Decision-Focused Learning

The Main Challenge

We are now ready to tackled decision-focused learning

Let's start from the "holy grail" problem:

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

Unfortunately, the argmin **used to define** $z^*(y_i)$ **is non-differentiable**

- A small change in the prediction vector y_i
- ...May cause a large/discrete change in the optimal solution z_i

This is certainly the case for our example problem

How are we going to deal with this?

Towards a Solution

A possible solution consists in using a surrogate loss

For the i-th example:

- Since $z^*(\hat{y}_i)$ is the true optimal solution for the true costs $\hat{y}_i$
- We expect that to remain optimal for any good vector y_i of predicted

paramters

In practice, we could train the model to minimize this contrastive loss:

$$c(z^*(\hat{y}_i), y_i) - c(z^*(y_i), y_i)$$

$z^*(y_i)$ is the cost minimizer for the estimated parameters y_i

- I.e. our model thinks that this is the correct solution for the i-th example
- ..But $z^*(\hat{y}_i)$ is the true optimum for the example

Towards a Solution

Let's consider again our contrastive loss:

$$c(z^*(\hat{y}_i), y_i) - c(z^*(y_i), y_i)$$

We wish to backpropagata by differentiating over $y_i = f(\hat{x}_i, \theta)$

- The loss contains a constant, i.e. $z^*(\hat{y}_i)$
- ...A non-differentiable term, i.e. $z^*(y_i)$ that still depends on y_i
- ...And finally a naturally differentiable term, i.e. $c(\cdot, y_i)$

This will be enough for us

- We will pretend that $z^*(y_i)$ is fixed, even if it depends on y_i
- It can be proved that, under some assumptions, this yields a valid subgradient

An Example on Our Market Problem

Let's use our market problem, for the i-th example

$$\text{argmin}_z \{ y_i^T z \mid v^T z \geq r, z \in \{0, 1\}^n \}$$

This satisfied the required assumption

- In particular, the cost expression (i.e. $y_i^T z$) is differentiable in y_i

Therefore, we can get a valid subgradient:

- First we compute the optimal solution $z_i = z^*(y_i)$ ("in the forward pass")
- Then we compute $\nabla_y (y^T z_i^*(\hat{y}_i) - y^T z_i) = z_i^*(\hat{y}_i) - z^*(y_i)$
- I.e. the difference between optima w.r.t. the true and the predicted costs

We can do this by relying on automatic differentiation

Almost There...

Let's recap our plan

- When we evaluate our ML model, we need to solve the market problem
- ...So as to compute $z^*(y_i)$ for each example (in the mini-batch)
- Then we compute the loss:

$$L_C(y, \hat{y}) = \sum_{i=1}^{m} y_i^T (z^*(\hat{y}_i) - z^*(y_i))$$

Finally we can use automatic differentiation (as usual) to get the subgradient

Almost There...

Let's recap our plan

- When we evaluate our ML model, we need to solve the market problem
- ...So as to compute $z^*(y_i)$ for each example (in the mini-batch)
- Then we compute the loss:

$$L_C(y, \hat{y}) = \sum_{i=1}^{m} y_i^T (z^*(\hat{y}_i) - z^*(y_i))$$

Finally we can use automatic differentiation (as usual) to get the subgradient

Except that with linear costs this plan has a fatal flow

There, Finally!

The problem is that our loss admits a trivial solution

$$L_C(y, \hat{y}) = \sum_{i=1}^{m} y_i^T (z^*(\hat{y}_i) - z^*(y_i))$$

- All contrastive terms are non-negative by definition
- ...And it's easy to make them null by just predicting $y_i = 0$ for all examples

A possible fix consists in using this modified function

$$L_{CR}(y, \hat{y}) = \sum_{i=1}^{m} y_i^T (z^*(\hat{y}_i) - z^*(y_i)) + \hat{y}_i^T (z^*(y_i) - z^*(\hat{y}_i))$$

- This is another surrogate loss (ready for subgradient computation)

There, Finally!

