Motivation for Decision-Focused Learning

Remember that thing about the big picture?

Prediction and Optimization in the Wild

Real world problems typically rely on estimated parameters

E.g. travel times, demands, item weights/costs...

However, sometimes we have access to a bit more information

Prediction and Optimization in the Wild

Take traffic-dependent travel times as an example

If we know the time of the day we can probably estimate them better

Let's see how these problems are typically addressed

Predict, then Optimize

First, we train an estimator for the problem parameters:

$$\text{argmin}_\omega \left\{ L(y, \hat{y}) \mid y = f(\hat{x}; \omega) \right\}$$

- L is the loss function
- f is the ML model with parameter
- $\hat{x}, \hat{y}$ are the training set input/output

In our example:

- x would be the time of the day
- y would be a vector of travel times
- L may be a classical MSE loss
- f may be a linear regressor or neural network

Predict, then Optimize

Then, we solve the optimization problem with the estimated parameters

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

- z is the vector of variables of the optimization problem
- c is the cost function
- F is the feasible space
- In general, both c and F may depend on the estimated parameters

In our example

- z may represent routing decisions
- c may be the total travel time
- F may encode a deadline constraint

Predict, then Optimize

This approach is sometimes referred to as "Predict, then Optimize"

It is simple and it makes intuitively sense

- The more accurate we are, the better we will estimate the parameters
- ...And in turn we should get better optimization results

Let $L^*(\hat{y})$ be the best possible loss value, for any ML model

- For any reasonable loss function, better training leads to better predictions

$$y \xrightarrow[L(y,\hat{y}) \to L^*(\hat{y})]{\qquad\qquad} \hat{y}$$

- ...And therefore, eventually we are guaranteed to find the best solution

$$z^*(y) \xrightarrow[L(y,\hat{y}) \to L^*(\hat{y})]{\qquad\qquad} z^*(\hat{y})$$

"Predict, then Optimize": Limitations

However, things are not really that simple!

Why is that the case?

"Predict, then Optimize": Limitations

However, things are not really that simple!

Why is that the case?

The relation:

$$z^*(y) \xrightarrow[L(y,\hat{y}) \to L^*(\hat{y})]{} z^*(\hat{y})$$

...Holds only asymptotically

- In practice, our model may not be capable of reaching mimimum loss
- ...And this is even more true for unseen example

In this situation, it is unclear how imperfect predictions impact the cost

"Predict, then Optimize": Limitations

Say we want to move from location A to B, using one of two routes

Based on the time of the day (x-axis)

Image from "Smart Predict, then Optimize"

...The travel time changes (y-axis)

"Predict, then Optimize": Limitations

We need to pick the best route

Image from "Smart Predict, then Optimize"

- The dashed line shows the input value that causes the optimal choice to switch

"Predict, then Optimize": Limitations

If we train an optimal Linear Regression, we get these estimates

- The estimator is most accurate possible
- ...But we get the switching point wrong!

"Predict, then Optimize": Limitations

By contrast, consider this second estimator

- The accuracy is awful
- ...But we get the switching point right!

Decision Focused Learning

Addressing these issues is the goal of decision focused learning

- The general idea is to account for the optimization problem during training
- ...And the "holy grail" of the DFL is solving:

$$\text{argmin}_\omega \left\{ \sum_{i=1}^{m} c(z^*(y_i), \hat{y}_i) \mid y = f(\hat{x}, \omega) \right\}$$

- The field was kicked off by this paper
- ...And many other have followed

A good entry point are the works by prof. Guns and references therein

Before discussing DFL, however, let's establish a baseline

A Baseline Approach

We'll need to do better than this

Target Problem

We will consider an "optimal purchase" problem

Given a set of objects with values v_i and cost y_i

- We need to buy items for a value of at least v_{min}
- ...While minimizing the purchase cost

