Knowledge Injection in ML

Data ⊂ Knowledge

ML methods excel at taking advantage of implicit knowledge from data

...But not all knowledge comes in the form of datasets!

- Rules of thumb, rough estimates
- Know correlations and causal factors
- Laws of physics
- ...

Knowledge from these sources is typically in explicit form

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Exploiting this information is critical in many practical applications

Many domains can boast decades of field knowledge and specialized methods

- Trying to replace those with pure data-driven approaches can be challenging
- ...And it can encounter a lot of resistance

Knowledge Injection in ML

It would be far preferable to account for all available information

...Including both explicit and implicit knowledge

- Implicit knowledge (data) is well-covered by ML methods
- ...But explicit knowledge used to be the domain of symbolic AI

How can we combined both?

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- Implicit knowledge (data) is well-covered by ML methods
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How can we combined both?

We could go for a "generative" approach

- We rely on symbolic knowledge for generating new examples
- ...Then we proceed as usual in ML

This how things are done in data augentation

...But is that really the only approach?

Knowledge as Constraints

Knowledge can be though of as a constraint

E.g. predictions should satisfy certain symbolic properties

- Predictions should lay within an interval
- Predictions should be robust w.r.t. variations
- ...

So, enforcing constraints is a way to "inject knowledge" in ML

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So, enforcing constraints is a way to "inject knowledge" in ML

The enforced constraints can be hard or soft:

- Hard constraints should always hold
- Soft constraints are expected to be violated to a some degree

Let's revisit one of our use cases to see an example of this idea

Scarce Labels in RUL Predictions

RUL estimation is the holy grail of predictive maintenance

RUL stands for "Remaining Useful Life"

- If you can predict when a machine will fail
- ...Then you can plan maintenance in the best possible way

However, ground truth for RUL is hard to come by

...Since it requires performing run-to-failure experiments

- These are time-consuming (machines are not designed to break)
- ...Costly (machines can be expensive)
- ...And difficult to perform (e.g. for complex machines)

Typically, only a few runs are available

Scarce Labels in RUL Predictions

On the other hand, data about normal operation is abundant

This may come from test runs, installed machines, etc.

- Those machines will not be in a critical state
- ...But they will still show sign of component wear

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In practice:, for normal operation

- We have access to the same observable as in run-to-failure experiments
- ...But we have no ground truth

Can we still take advantage of this data?

Data Loading and Preparation

We will rely again on the NASA C-MAPPS dataset

...Which contains simulated run-to-failure experiments for turbo-fan engines

In [5]:
```
data.head()
```

Out[5]:

	src	machine	cycle	p1	p2	p3	s1	s2	s3	s4	...	s13	s14	s15	s16	s
0	train_FD004	1	1	42.0049	0.8400	100.0	445.00	549.68	1343.43	1112.93	...	2387.99	8074.83	9.3335	0.02	3
1	train_FD004	1	2	20.0020	0.7002	100.0	491.19	606.07	1477.61	1237.50	...	2387.73	8046.13	9.1913	0.02	3
2	train_FD004	1	3	42.0038	0.8409	100.0	445.00	548.95	1343.12	1117.05	...	2387.97	8066.62	9.4007	0.02	3
3	train_FD004	1	4	42.0000	0.8400	100.0	445.00	548.70	1341.24	1118.03	...	2388.02	8076.05	9.3369	0.02	3
4	train_FD004	1	5	25.0063	0.6207	60.0	462.54	536.10	1255.23	1033.59	...	2028.08	7865.80	10.8366	0.02	3

5 rows × 28 columns

- There are four sub-datasets (column `src`)
- Columns **`p1–3`** represent control parameters
- Columns **`s1–21`** are sensor readings

Data Loading and Preparation

We will focus on the FD004 dataset (the hardest)

In [8]:
```
data_by_src = util.partition_by_field(data, field='src')
dt = data_by_src['train_FD004']
```

Then we separate two sets for training and one for testing

- The first trainign set will contain finished experiments (supervised)
- ...The second will contain data for still running machines (unsupervised)

In [11]:
```
trs_ratio = 0.03 # Supervised experiments / all experiments
tru_ratio = 0.6 # Unsupervised experiments / remaining experiments
trs, tmp = util.split_datasets_by_field(dt, field='machine', fraction=trs_ratio, seed=42)
tru, ts = util.split_datasets_by_field(tmp, field='machine', fraction=tru_ratio, seed=42)

trs_mcn, tru_mcn, ts_mcn = trs['machine'].unique(), tru['machine'].unique(), ts['machine'].u
print(f'Num. machine: {len(trs_mcn)} (supervised), {len(tru_mcn)} (unsupervised), {len(ts_mc
```

```
Num. machine: 7 (supervised), 145 (unsupervised), 97 (test)
```

