Decision-Focused Learning

Where we discover that things ain't that easy

The Main Challenge

We are now ready to tackled decision-focused learning

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

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

Unfortunately, the $\textbf{argmin}$ 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 $\boldsymbol{i}$-th example:

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

In practice, we could train the model to minimize the regret:

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

- This quantity is always non-negative (since $z^*(y_i)$ is a cost minimizer w.r.t. y_i)
- It becomes 0 when the two solutions match
- It contains a naturally differentiable term, i.e. $y_i = f(\hat{x}_i)$

...But unfortunately also a non-differentiable term, i.e. $z^*(y_i)$

Towards a Solution

We can view the regret computation as a maximization problem

$$r_i^*(y_i) = \max_{z \in F(y_i)} r_i(z, y_i)$$

$$\text{with: } r_i(z, y_i) = c(z^*(\hat{y}_i), y_i) - c(z, y_i)$$

This enables casting the "holy grail" problem as bi-level optimization:

$$\text{argmin}_\omega \left\{ \sum_{i=1}^{m} \max_{z \in F(y_i)} r_i(z, y_i) \mid y = f(\hat{x}, \omega) \right\}$$

...And for bi-level optimization problem we can rely on two great results

- That are remarkably easy to use
- ...But have a mildly complicated proof and require some assumptions

Bi-level Optimization and Subgradient

First of all, let simplify the problem by assuming a fixed feasible set

$$F(y_i) = F$$

- This assumption limits the approach applicability
- ...But it remains useful on many real world problems

Then, let's focus on a single example

We have that, for a generic prediction vector y:

$$\max_{z \in F} r_i(z, y) \geq r_i(z_i, y)$$

- Where z_i is a compact notation for $z^*(y_i)$
- The result stands since z_i is not necessarily optimal w.r.t. y

Bi-level Optimization and Subgradient

If $r_i(z, y)$ is differentiable, we can expand it via Taylor's theorem

We will use as a reference the current prediction vector y_i:

$$r_i(z_i, y) = r_i(z_i, y_i) + \nabla_y r_i(z_i, y_i)(y - y_i) + o(\|y - y_i\|)$$

Therefore we will have:

$$\max_{z \in F} r_i(z, y) \geq r_i(z_i, y_i) + \nabla_y r_i(z_i, y_i)(y - y_i) + o(\|y - y_i\|)$$

- For $y \to y_i$ the term $o(\|y - y_i\|)$ will be come vanishingly small
- Meaning that we will approximately have

$$\max_{z \in F} r_i(z, y) - \max_{z \in F} r_i(z, y_i) \geq \nabla_y r_i(z_i, y_i)(y - y_i)$$

Bi-level Optimization and Subgradient

Let's look again at the last (local, approximate) inequality

$$\max_{z \in F} r_i(z, y) - \max_{z \in F} r_i(z, y_i) \geq \nabla_y r_i(z_i, y_i)(y - y_i)$$

- We are saying that the regret difference locally admits a linear under approximation
- ...Which uses $\nabla_y r_i(z_i, y_i)$ as a coefficient vector

Formally, this means that $\nabla_y r_i(z_i, y_i)$ is a local subgradient

...But what is $\nabla_y r_i(z_i, y_i)$ exactly?

- It's what you get by taking the regret expression $r(z, y)$
- Plugging in z_i for z
- Differentiating over y
- ...And finally plugging in y_i for y

Bi-level Optimization and Pseudo-convexity

If $r_i(z, y)$ is convex in y, then:

- The for the Taylor expansion we have:

$$r_i(z_i, y) \geq r_i(z_i, y_i) + \nabla_y r_i(z_i, y_i)(y - y_i)$$

- ...And our main inequality holds everywhere:

$$\max_{z \in F} r_i(z, y) - \max_{z \in F} r_i(z, y_i) \geq \nabla_y r_i(z_i, y_i)(y - y_i)$$

This means our inner optimization function is pseudo-convex

A pseudo-convex function behaves as convex for the purpose of optimization

- I.e. If we could freely control y_i...
- ...Then we could optimally solve $\min_{y_i} \max_{z \in F} r_i(z, y_i)$
- ...Via simple sub-gradient descent

Both result hold for bi-level optimization in general!