Let's examine the modified loss

$$L_{CR}(y, \hat{y}) = \sum_{i=1}^{m} \underbrace{y_i^T(z^*(\hat{y}_i) - z^*(y_i))}_{\text{contrastive}} + \underbrace{\hat{y}_i^T(z^*(y_i) - z^*(\hat{y}_i))}_{\text{regret}}$$

The new term $\hat{y}_i^T(z^*(y_i) - z^*(\hat{y}_i))$ is the regret:

- I.e. it's the additional cost we pay (under the true parameter values $\hat{y}_i$
- ...For not having guessed correctly the true optimal solution

Both terms are guaranteed non-negative and therefore $L_{CR}(y, \hat{y}) \geq 0$

We wish both terms to be small (hence the loss is valid)

There, Finally!

It is convenient to rewrite the loss as:

$$L_{CR}(y, \hat{y}) = \sum_{i=1}^{m} (y_i - \hat{y}_i)^T (z^*(\hat{y}_i) - z^*(y_i))$$

This clarifies that it can be minimized in two ways:

- Either by making the two solutions as similar as possible, i.e. $z^*(\hat{y}_i) \simeq z^*(y_i)$
- ...Or by making the two costs as similar as possible, i.e. $y_i \simeq \hat{y}_i$

Importantly, $y = 0$ is no longer a minimizer

A DFL Implementation

A Decision Focused Learning Implementation

An implementation of the method is available in the `util` module

The code relies (again) on subclassing the `keras.Model` class

```
class DFLModel(keras.Model):
    def __init__(self, prb, ..., **params):
        super(DFLModel, self).__init__(**params)
        self.prb = prb
        ...
```

At construction time, we need to pass the optimization problem as an argument

```
nnin = keras.Input(input_size)
nnout = nnin
for h in hidden:
    nnout = layers.Dense(h, activation='relu')(nnout)
nnout = layers.Dense(output_size, activation=output_activation)(nnout)
model = DFLModel(problem, inputs=nnin, outputs=nnout, ...)
```

A Decision Focused Learning Implementation

The `fit` function is overloaded

- We compute all the optimal solutions w.r.t. the true costs, i.e. $z^*(\hat{y}_i)$
- Then we calling the parent `fit` function

```
def fit(self, X, y, **kwargs):
    # Precompute all solutions for the true costs
    self.sol_store = []
    for c in y:
        sol, closed = self.prb.solve(c, tlim=self.tlim)
        self.sol_store.append(sol)
    self.sol_store = np.array(self.sol_store)
    # Call the normal fit method
    return super(DFLModel, self).fit(X, y, **kwargs)
```

A Decision Focused Learning Implementation

In the `train_step` method, we compute the surrogate loss

```
def train_step(self, data):
    x, costs_true = data
    ...
    with tf.GradientTape() as tape:
        costs = self(x, training=True) # obtain predictions
        sols, tsols = [], []
        for c, tc in zip(costs.numpy(), costs_true.numpy()):
            sol, closed = prb.solve(c, ...) # Best w.r.t. predictions
            sols.append(sol)
            tsol = self._find_best(tc) # Best w.r.t. true costs
            tsols.append(tsol)
        sols, tsols = np.array(sols), np.array(tsols)
        cdiff = costs - costs_true # cost difference
        sdiff = tsols - sols # solution difference
```