Data Loading and Preparation

Then we standardize the input data

In [12]:
```
sscaler, nscaler = StandardScaler(), MinMaxScaler()
trs_s, tru_s, ts_s = trs.copy(), tru.copy(), ts.copy()
trs_s[dt_in] = sscaler.fit_transform(trs[dt_in])
tru_s[dt_in], ts_s[dt_in] = sscaler.transform(tru[dt_in]), sscaler.transform(ts[dt_in])
trs_s[['rul']] = nscaler.fit_transform(trs[['rul']])
tru_s[['rul']], ts_s[['rul']] = nscaler.transform(tru[['rul']]), nscaler.transform(ts[['rul

maxrul = nscaler.data_max_[0]
display(trs_s.head())
```

	src	machine	cycle	p1	p2	p3	s1	s2	s3	s4	...	s13	
1725	train_FD004	7	1	-1.688818	-1.924463	0.445653	1.811019	1.784571	1.676983	1.834240	...	0.445850	0.74
1726	train_FD004	7	2	-0.320795	0.385443	0.445653	0.754416	0.824865	0.604660	0.459056	...	0.445776	-0.1
1727	train_FD004	7	3	-1.688920	-1.925123	0.445653	1.811019	1.768351	1.668955	1.823341	...	0.445477	0.68
1728	train_FD004	7	4	1.184267	0.844852	0.445653	-1.021583	-0.742836	-0.576936	-0.541685	...	0.443309	0.07
1729	train_FD004	7	5	-1.688948	-1.925453	0.445653	1.811019	1.767810	1.726472	1.761244	...	0.445402	0.67

5 rows × 28 columns

Later, we will need the maximum RUL value on the training set

Removing RUL Values

Next, we simulate the lack of RUL values on the unsupervised data

- We copy the unsupervised data and remove number of their last entries
- Then, we replace RUL values with -1 (invalid)
- Finally, we merge supervised and unsupervised data in a single dataset

In [15]:
```
tru_s2 = util.rul_cutoff_and_removal(tru_s, cutoff_min=20, cutoff_max=60, seed=42)
tr_s2 = pd.concat((trs_s, tru_s2))
tr_s2.head()
```

Out[15]:

	src	machine	cycle	p1	p2	p3	s1	s2	s3	s4	...	s13	
1725	train_FD004	7	1	-1.688818	-1.924463	0.445653	1.811019	1.784571	1.676983	1.834240	...	0.445850	0.74
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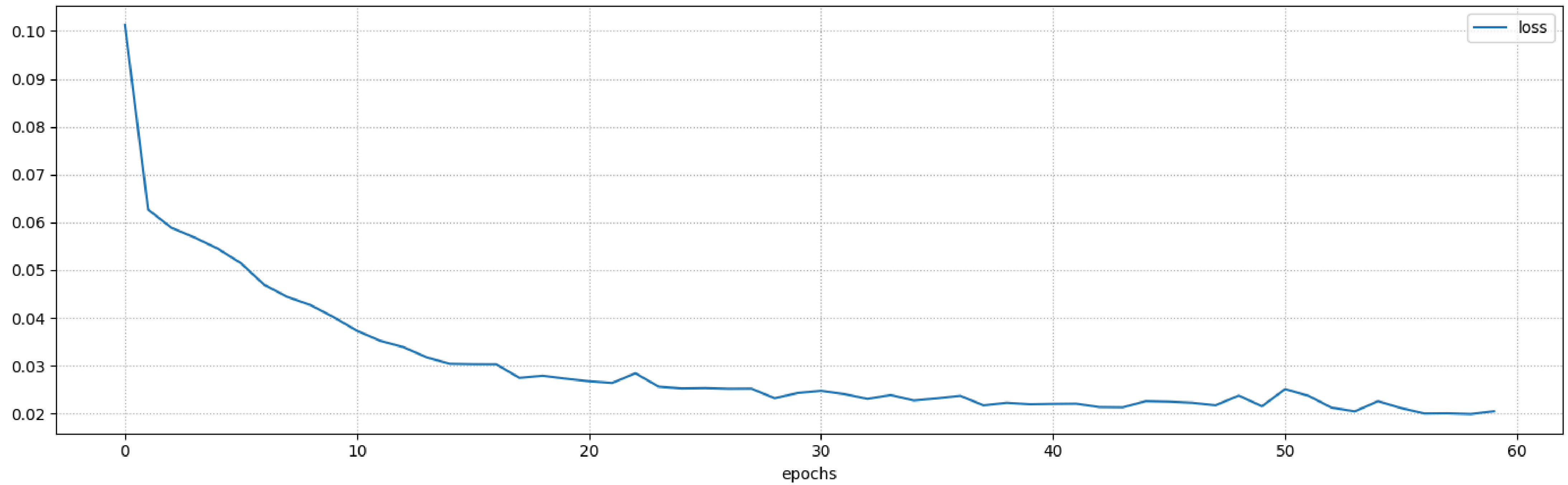
MLP with Scarce Labels