Beyond Decision Focused Learning

These are general results

Given a bi-level optimization in the form:

$$\min_{y \in Y} \max_{x \in X} f(x, y)$$

With:

$$x^*(y) = \text{argmin}_{x \in X} f(x, y)$$

Then:

- If f is differentiable, $\nabla_y f(x^*(y), y)$ is a valid subgradient w.r.t. y
- If f is linear, $f^*(y) = \max_{x \in X} f(x, y)$ is pseudo-convex

An Example on Our Market Problem

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

$$\text{argmin}_z \{ y_i^T z \mid \|z\|_1 \geq r, z \in \{0, 1\}^n \}$$

- The feasible space does not depend on the predicted costs, hence $F(y_i) = F$
- The regret expression is $r_i^*(z, y) = y^T z_i^*(\hat{y}_i) - y^T z$
- ...Which is differentiable and linear

Therefore, we can get a valid subgradient:

- First we compute the optimal solution z_i ("in the forward pass")
- Then we compute $\nabla_y (y^T z_i^*(\hat{y}_i) - y^T z_i) = z_i^*(\hat{y}_i) - z_i$
- Since there is dependence on y, our subgradient is $z_i^*(\hat{y}_i) - z_i$

...I.e. just the difference between optima w.r.t. the true and the predicted costs

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:

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

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

Except that with a linear cost this plan has a fatal flow

There, Finally!

The problem is that our loss admits a trivial solution

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

- All regret 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

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

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

There, Finally!

Let's examine the modified loss

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

- The term $y_i^T (z^*(\hat{y}_i) - z^*(y_i))$ is the regret w.r.t. the predicted costs y_i
- The term $\hat{y}_i^T (z^*(y_i) - z^*(\hat{y}_i))$ is the regret w.r.t. the true costs $\hat{y}_i$
- Both terms are guaranteed non-negative and therefore $L_{NCE}(y, \hat{y}) \geq 0$

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

- We did not use $\hat{y}_i^T (z^*(y_i) - z^*(\hat{y}_i))$ before...
- ...Because it lack a naturally differentiable term

The corresponding subgradient would not lead to back-propagation

There, Finally!

It is convenient to rewrite the loss as:

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

This clarifies that the loss 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, $y_i = 0, \forall i = 1..m$ **is no longer a minimizer**

- There are other viable surrogate losses (e.g. $SPO+$ from this paper)
- ...But we will limit our analysis to this one

A Decision Focused Learning Implementation

For those who, like me, understand code better

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 model construction time, we need to specify the optimization problem

```
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 was overloaded

- We compute all the optimal solutions w.r.t. the true costs, i.e. $z^*(\hat{y}_i)$
- Then we calling the usual `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
        loss = tf.reduce_mean(tf.reduce_sum(cdiff * sdiff, axis=1))
    ...
```

Early Training

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

In [4]:
```
dfm_early = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, hidden=[], na
%time history = util.train_dfo_model(dfm_early, tr_in, tr_out, epochs=30, verbose=1, validation_
```