This is essentially the dual of the classical knapsack problem

The costs depend on the market state

I.e. we have:

$$y = f(x)$$

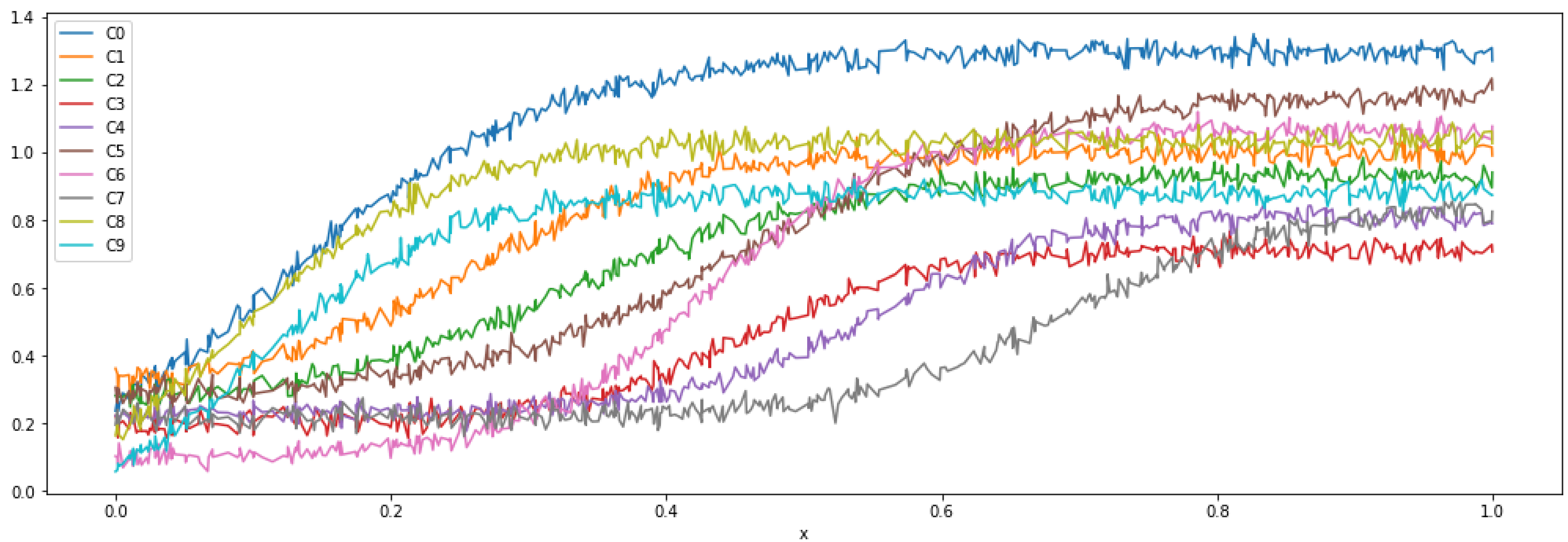
- We will assume that the market state if captured by a single number
- ...And that historical data is available for training an estimator

Dataset Generation

We will start by generating a training set

We will assume that the dependency on x is captured by sigmoid curves

In [2]:
```
nitems, nsamples = 10, 500
data = util.generate_market_dataset(nsamples, nitems, seed=2, noise=.02)
util.plot_df_cols(data, figsize=figsize)
```



Dataset Generation

Let's check the dataset structure

In [3]:
```python
data.head()
```

Out[3]:

x	C0	C1	C2	C3	C4	C5	C6	C7	C8	C9
0.000124	0.237339	0.362793	0.283177	0.223027	0.223313	0.306461	0.103802	0.196172	0.164807	0.058347
0.001541	0.273677	0.346396	0.269355	0.204457	0.221878	0.261104	0.099676	0.241537	0.195367	0.063215
0.001883	0.235295	0.298894	0.282876	0.158408	0.218716	0.304677	0.080486	0.190402	0.183731	0.081783
0.002583	0.250008	0.341717	0.278371	0.200027	0.218275	0.298575	0.142006	0.204406	0.167427	0.073985
0.005544	0.290177	0.340446	0.279034	0.207337	0.232551	0.260204	0.070202	0.241806	0.152773	0.081679

- The input value is stored as the index
- Each `CX` column refers to the cost for a given item
- x naturally ranges in $[0, 1]$, while the costs are not normalized
- ...But their range is fine enough to avoid issues with gradient descent

Data Preparation

Therefore, we just need to split our data for training and test

In [4]:
```
data_tr, data_ts = util.train_test_split(data, test_size=0.3, seed=42)
print(f'#Examples: {len(data_tr)} (training), {len(data_ts)} (test)')
```

```
#Examples: 350 (training), 150 (test)
```

We do not have many examples

- This is actually fairly realistic
- ...Since it's not easy to collect instances for decision problems

Next, we separate input and output

In [5]:
```
tr_in, tr_out = data_tr.index.values, data_tr.values
ts_in, ts_out = data_ts.index.values, data_ts.values
```