As a baseline, we will train a MLP model on the supervised data

We do not split a validation set, given we have scarce data

In [22]:
```
nn = util.build_nn_model(input_shape=(len(dt_in),), output_shape=(1,), hidden=[32, 32])
history = util.train_nn_model(nn, trs_s[dt_in], trs_s['rul'], loss='mse', validation_split=(
util.plot_training_history(history, figsize=figsize)
```

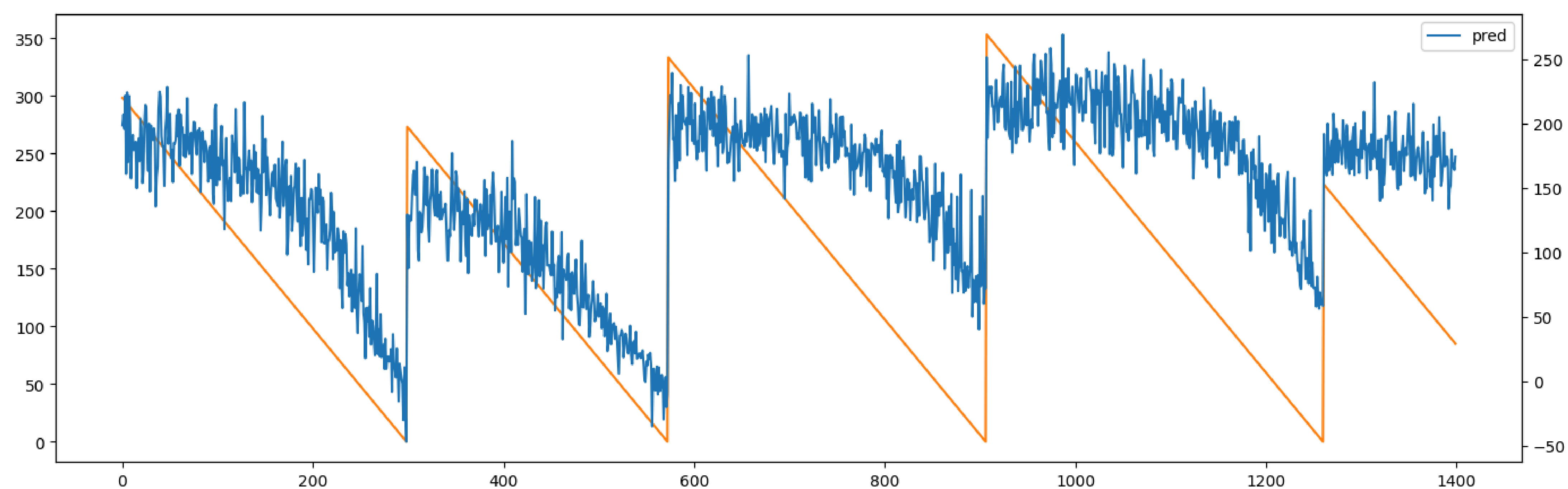



```
Final loss: 0.0205 (training)
```

Evaluation

Let's have a look at the predictions

In [25]:
```
stop = 1400
ts_pred = nn.predict(ts_s[dt_in], verbose=0).ravel() * maxrul
util.plot_rul(ts_pred[:stop], ts['rul'].iloc[:stop], same_scale=False, figsize=figsize)
```



- The predictions have a decreasing trend (which is good)
- ...But they are very noisy (which is bad)

Cost Model

The RUL estimator is meant to be used to define a policy

Namely, we stop operations when:

$$f(x; \theta) \leq \varepsilon$$

- Where $f(x; \theta)$ is the estimated output and ε is threshold

Calibrating ε is best done by relying on a cost model

- We assume that operating for a time step generates 1 unit of profit
- ...And that failing looses C units of profits w.r.t. performing maintenance
- We also assume we never stop a machine before a "safe" interval s

Both C and s are calibrated on data in our example:

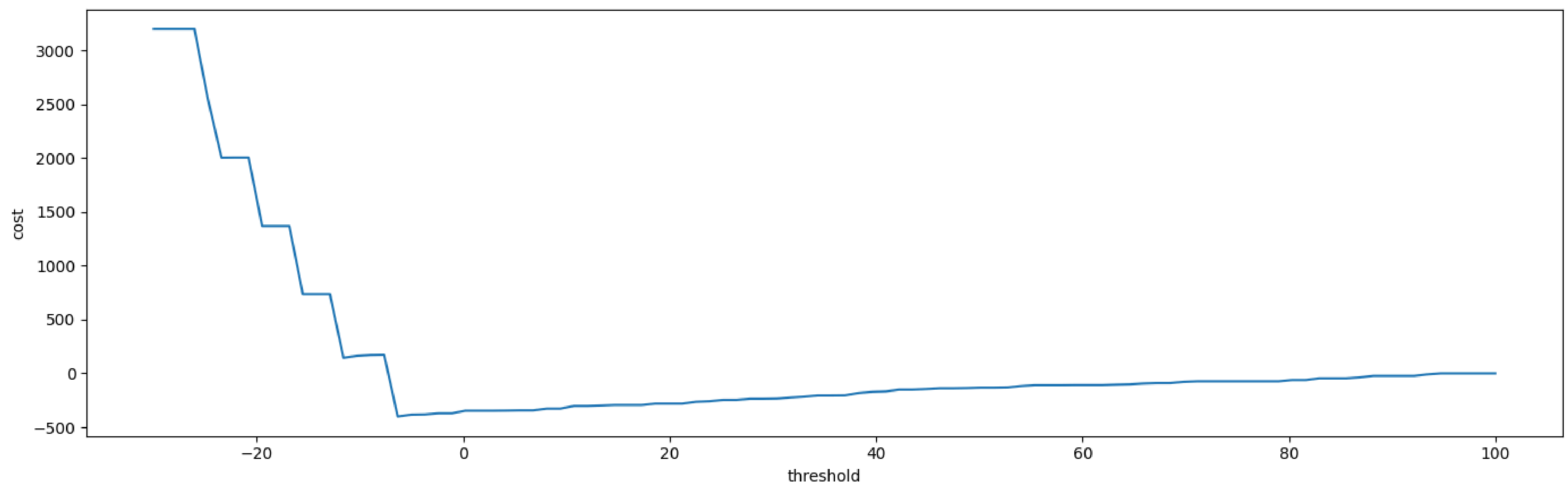
In [26]:
```
failtimes = dt.groupby('machine')['cycle'].max()
safe_interval, maintenance_cost = failtimes.min(), failtimes.max()
```

Cost Model and Threshold Optimization

We then proceed to choose ε to optimize the cost

In [29]:
```
trs_pred = nn.predict(trs_s[dt_in], verbose=0).ravel() * maxrul
cmodel = util.RULCostModel(maintenance_cost=maintenance_cost, safe_interval=safe_interval)
th_range = np.linspace(-30, 100, 100)
trs_thr = util.optimize_threshold(trs_s['machine'].values, trs_pred, th_range, cmodel, plot=
print(f'Optimal threshold for the training set: {trs_thr:.2f}')
```

```
Optimal threshold for the training set: -6.36
```



Cost Results

Let's now check the costs on all datasets

```
In [30]: trs_c, trs_f, trs_sl = cmodel.cost(trs_s['machine'].values, trs_pred, trs_thr, return_margi
         ts_c, ts_f, ts_sl = cmodel.cost(ts['machine'].values, ts_pred, trs_thr, return_margin=True)
         print(f'Avg. cost: {trs_c/len(trs_mcn):.2f} (supervised), {ts_c/len(ts_mcn):.2f} (test)')

         Avg. cost: -57.29 (supervised), 199.53 (test)
```

- The cost for the training set is good (negative)
- ...But that is not the case for the training set

```
In [31]: trs_nm, tru_nm, ts_nm = len(trs_mcn), len(tru_mcn), len(ts_mcn)
         print(f'Avg. fails: {trs_f/trs_nm:.2f} (supervised), {ts_f/ts_nm:.2f} (test)')
         print(f'Avg. slack: {trs_sl/trs_nm:.2f} (supervised), {ts_sl/len(ts_mcn):.2f} (test)')

         Avg. fails: 0.00 (supervised), 0.44 (test)
         Avg. slack: 11.29 (supervised), 7.47 (test)
```

- In particular, there is a very high failure rate on unseen data

Ok, now we are supposed to inject knowledge in ML

So, what do we know?

From Domain Knowledge...

We know that the RUL decreases at a fixed rate

- After 1 time step, the RUL will have decreased by 1 unit
- After 2 time steps, the RUL will have decreased by 2 units and so on

In general, let's consider pairs of examples (x_i, y_i) and (x_j, y_j)

Then we know that:

$$y_i - y_j = j - i \qquad \forall i, j = 1..m \ \text{ with: } c_i = c_j$$

- c_i, c_j are the machine for the two samples
- The left-most terms is the difference between the RULs
- $j - i$ is the difference between the sequential indexes of the two samples
- ...Which by construction should be equal to the RUL difference

...To Constraints

We can use the observation to define a constraint on the model output

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

- It's best to treat this as a soft constraint
- ...Since the predictions are subject to errors

Hence, one way to account for domain knowledge

...Is to move from training to constrained training:

$$\operatorname*{argmin}_{\theta} \ L(y, f(x; \theta))$$

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

But how can we deal with constraints at training time?