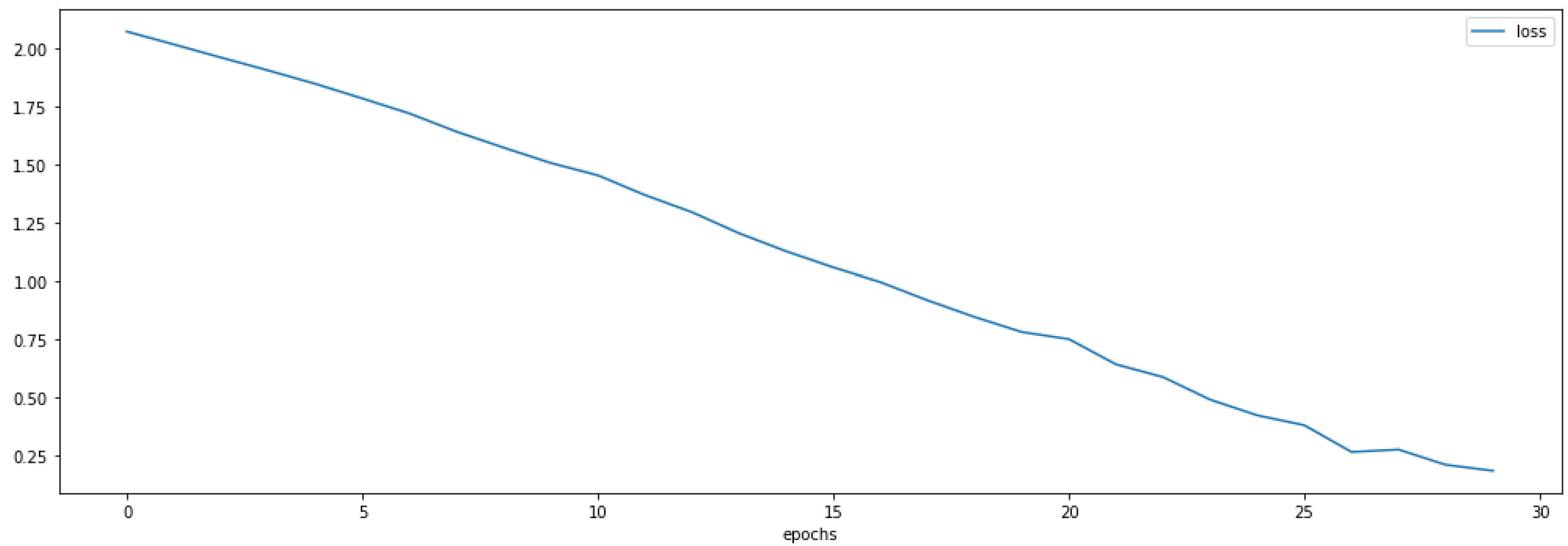
```
Epoch 1/30
11/11 [==============================] - 1s 65ms/step - loss: 2.0735
Epoch 2/30
11/11 [==============================] - 1s 68ms/step - loss: 2.0181
Epoch 3/30
11/11 [==============================] - 1s 67ms/step - loss: 1.9616
Epoch 4/30
11/11 [==============================] - 1s 70ms/step - loss: 1.9063
Epoch 5/30
11/11 [==============================] - 1s 74ms/step - loss: 1.8487
Epoch 6/30
11/11 [==============================] - 1s 77ms/step - loss: 1.7855
Epoch 7/30
11/11 [==============================] - 1s 82ms/step - loss: 1.7207
Epoch 8/30
11/11 [==============================] - 1s 90ms/step - loss: 1.6423
Epoch 9/30
11/11 [==============================] - 1s 92ms/step - loss: 1.5737
Epoch 10/30
11/11 [==============================] - 1s 97ms/step - loss: 1.5077
Epoch 11/30
11/11 [==============================] - 1s 102ms/step - loss: 1.4546
```

What We Loose

It works, but there are some issues

We will highlight them now and address one of them later

In [5]:
```
util.plot_training_history(history, figsize=figsize)
```




```
Model loss: 0.1838 (training)
```

What We Loose

We also loose a lot in terms of accuracy

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

In [6]:
```
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: -1.39, MAE: 0.3, RMSE: 0.41 (training)
R2: -1.46, MAE: 0.3, RMSE: 0.41 (test)
```

