

```
In [1]: # =====
# Notebook setup
# =====

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(14, 4)

from util import util
import os
import numpy as np
from tensorflow.keras import callbacks
import warnings
import pandas as pd
warnings.simplefilter("ignore")

# Load data
data_folder = os.path.join '..', 'data'
data = util.load_cmapss_data(data_folder)

# Focus on a subset of the data
data_by_src = util.split_by_field(data, field='src')
dt = data_by_src['train_FD004']

# Split training and test machines
tr_ratio = 0.75
np.random.seed(42)
machines = dt.machine.unique()
np.random.shuffle(machines)

sep = int(tr_ratio * len(machines))
tr_mcn = machines[:sep]
ts_mcn = machines[sep:]

tr, ts = util.partition_by_machine(dt, tr_mcn)
```

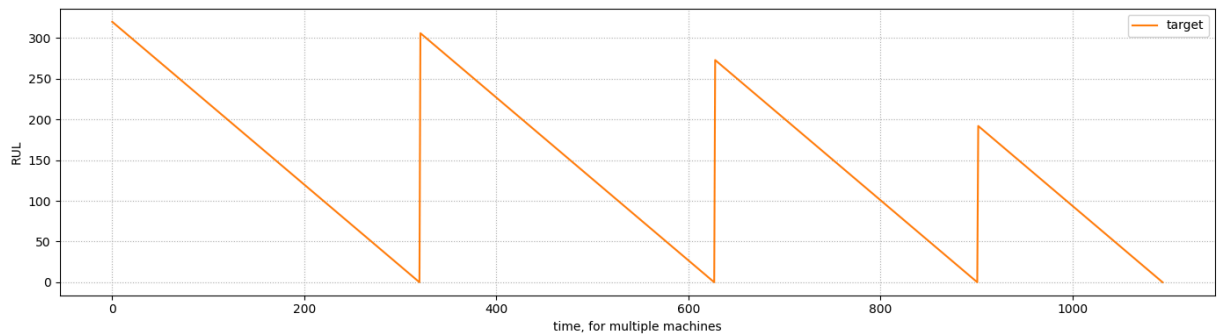
Probabilistic RUL Estimation

RUL Estimation, Again

Let's consider again our RUL-based policy use case

We first tackled that by using a regressor to estimate this kind of function:

```
In [2]: stop = 1095
util.plot_rul(target=tr['rul'][:stop], figsize=figsize, xlabel='time, for mu
```



...Then we tuned a threshold to define a simple maintenance policy

It worked well enough, but not perfectly

What did we fail to achieve?

Limitations

The RUL estimation was of very poor quality

- Our model was good enough for defining a policy
- ...But not usable to provide a real-time RUL estimate

Why did we fail? Here are a few potential culprits

- Are we sure our target is correct? What if the defect arises late?
- Our target looks deterministic: are we accounting for uncertainty?
- Are we providing all the necessary input?

It's not easy to tell where the problem lays

...Because *we didn't think enough before solving!*

Back to the Drawing Board

Here's what the correct approach should be:

- We start by defining a *probabilistic model*
- We use *ML to approximate* key components of such model
- We use the model + the approximators to make *probabilistic predictions*

This approach can be significantly more challenging

...But it comes with several benefits:

- You have both predictions *and confidence*
- You exploit a degree of *domain knowledge*
- You get a *more interpretable* model

- If you choose to *ignore* an element (e.g. because it is too difficult to model)
- ...At least you *know* that you have done so

A Survival Analysis Model

We are interested in the "survival time" of an entity

We can start by modeling that as a single random variable T with unknown distribution

$$T \sim P(T) \quad (\text{draft 1})$$

- T (with \mathbb{R}^+ as support) represents the survival time

To be specific, we want T to be *remaining* survival time

...With respect to time t when we perform the estimation. Formally:

$$T \sim P(T \mid t) \quad (\text{draft 2})$$

- Now the distribution is conditioned on t (which we can access)

A Survival Analysis Model

Survival depends on additional factors

E.g. on the lifestyle of a person, or on how industrial equipment is used

- We can model these factors as additional random variables
- We can distinguish between behavior in the past $X_{\leq t}$ and the future $X_{>t}$

Formally, we have:

$$T \sim P(T \mid X_{\leq t}, t, X_{>t}) \quad (\text{draft 3})$$

For now we focus on *capturing the elements that affect the estimate*

- We not not care (yet) about the fact that we can access them
- The idea is to focus on *one problem at a time*

A Survival Analysis Model

...But of course whether a quantity can be accessed or not does matter

In particular, *future behavior cannot be accessed* at estimation time

- Intuitively, future behavior affects the estimate as *noise*
- Formally, we can *average out* its effect

This operation is called **marginalization** and leads to:

$$T \sim \mathbb{E}_{X_{>t}} [P(T \mid X_{\leq t}, t, X_{>t})] \quad (\text{draft 4})$$

This is a good model for the distribution of the variable we wish to estimate

- The "sawtooth like" target that we used earlier for RUL regression
-Corresponds to *samples from* $P(T \mid X_{\leq t}, t, X_{>t})$

In other words, we are saying our target was correct!