Building a ML Estimator

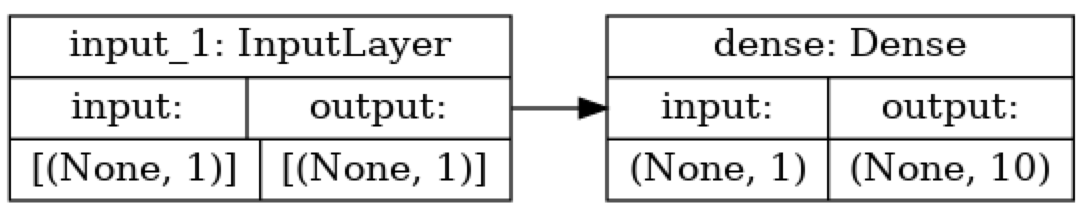
We will train a linear regression model

- This is on purpose: the strong bias in the model
- ...Will prevent a very accurate approximation of the data

...So that we get some mistakes even for this very simple problem

```
In [6]: fsm_early = util.build_ml_model(input_size=1, output_size=nitems, hidden=[], name='FSM', ou
        util.plot_ml_model(fsm_early)
```

Out[6]:



- Specifically, we have one linear regressor per item

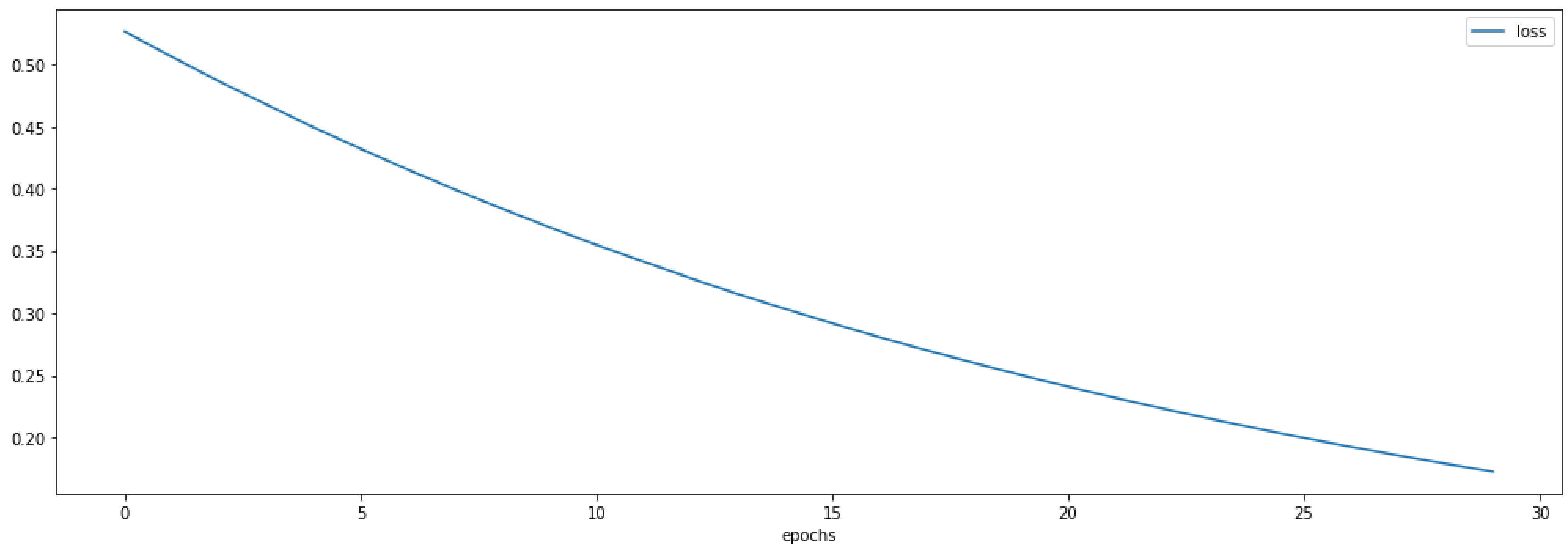
Training the Estimator

We will investigate early and later convergence

Therefore, let's make a first training attempt for just a few epochs

In [7]:
```
history = util.train_ml_model(fsm_early, tr_in, tr_out, epochs=30, validation_split=0)
fsm_early.save('fsm_early')
util.plot_training_history(history, figsize=figsize)
```

```
INFO:tensorflow:Assets written to: fsm_early/assets
```




```
Model loss: 0.1725 (training)
```