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

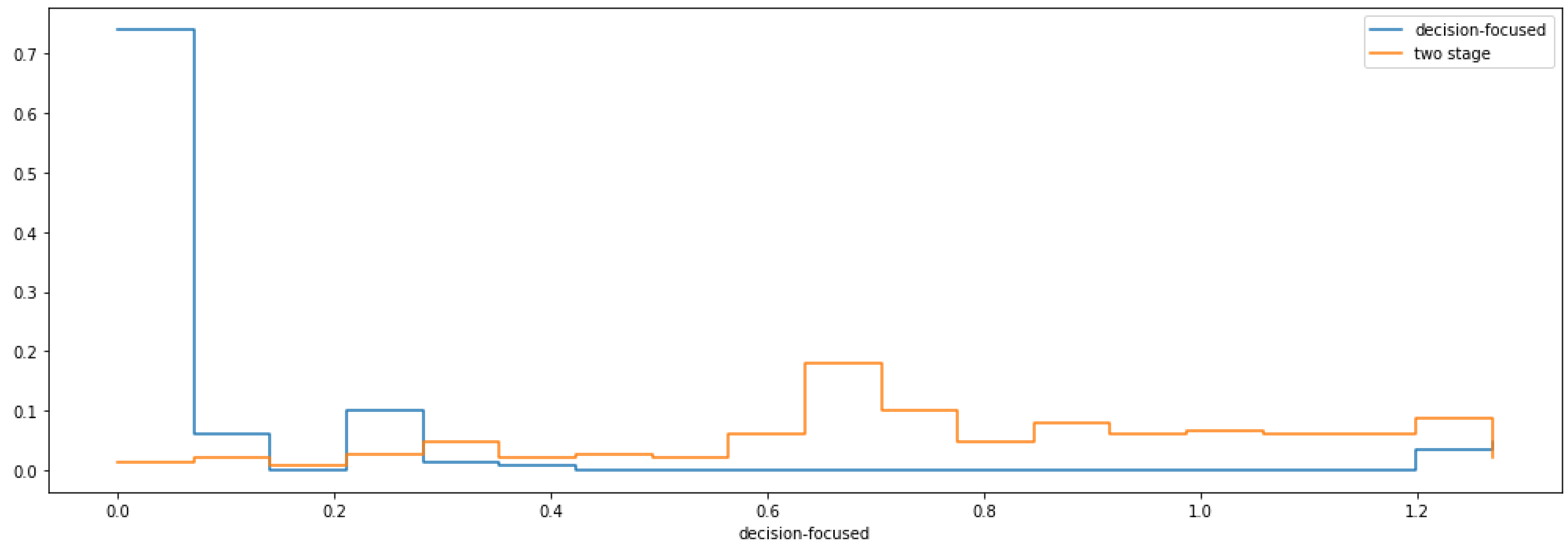
In [7]:
```
r2, mae, rmse = util.get_ml_metrics(dfm_early, tr_in, tr_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
r2, mae, rmse = util.get_ml_metrics(dfm_early, ts_in, ts_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')
```

```
R2: -6.45, MAE: 0.62, RMSE: 0.70 (training)
R2: -6.64, MAE: 0.63, RMSE: 0.70 (test)
```

What We Gain

But in terms of regret, we are doing much better

In [8]:
```
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: 0.142 (decision-focused), 0.785 (two stage)
```

Speeding Up the Process

Training speed is a major bottleneck for decision-focused learning

One possibility is to use a relaxation that is easier to solve

- For a MILP, this would be the LP relaxation
- In general, given a relaxed feasible space $\tilde{F}$, we compute $z^*(y_i)$ as:

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

Another possibility consists in keeping a solution cache

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

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

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

Speeding Up the Process

For MILPs, the two approaches have a nice interpretation

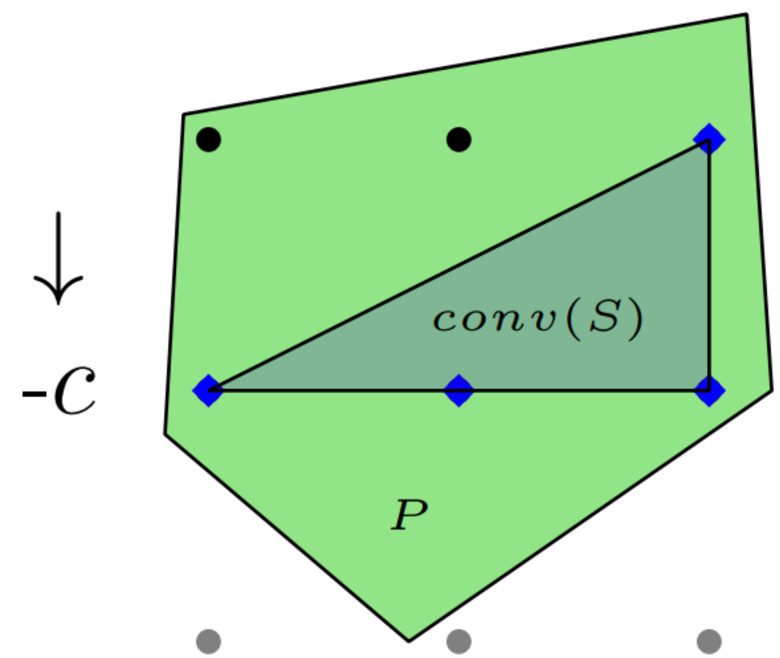


Image from this paper

Given the true feasible space (discrete points in the polytope in the figure)

- The relaxation leads to an outer approximation (green), hence a lower bound
- The cache provides an inner approximation (blue), hence an upper bound

Implementing Solution Caching

A solution caching mechanism is implemented in our code

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

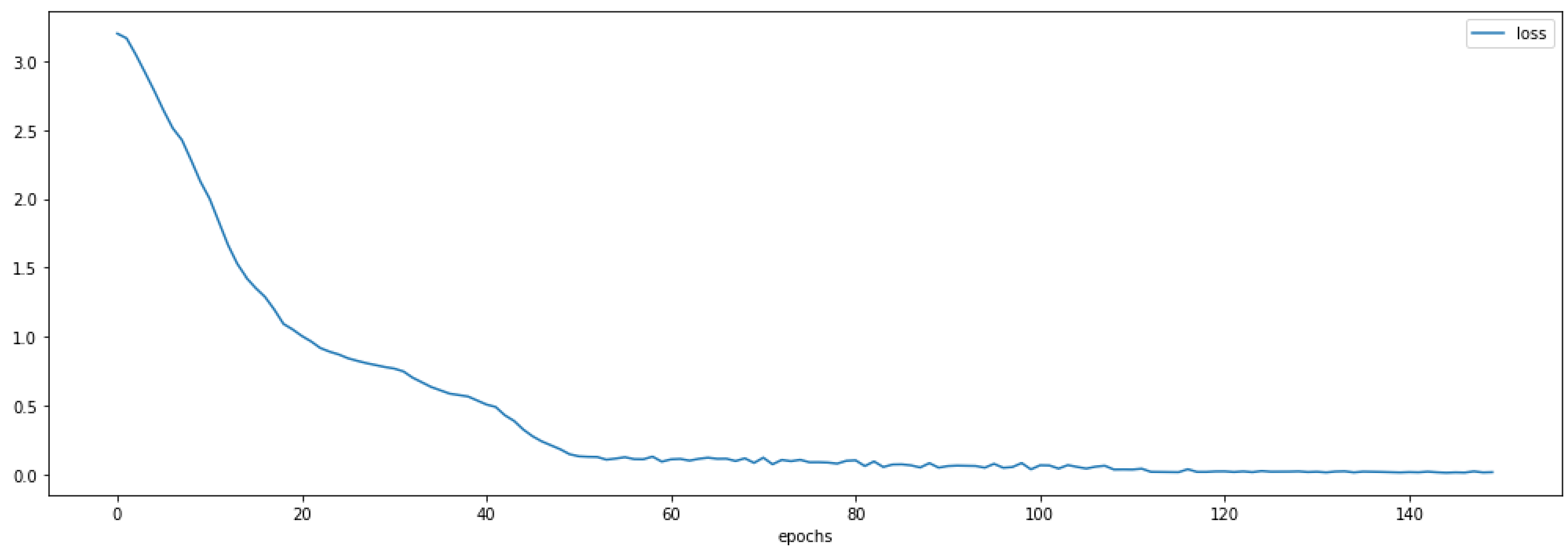
```
def train_step(self, data):
    ...
    with tf.GradientTape() as tape:
        ...
        for c, tc in zip(costs.numpy(), costs_true.numpy()):
            if np.random.rand() < self.recompute_chance: # guard
                sol, closed = prb.solve(c, tlim=self.tlim) # recompute
                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 [9]:
```
dfm_late = util.build_dfl_ml_model(input_size=1, output_size=nitems, problem=prb, recompute_char
%time history = util.train_dfo_model(dfm_late, tr_in, tr_out, epochs=150, verbose=0, validation_
util.plot_training_history(history, figsize=figsize)
```