So, why did we get strange results in the RUL lecture?

Looking Back to Our Model

In the RUL lecture we trained a regressor

...With the current parameters/sensors as input and an MSE loss

- Meaning the *our estimator* is making implicitly use of this model:

$$T \sim \mathcal{N}(\mu(X_t), \sigma)$$

- \mathcal{N} denotes the Normal distribution, $\mu(\cdot)$ represents our old regressor

Now, compare it with our "ideal" probabilistic model:

$$T \sim \mathbb{E}_{X_{>t}} [P(T \mid X_{\leq t}, t, X_{>t})]$$

- Let's try to spot together any major difference

Implicit Assumptions

We made several implicit assumptions:

$$T \sim \mathcal{N}(\mu(X_t), \sigma) \quad \text{vs} \quad T \sim \mathbb{E}_{X_{>t}} [P(T \mid X_{\leq t}, t, X_{>t})]$$

We considered a *single* $X_{\{t\}}$, rather than $X_{\{\leq t\}}$

- Actually, we tried that by using sequence input (it helped, but not much)

We *disregarded time* as an input

- ...And thankfully this is easy to fix

We assumed a *Normal distribution* with *fixed variance*

- It's unclear how to relax the normality assumption
- ...But we know we can fix the variance this using a neuro-probabilistic model!

About Time

Let's fix one mistake by adding *time as an input*

In our dataset, time corresponds to the "cycle" field

```
In [3]: # Identify parameter and sensor columns
dt_in = list(data.columns[3:-1])

# Standardize parameters and sensors
trmean = tr[dt_in].mean()
trstd = tr[dt_in].std().replace(to_replace=0, value=1) # handle static fields
ts_s = ts.copy()
ts_s[dt_in] = (ts_s[dt_in] - trmean) / trstd
tr_s = tr.copy()
tr_s[dt_in] = (tr_s[dt_in] - trmean) / trstd

# Normalize RUL and time (cycle)
trmaxrul = tr['rul'].max()
ts_s['cycle'] = ts_s['cycle'] / trmaxrul
tr_s['cycle'] = tr_s['cycle'] / trmaxrul
ts_s['rul'] = ts['rul'] / trmaxrul
tr_s['rul'] = tr['rul'] / trmaxrul

# Add time (cycle) to the input columns
dt_in = dt_in + ['cycle']
```

Estimated Variance

Then we can make our ML model capable of *estimating variance*

In particular, we can use a neuro-probabilistic ML model

- The underlying probabilistic model is:

$$T \sim \mathcal{N}(\mu(X_t, t), \sigma(X_t, t))$$

In practice:

- We use conventional ML model (a network) to estimate μ and σ
- ...Then we feed both parameters to a `DistributionLambda` layer

Our model will be able to learn how σ depends on the input

- This will be more challenging, but also more flexible
- ...And it will provide us confidence intervals

Building a Neuro-Probabilistic Model

Code to build the model can found in the `util` module

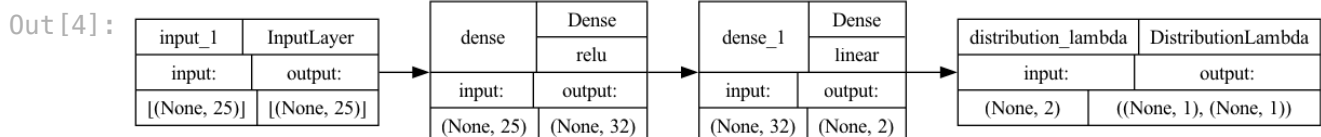
```
def build_nn_normal_model(input_shape, hidden, stddev_guess=1):
    model_in = keras.Input(shape=input_shape, dtype='float32')
    x = model_in
    for h in hidden:
        x = layers.Dense(h, activation='relu')(x)
    mu_logsigma = layers.Dense(2, activation='linear')(x)
    lf = lambda t: tfp.distributions.Normal(loc=t[:, :1],
scale=stddev_guess*tf.math.exp(t[:, 1:]))
    model_out = tfp.layers.DistributionLambda(lf)(mu_logsigma)
    model = keras.Model(model_in, model_out)
    return model
```

- Note the way the input tensor `t` is split in the `lambda` function
- That is needed to obtain the correct tensor shapes (columns)

Building a Neuro-Probabilistic Model

Let's build a simple neuro-probabilistic model

```
In [4]: tr_rul_std = tr_s['rul'].std()
nnp = util.build_nn_normal_model(input_shape=(len(dt_in), ), hidden=[32], st
util.plot_nn_model(nnp)
```

