Knowledge Injection in RUL

Let's see the last approach in action

Domain Knowledge as Constraints

Our soft constraint is in the form:

$$f(x_i;\theta) - f(x_j;\theta) \simeq j - i \qquad \forall i, j = 1..m \text{ s.t. } c_i = c_j$$

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From which we can derive the penalizer:

$$\lambda \sum_{\substack{i,j=1..m \\ c_i = c_j}} \left(f(x_i; \theta) - f(x_j; \theta) - (j - i) \right)^2$$

- For sake of simplicity, we are using the same λ for all pairs
- ...Meaning the same standard deviation using a Normal semantic

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- ...Meaning the same standard deviation using a Normal semantic

There's large number of constraints, but many are redundant

Our Regularizer

For example, we can focus on subsequent pairs

$$L(\hat{y}) + \lambda \sum_{\substack{i \prec j \\ c_i = c_j}} \left(f(x_i; \theta) - f(x_j; \theta) - (j - i) \right)^2$$

- Where $i \prec j$ iff j is the next sample for after i for a given machine
- This approach requires a linear (rather than quadratic) number of constraints

This method can work with mini-batches

- In this case, $\prec$ will refer to contiguous samples in the same batch
- ...And of course for the same component

We will now see how to implement this approach

Generating Batches from the Same Machine

Our regularizer requires to have sorted samples from the same machine

The easiest way to ensure we have enough is using a custom `DataGenerator`

```
class SMBatchGenerator(tf.keras.utils.Sequence):
    def __init__(self, data, in_cols, batch_size, seed=42): ...
    def __len__(self): ...
    def __getitem__(self, index): ...
    def on_epoch_end(self): ...
    def __build_batches(self): ...
```

- `__len__` is called to know how many batches are left
- `__getitem__` should return one batch
- `on_epoch_end` should take care (e.g.) of shuffling

Generating Batches from the Same Machine

The `__init__` method takes care of the initial setup

```python
def __init__(self, data, in_cols, batch_size, seed=42):
    super(SMBatchGenerator).__init__()
    self.data = data
    self.in_cols = in_cols
    self.dpm = split_by_field(data, 'machine')
    self.rng = np.random.default_rng(seed)
    self.batch_size = batch_size
    # Build the first sequence of batches
    self.__build_batches()
```

- We store some fields
- We split the data by machine
- We build a dedicated RNG
- ...And finally we call the custom-made `__build_batches` method

Generating Batches from the Same Machine

The `__build_batches` method prepares the batches for one full epoch

```python
def __build_batches(self):
    self.batches, self.machines = [], []
    mcns = list(self.dpm.keys())
    self.rng.shuffle(mcns) # sort the machines at random
    for mcn in mcns: # Loop over all machines
        index = self.dpm[mcn].index # sample indexes for this machine
        ...
        self.rng.shuffle(idx) # shuffle sample indexes for this machine
        bt = idx.reshape(-1, self.batch_size) # split into batches
        bt = np.sort(bt, axis=1) # sort every batch individually
        self.batches.append(bt) # store the batch
        self.machines.append(np.repeat([mcn], len(bt))) # add machine information
    self.batches = np.vstack(self.batches) # concatenate
    self.machines = np.hstack(self.machines)
```

Generating Batches from the Same Machine

We rebuild batches after each epoch

```
def on_epoch_end(self):
    self.__build_batches()
```

Most of the remaining work is done in the `__getiitem__` method:

```
def __getitem__(self, index):
    idx = self.batches[index]
    x = self.data[self.in_cols].loc[idx].values
    y = self.data['rul'].loc[idx].values
    flags = (y != -1)
    info = np.vstack((y, flags, idx)).T
    return x, info
```

- The RUL value is -1 for the unsupervised data: we flag the meaningful RULs
- ...We pack indexes, RUL values, and flags into a single `info` tensor

Custom Training Step

We then enforce the constraints by means of a custom training step

```python
class CstRULRegressor(keras.Model):
    def __init__(self, rul_pred, alpha, beta, maxrul): ...

    def train_step(self, data): ...

    def call(self, data): return self.rul_pred(data)

    ...
```

- We use a custom `keras.Model` subclass
- ...And accept an externally built RUL prediction model (`rul_pred`)
- The custom training step is implemented in `train_step`
- The `call` method relies on the external model for RUL prediction