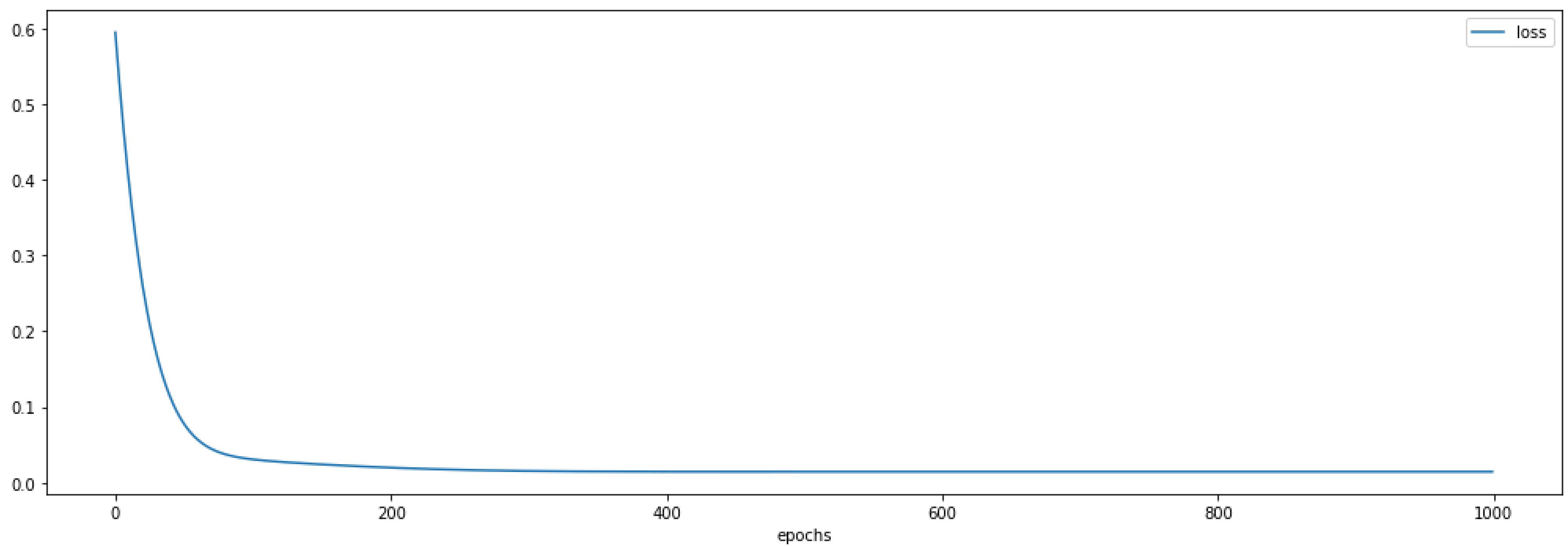
Training the Estimator

We will investigate early and later convergence

...And then let's train to (approximate) convergence

In [8]:
```
fsm_late = keras.models.clone_model(fsm_early)
history = util.train_ml_model(fsm_late, tr_in, tr_out, epochs=1000, validation_split=0)
fsm_late.save('fsm_late')
util.plot_training_history(history, figsize=figsize)
```

```
INFO:tensorflow:Assets written to: fsm_late/assets
```




```
Model loss: 0.0143 (training)
```

Evaluating the Estimator

Let's evaluate the accuracy of the two models

Here are the metrics for the "early" stage of training:

In [9]:
```
r2, mae, rmse = util.get_ml_metrics(fsm_early, tr_in, tr_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
r2, mae, rmse = util.get_ml_metrics(fsm_early, ts_in, ts_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')
```

```
R2: -1.02, MAE: 0.29, RMSE: 0.41 (training)
R2: -1.07, MAE: 0.29, RMSE: 0.42 (test)
```

...And here for the "late" stage:

In [10]:
```
r2, mae, rmse = util.get_ml_metrics(fsm_late, tr_in, tr_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
r2, mae, rmse = util.get_ml_metrics(fsm_late, ts_in, ts_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')
```

```
R2: 0.79, MAE: 0.097, RMSE: 0.12 (training)
R2: 0.78, MAE: 0.1, RMSE: 0.12 (test)
```