Early Training

Let's train our decision-focused model for a few epochs

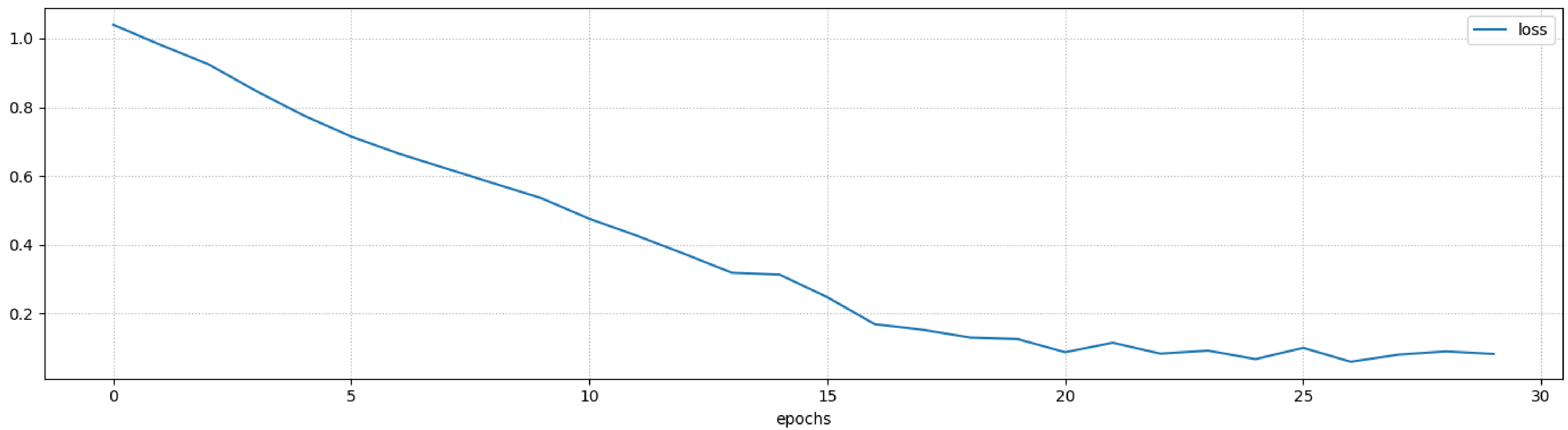
```
In [12]: dfm_early = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[], na
         %time history = util.train_dfl_model(dfm_early, tr_in, tr_out, epochs=30, verbose=1, validation_
```

```
Epoch 1/30
11/11 [==============================] - 1s 58ms/step - loss: 1.0399
Epoch 2/30
11/11 [==============================] - 1s 63ms/step - loss: 0.9810
Epoch 3/30
11/11 [==============================] - 1s 80ms/step - loss: 0.9249
Epoch 4/30
11/11 [==============================] - 1s 92ms/step - loss: 0.8474
Epoch 5/30
11/11 [==============================] - 1s 101ms/step - loss: 0.7762
Epoch 6/30
11/11 [==============================] - 1s 117ms/step - loss: 0.7148
Epoch 7/30
11/11 [==============================] - 1s 124ms/step - loss: 0.6652
Epoch 8/30
11/11 [==============================] - 1s 126ms/step - loss: 0.6217
Epoch 9/30
11/11 [==============================] - 1s 130ms/step - loss: 0.5786
Epoch 10/30
11/11 [==============================] - 1s 128ms/step - loss: 0.5353
Epoch 11/30
11/11 [==============================] - 1s 130ms/step - loss: 0.4757
```

What We Loose

It works, but there are some issues

```
In [13]: util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.0826 (training)
```

- The loss curve is less smooth (since we are using a sub-gradient)
- Training takes longer (since we need to solve optimization problems)

What We Loose

We also loose a lot in terms of accuracy

These are the results for our previous "early" training model

```
In [14]: 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: -1.86, MAE: 0.32, RMSE: 0.43 (training)
         R2: -1.92, MAE: 0.32, RMSE: 0.43 (test)
```

...And these are the results for the decision-focused model

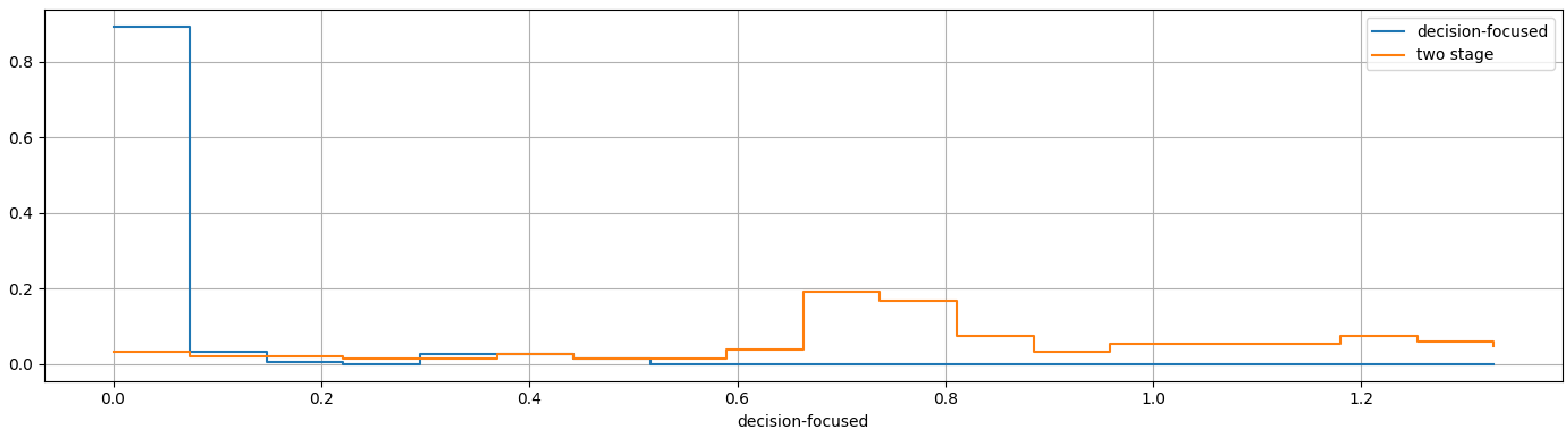
```
In [15]: r2, mae, rmse = util.get_ml_metrics(dfm_early, tr_in, tr_out)
         print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
         r2, mae, rmse = util.get_ml_metrics(dfm_early, ts_in, ts_out)
         print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')

         R2: -5.24, MAE: 0.6, RMSE: 0.65 (training)
         R2: -5.37, MAE: 0.6, RMSE: 0.66 (test)
```