Custom Training Step

In the `__init__` function:

```python
def __init__(self, rul_pred, alpha, beta, maxrul):
    super(CstRULRegressor, self).__init__(input_shape, hidden)
    # Store the base RUL prediction model
    self.rul_pred = rul_pred
    # Weights
    self.alpha = alpha
    self.beta = beta
    self.maxrul = maxrul
    ...
```

- `beta` is the regularizer weight, `alpha` is a weight for the loss function itself
- We also store the maximum RUL

Custom Training Step

In the custom training step:

```
def train_step(self, data):
    x, info = data
    y_true, flags, idx = info[:, 0:1], info[:, 1:2], info[:, 2:3]
    with tf.GradientTape() as tape:
        y_pred = self(x, training=True) # predictions
        mse = tf.math.reduce_mean(flags * tf.math.square(y_pred-y_true)) # MSE loss
        delta_pred = y_pred[1:] - y_pred[:-1] # pred. difference
        delta_rul = -(idx[1:] - idx[:-1]) /self.maxrul # index difference
        deltadiff = delta_pred - delta_rul # difference of differences
        cst = k.mean(k.square(deltadiff)) # regualization term
        loss = self.alpha * mse + self.beta * cst # loss
    ...
```

- We unpack the `info` tensor
- Inside a `GradientTape`, we construct our regularized loss

Custom Training Step

In the custom training step:

```
def train_step(self, data):
    ...
    tr_vars = self.trainable_variables
    grads = tape.gradient(loss, tr_vars) # gradient computation

    self.optimizer.apply_gradients(zip(grads, tr_vars)) # weight update

    ...
```

- We then apply the (Stochastic) Gradient Descent step
- Then we update and retun the loss trackers

Training the Lagrangian Approach

We can now test our approach

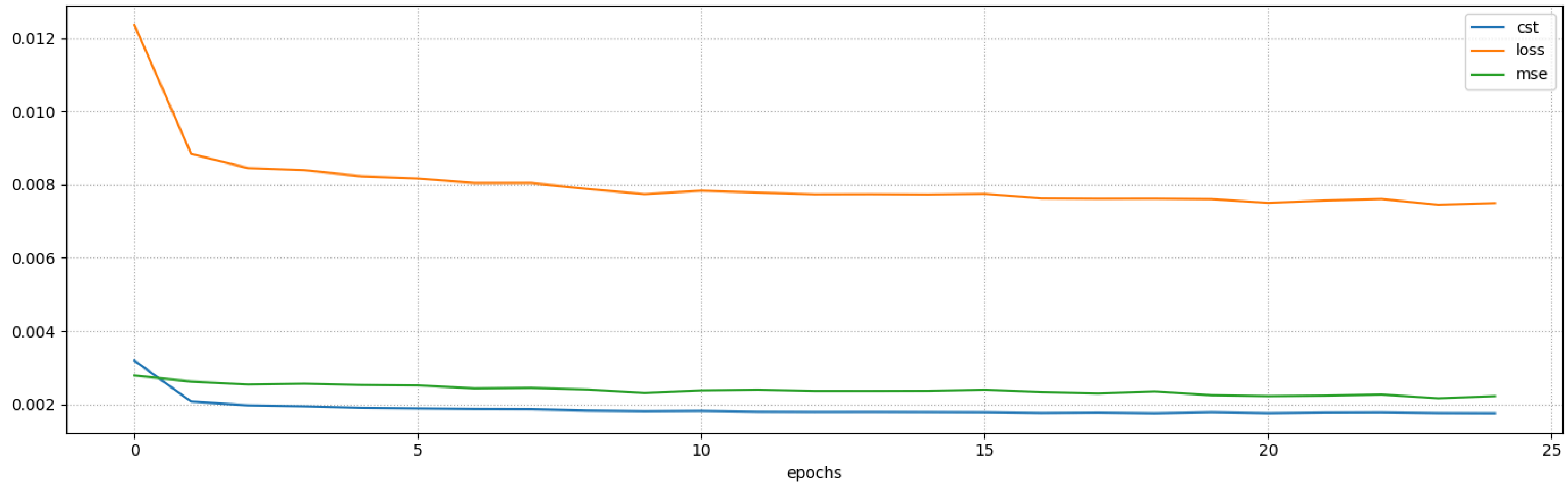
In [22]:
```
nn_aux = util.build_nn_model(input_shape=(len(dt_in),), output_shape=(1,), hidden=[32, 32])
nn2 = util.CstRULRegressor(rul_pred=nn_aux, alpha=1, beta=3, maxrul=maxrul)
batch_gen = util.CstBatchGenerator(tr_s2, dt_in, batch_size=32)
history = util.train_nn_model(nn2, X=batch_gen, y=None, loss=None, validation_split=0., epo
```

```
Epoch 1/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0072 - loss: 0.0250 - mse: 0.0034
Epoch 2/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0021 - loss: 0.0088 - mse: 0.0026
Epoch 3/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0019 - loss: 0.0086 - mse: 0.0028
Epoch 4/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0019 - loss: 0.0078 - mse: 0.0020
Epoch 5/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 2ms/step - cst: 0.0019 - loss: 0.0083 - mse: 0.0025
Epoch 6/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0019 - loss: 0.0073 - mse: 0.0017
Epoch 7/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 2ms/step - cst: 0.0019 - loss: 0.0078 - mse: 0.0022
Epoch 8/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0019 - loss: 0.0079 - mse: 0.0022
Epoch 9/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0018 - loss: 0.0079 - mse: 0.0024
Epoch 10/25
1071/1071 ━━━━━━━━━━━━━━━━━━━━ 2s 1ms/step - cst: 0.0019 - loss: 0.0079 - mse: 0.0023
Epoch 11/25
```