Solving the Optimization Problem

The predictions $y = f(x)$ are used to solve an optimization problem

...Which can be stated in the form:

$$\text{argmin}_z \{ y^T z \mid v^T z \geq v_{min}, z \in \{0, 1\}^n \}$$

- This is Integer Linear Program (ILP)
- ...Which we tackle in our code using Or-tools/CBC:

```
slv = pywraplp.Solver.CreateSolver('CBC')
x = [slv.IntVar(0, 1, f'x_{i}') for i in range(nv)]
rcst = slv.Add(sum(values[i] * x[i] for i in range(nv)) >= req)
slv.Minimize(sum(costs[i] * x[i] for i in range(nv)))
```

The code is wrapped in the class `MarketProblem`

Solving the Optimization Problem

First, let's generate an instance where we need to select 50% of the items

In [11]:
```python
prb = util.generate_market_problem(nitems=nitems, rel_req=0.5, seed=42)
```

Then, let's check the solution for two distinct market states:

In [12]:
```python
costs = data.iloc[0]
print('costs:', ', '.join(f'{v:.2}' for v in costs))
sol, closed = prb.solve(costs, tlim=10, print_solution=True)
```

```
costs: 0.24, 0.36, 0.28, 0.22, 0.22, 0.31, 0.1, 0.2, 0.16, 0.058
Selected items: 3, 6, 7, 8, 9
Cost: 2.16, Value: 5.57, Requirement: 5.52, Closed: True
```

In [13]:
```python
costs = data.iloc[200]
print('costs:', ', '.join(f'{v:.2}' for v in costs))
sol, closed = prb.solve(costs, tlim=10, print_solution=True)
```

```
costs: 1.2, 0.85, 0.68, 0.34, 0.27, 0.54, 0.38, 0.24, 1.0, 0.84
Selected items: 1, 3, 4, 6, 7
Cost: 6.32, Value: 5.53, Requirement: 5.52, Closed: True
```

Regret

Using an accuracy metric for our estimator has lots of limits

This is basically the point of our current line of reasoning ;-)

- Now that we have a solver for our optimization problem
- We can evaluate our estimator in terms of regret

By regret we mean the cost difference w.r.t. the true solution

For the i-th example, this is given by:

$$\hat{y}_i^T z(y_i) - \hat{y}_i^T z(\hat{y}_i) \quad \text{with } y_i = f(x_i)$$

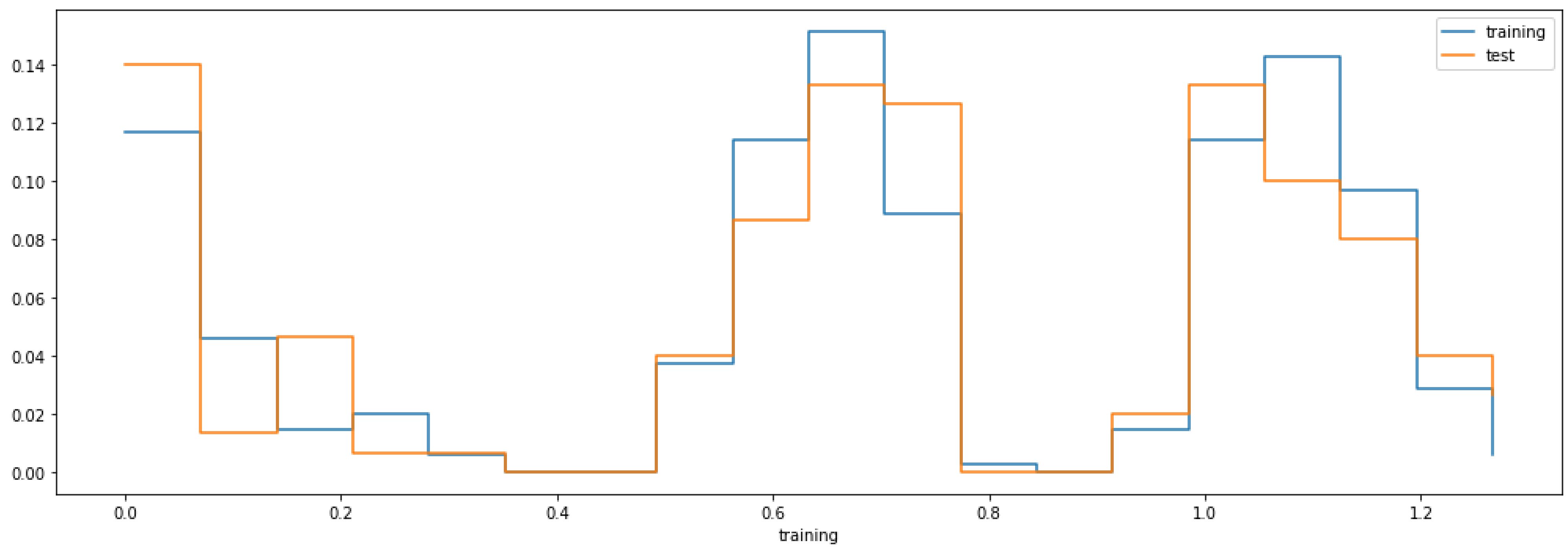
- $\hat{y}_i$ is the true cost vector
- $z(\hat{y}_i)$ is the true optimal solution
- $z(y_i)$ is the optimal solution for the predicted costs