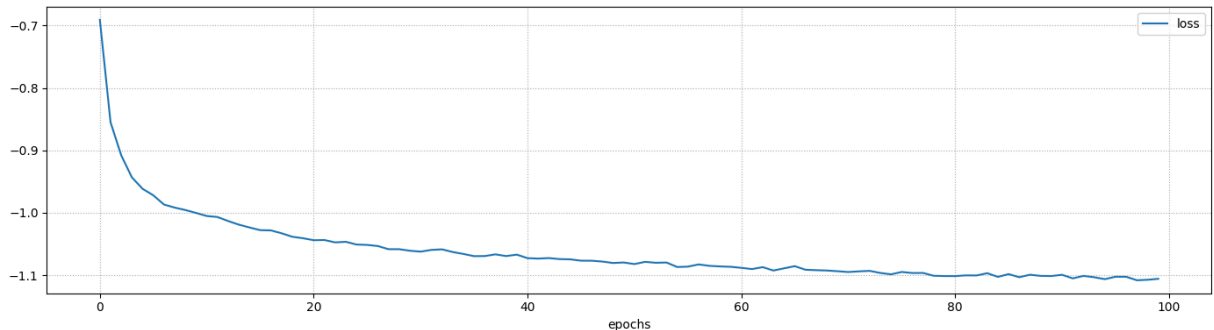


- There is a single hidden layer
- As a guess for σ , we provide the standard deviations over the training set

Training the Neuro-Probabilistic Model

We can train the model as in our previous example

```
In [5]: negloglikelihood = lambda y_true, dist: -dist.log_prob(y_true)
nnp = util.build_nn_normal_model(input_shape=(len(dt_in), ), hidden=[32], st
history = util.train_nn_model(nnp, tr_s[dt_in], tr_s['rul'], loss=negloglike
util.plot_training_history(history, figsize=figsize)
```



Final loss: -1.1057 (training)

Evaluation

We care about the estimated distributions (not about sampling)

...Therefore we call the model rather than using the `predict` method

```
In [6]: nn_pred_ts = nnp(tr_s[dt_in].values)
nn_pred_ts
```

```
Out[6]: <tfp.distributions._TensorCoercible 'tensor_coercible' batch_shape=[45385,
1] event_shape=[] dtype=float32>
```

From the distribution objects we can obtain means and standard deviations

```
In [7]: np_pred_ts_mean = nn_pred_ts.mean().numpy().ravel() * trmaxrul
np_pred_ts_std = nn_pred_ts.stddev().numpy().ravel() * trmaxrul
```

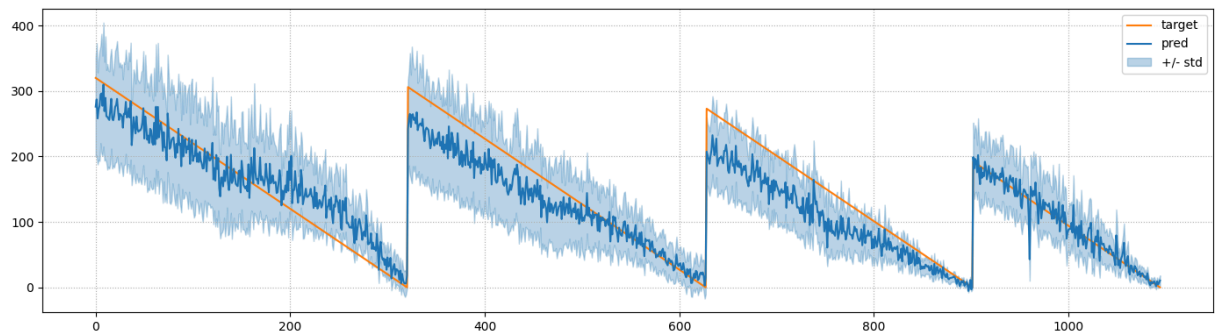
- For sake of keeping it short, we will just inspect the predictions
- ...Rather than making a full evaluation

That said, we could do it (and the results would be similar to the old ones)

Evaluation

Let's inspect the predictions on a portion of the test set

```
In [8]: stop = 1095
util.plot_rul(target=tr_s['rul'].iloc[:stop]*trmaxrul, pred=np_pred_ts_mean,
stddev=np_pred_ts_std[:stop], figsize=figsize)
```



- The initial plateaus in the predictions have disappeared
- ...And the true RUL is typically within 1σ from the predicted mean

Neuro-probabilistic Models vs Sample Weights

The approach we have seen works already very well

- We get a predicted mean (as usual)
- ...But also an input-dependent standard deviation

But can't we do the same with sample weights?

Yes, but it's not the same

- Sample weights allow use to control the standard deviation with an MSE loss
- ...But we need to *pre-compute them* using another model (or assumption)

They cannot be learned in an end-to-end fashion!