Training the Lagrangian Approach

...And we can check the training curve

In [23]:
```
util.plot_training_history(history, figsize=figsize)
```

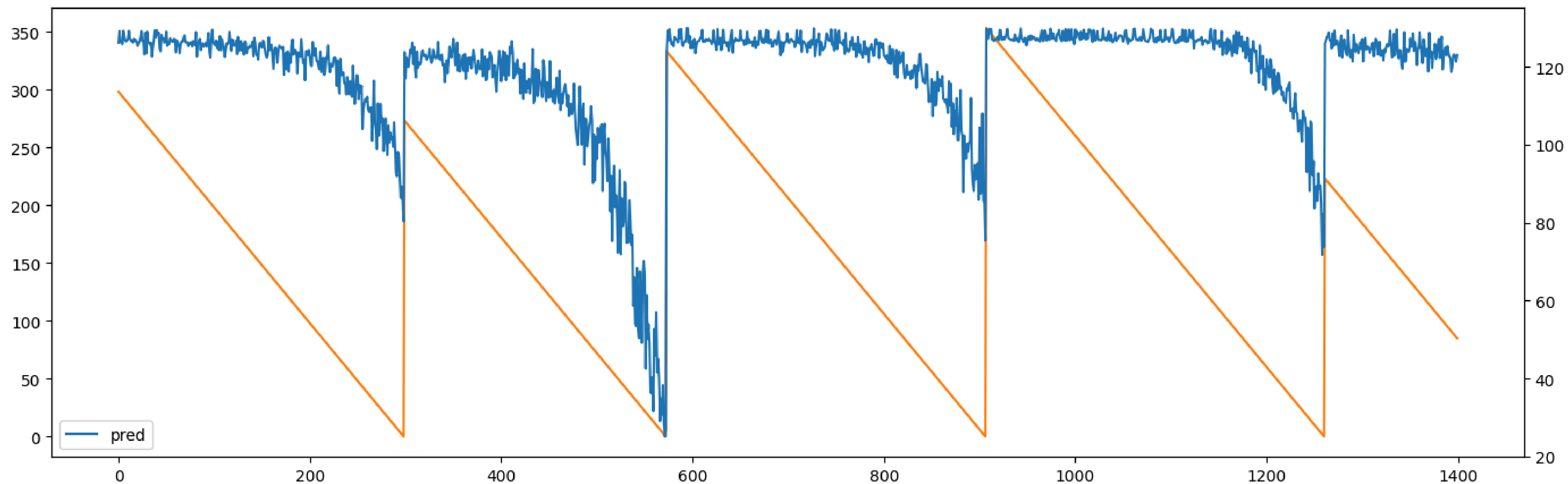



```
Final loss: 0.0075 (training)
```

Inspecting the Predictions

Let's have a look at the predictions on the test data

```
In [24]: ts_pred2 = nn2.predict(ts_s[dt_in], verbose=0).ravel() * maxrul
         util.plot_rul(ts_pred2[:stop], ts["rul"].iloc[:stop], same_scale=False, figsize=figsize)
```