Regret

Let's check the regret on the training and test set

We'll do this for the "early" model...

In [14]:
```
r_tr = util.compute_regret(prb, fsm_early, tr_in, tr_out)
r_ts = util.compute_regret(prb, fsm_early, ts_in, ts_out)
util.plot_histogram(r_tr, figsize=figsize, label='training', data2=r_ts, label2='test', pri
```



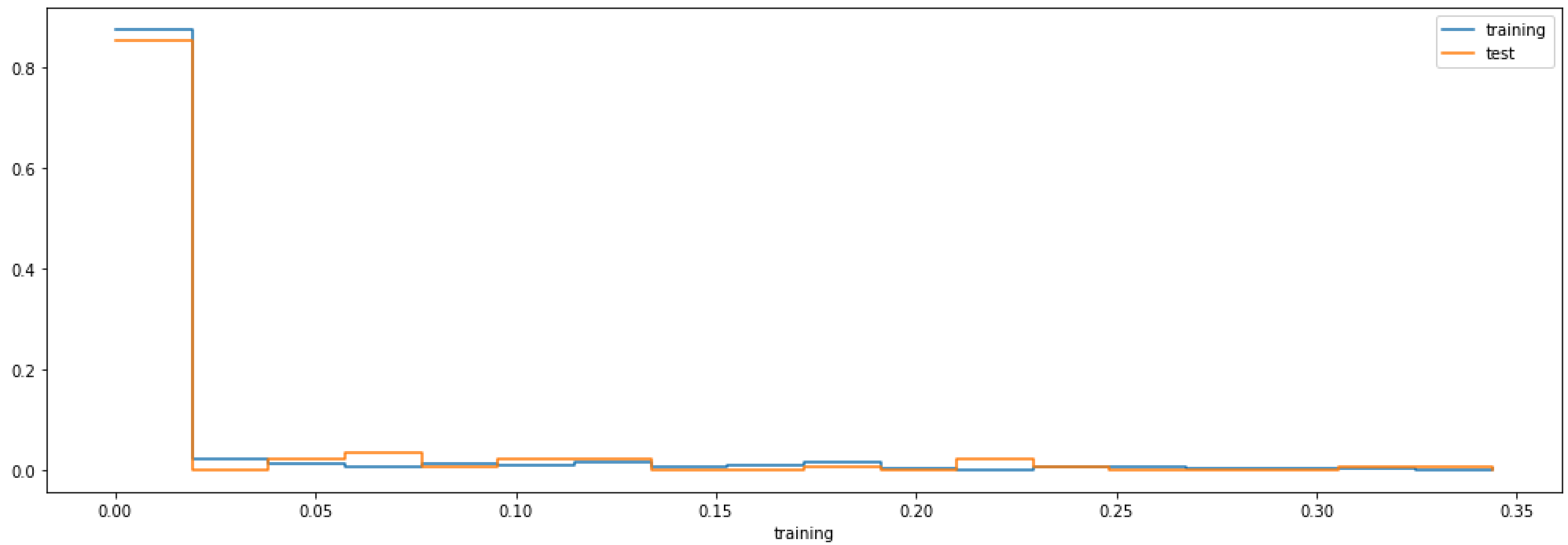

```
Mean: 0.712 (training), 0.711 (test)
```

Regret

Let's check the regret on the training and test set

...And for the "late" one

In [15]:
```
r_tr = util.compute_regret(prb, fsm_late, tr_in, tr_out)
r_ts = util.compute_regret(prb, fsm_late, ts_in, ts_out)
util.plot_histogram(r_tr, figsize=figsize, label='training', data2=r_ts, label2='test', pri
```




```
Mean: 0.017 (training), 0.020 (test)
```