```
CPU times: user 20.3 s, sys: 1.03 s, total: 21.3 s
Wall time: 20.9 s
```




```
Model loss: 0.0176 (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 [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)
```

In terms of accuracy we are doing still quite poorly

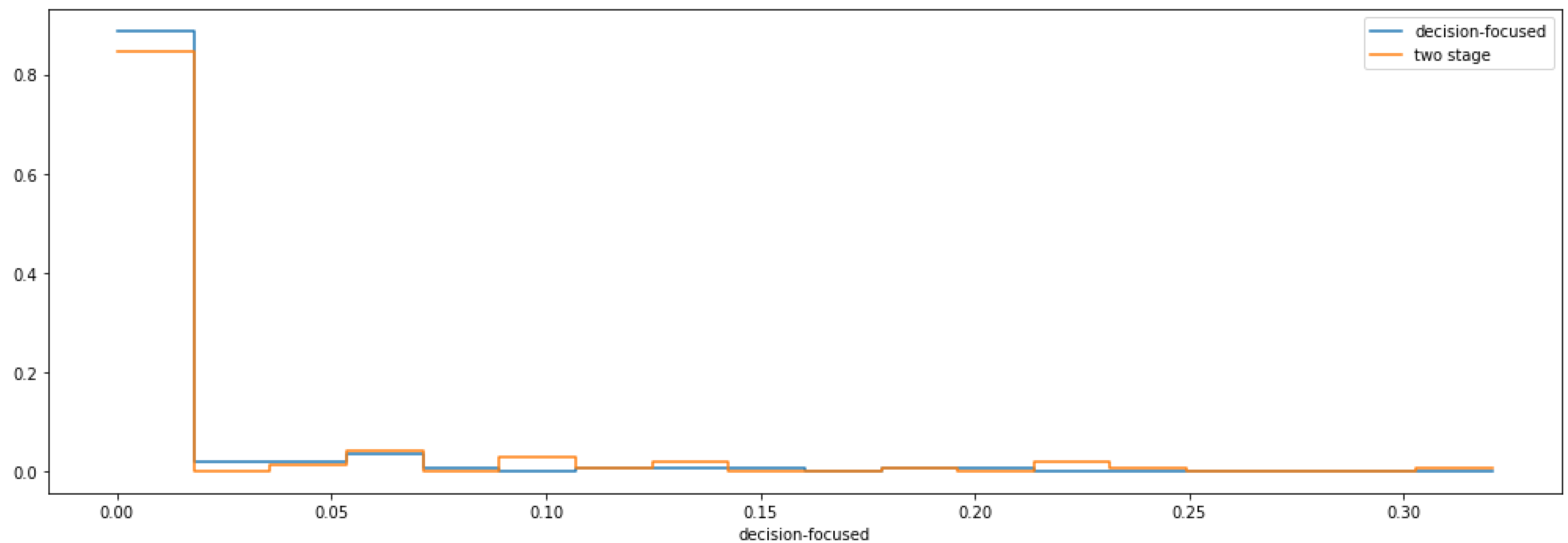
In [11]:
```
r2, mae, rmse = util.get_ml_metrics(dfm_late, tr_in, tr_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (training)')
r2, mae, rmse = util.get_ml_metrics(dfm_late, ts_in, ts_out)
print(f'R2: {r2:.2f}, MAE: {mae:.2}, RMSE: {rmse:.2f} (test)')
```