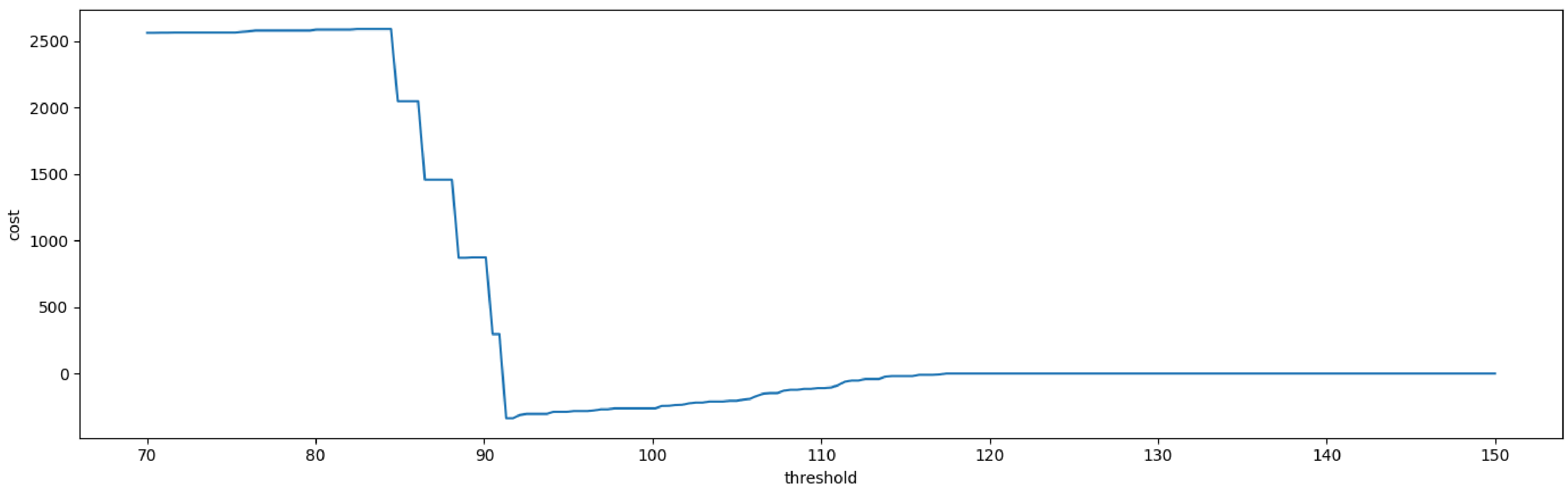
- The signal is much more stable
- The scale is still off, but we can fix that with a well chosen threshold

Threshold Optimization and Cost Evaluation

We can now optimize the threshold optimization (on the supervised data)

In [25]:
```
trs_pred2 = nn2.predict(trs_s[dt_in], verbose=0).ravel() * maxrul
cmodel = util.RULCostModel(maintenance_cost=maintenance_cost, safe_interval=safe_interval)
th_range2 = np.linspace(70, 150, 200)
trs_thr2 = util.optimize_threshold(trs_s['machine'].values, trs_pred2, th_range2, cmodel, p
print(f'Optimal threshold for the training set: {trs_thr2:.2f}')
```

```
Optimal threshold for the training set: 91.31
```



Threshold Optimization and Cost Evaluation

Finally, we can evaluate the SBR approach in terms of cost

```
In [26]: tru_pred2 = nn2.predict(tru_s[dt_in], verbose=0).ravel() * maxrul
         trs_c2, trs_f2, trs_sl2 = cmodel.cost(trs_s['machine'].values, trs_pred2, trs_thr2, return_r
         tru_c2, tru_f2, tru_sl2 = cmodel.cost(tru_s['machine'].values, tru_pred2, trs_thr2, return_r
         ts_c2, ts_f2, ts_sl2 = cmodel.cost(ts['machine'].values, ts_pred2, trs_thr2, return_margin=T
         print(f'Cost: {trs_c2/len(trs_mcn):.2f} (supervised), {tru_c2/len(tru_mcn):.2f} (unsupervise

         Cost: -48.14 (supervised), -77.90 (unsupervised), -70.34 (test)
```

```
In [27]: print(f'Avg. fails: {trs_f2/len(trs_mcn):.2f} (supervised), {tru_f2/len(tru_mcn):.2f} (unsu
         print(f'Avg. slack: {trs_sl2/len(trs_mcn):.2f} (supervised), {tru_sl2/len(tru_mcn):.2f} (uns

         Avg. fails: 0.00 (supervised), 0.04 (unsupervised), 0.04 (test)
         Avg. slack: 20.43 (supervised), 20.14 (unsupervised), 19.85 (test)
```

- The number of fails has decreased very significantly
- The slack is still contained

And we did this with just a handful of run-to-failure experiments