Training a DFL Approach

We traing a DFL with warm starting, but no solution cache

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

```
In [30]: sfge_2s = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[], name='sfge_2s')
@time history = util.train_dfl_model(sfge_2s, data_tr.index.values, data_tr.values, epochs=100,
util.plot_training_history(history, figsize=figsize_narrow, print_final_scores=False, excluded_r
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')
```

CPU times: user 4min 41s, sys: 34.8 s, total: 5min 16s  
Wall time: 5min 16s



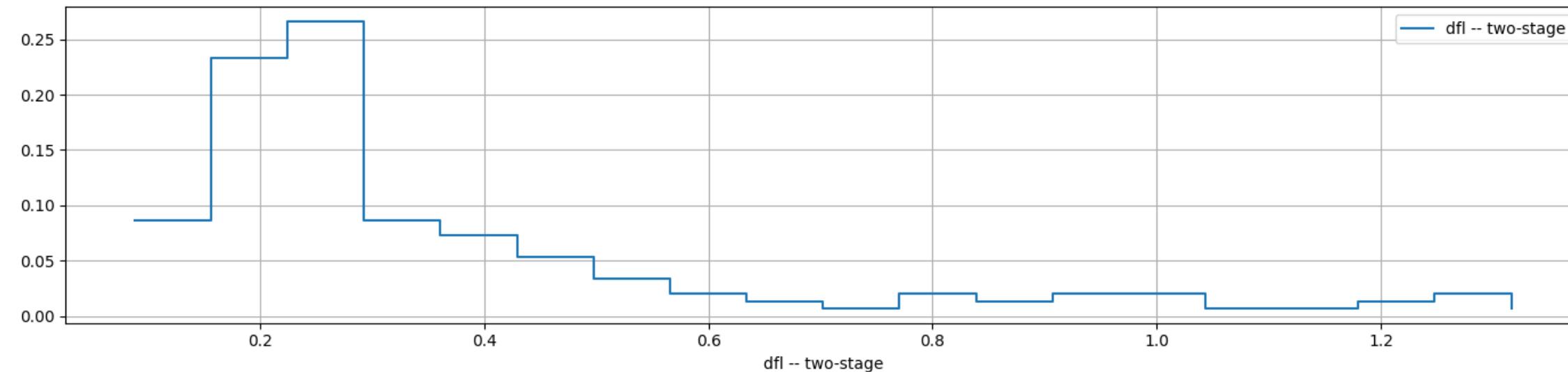
R2: 0.61, MAE: 0.095, RMSE: 0.12 (training)  
R2: 0.66, MAE: 0.081, RMSE: 0.10 (test)



# Evaluating the DFL Approach

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

```
In [31]: 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=True)
```



Mean: 0.382 (dfl -- two-stage)



## A More In-depth Comparison

### A more extensive experimentation will be found in [4]

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