What We Gain

But in terms of regret, we are doing better!

```
In [16]: r_ts_fsm_early = util.compute_regret(prb, fsm_early, ts_in, ts_out)
         r_ts_dfm_early = util.compute_regret(prb, dfm_early, ts_in, ts_out)
         util.plot_histogram(r_ts_dfm_early, figsize=figsize, label='decision-focused', data2=r_ts_fsm_ea
```




```
Mean: 0.034 (decision-focused), 0.825 (two stage)
```

Speeding Up the Process

Training speed is a major bottleneck for decision-focused learning

We will address that by keeping a solution cache

- We store all computed solutions in a set S
- Then we compute $z^*(y_i)$ via simple enumeration:

$$z^*(y_i) = \text{argmin}_{z \in S} c(z, y_i)$$

Occasionaly, we may compute a new solution and update the cache

E.g. we can trigger this with a low probability per sample

An alternative consists in using a problem relaxation

E.g. A Linear Programs instead of a Mixed Integer Linear Program

Implementing Solution Caching

A solution caching mechanism is implemented in our code

The computation of $z^*(y_i)$ is triggered with a controllable probability

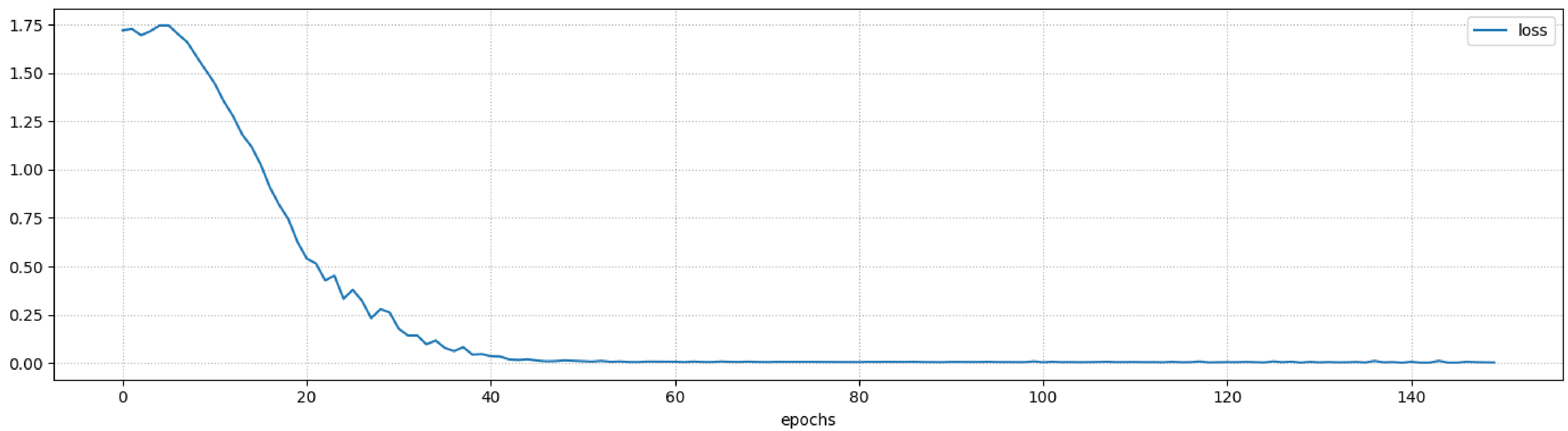
```
def train_step(self, data):
    ...
    with tf.GradientTape() as tape:
        ...
        for c, tc in zip(costs.numpy(), costs_true.numpy()):
            if np.random.rand() < self.recompute_chance: # guard
                sol, closed = prb.solve(c, tlim=self.tlim) # recompute
                if self.recompute_chance < 1: # update cache
                    if not (self.sol_store == sol).all(axis=1).any():
                        self.sol_store = np.vstack((self.sol_store, sol))
            else:
                sol = self._find_best(c) # look up in the cache
            ...
        ...
```