```
R2: -5.70, MAE: 0.61, RMSE: 0.69 (training)
R2: -5.87, MAE: 0.62, RMSE: 0.69 (test)
```

Regret Comparison

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

In [12]:
```
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
```

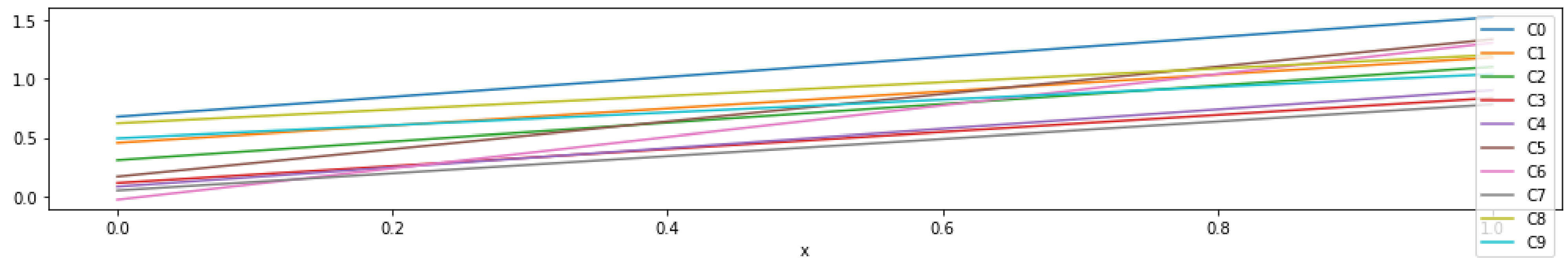


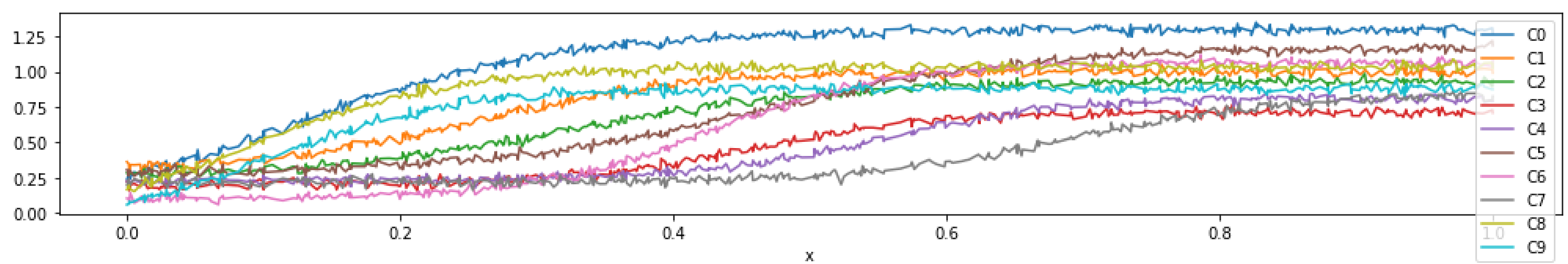

```
Mean: 0.009 (decision-focused), 0.020 (two stage)
```

A Deeper Look at the Predictions

It's interesting to the check the predictions for the "late" LR model

In [13]:
```
fsm_late_pred = pd.DataFrame(index=data.index, columns=data.columns, data=fsm_late.predict(data.
util.plot_df_cols(fsm_late_pred, figsize=(figsize[0], 0.5*figsize[1]))
util.plot_df_cols(data, figsize=(figsize[0], 0.5*figsize[1]))
```





A Deeper Look at the Predictions

It's interesting to the check the predictions for the "late" LR model

In [14]:
```
dfm_late_pred = pd.DataFrame(index=data.index, columns=data.columns, data=dfm_late.predict(data.
util.plot_df_cols(dfm_late_pred, figsize=(figsize[0], 0.5*figsize[1]))
util.plot_df_cols(data, figsize=(figsize[0], 0.5*figsize[1]))
```