Training With Solution Caching

Let's train the model with a solution cache and 5% recomputation chance

```
In [18]: dfm_late = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, recompute_char
         %time history = util.train_dfl_model(dfm_late, tr_in, tr_out, epochs=150, verbose=0, validation_
         util.plot_training_history(history, figsize=figsize)
```

```
CPU times: user 13.4 s, sys: 668 ms, total: 14.1 s
Wall time: 13.7 s
```




```
Final loss: 0.0023 (training)
```

Accuracy Comparison

Since we manage to train the model to (approximate) convergence

...It makes sense to compare with the "late" linear regression approach

```
In [20]: 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)
```

In terms of accuracy we are doing still quite poorly

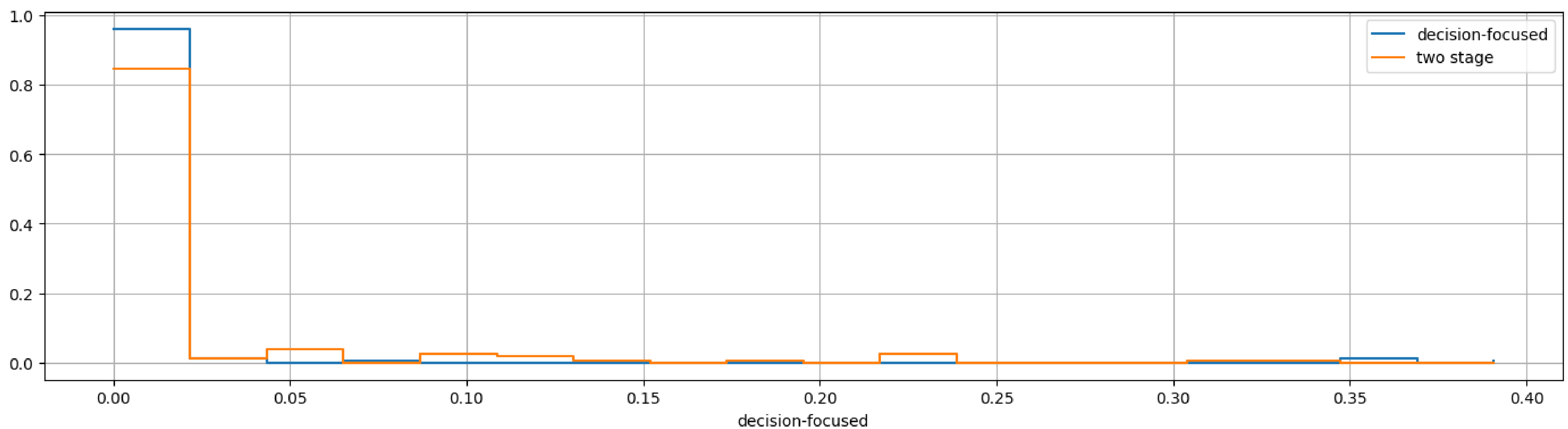
```
In [21]: r2, mae, rmse = util.get_ml_metrics(dfm_late, tr_in, tr_out)
         print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
         r2, mae, rmse = util.get_ml_metrics(dfm_late, ts_in, ts_out)
         print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')

         R2: -7.00, MAE: 0.66, RMSE: 0.74 (training)
         R2: -7.27, MAE: 0.66, RMSE: 0.74 (test)
```

Regret Comparison

Both approaches work well, but we beat LR by a factor of at least 2

In [22]:
```
r_ts_fsm_late = util.compute_regret(prb, fsm_late, ts_in, ts_out)
r_ts_dfm_late = util.compute_regret(prb, dfm_late, ts_in, ts_out)
util.plot_histogram(r_ts_dfm_late, figsize=figsize, label='decision-focused', data2=r_ts_fsm_lat
```




```
Mean: 0.009 (decision-focused), 0.020 (two stage)
```