Same Stop Chance

Same Stop Chance

Let's re-examine our RUL-regressor

- We have observed that poor accuracy for high RULs is not much of an issue
- ...But why is that the case?

We are going to use the RUL in a condition in the form

$$f(x, \lambda) < \theta$$

- Therefore, what really matters is not the RUL value itself
- ...But the probability that the condition is satisfied or violated

This depends entirely on the (lower) quantiles of the distribution of $f(x, \lambda)$

- ...And assumes a probabilistic interpretation for $f(x, \lambda)$
- But is our predictor probabilistic?

Same Stop Chance

Yes, of course! We have an MSE loss, therefore we know that:

$$\text{argmin}_\lambda \sum_{i=1}^{n} (f(\hat{x}_i, \lambda) - \hat{y}_i)^2 = \text{argmax}_\lambda \prod_{i=1}^{n} \phi(f(\hat{x}_i, \lambda) - \hat{y}_i)$$

- I.e. we are implicitly training a regressor with Normally distributed output
- ...Having mean $f(\hat{x}_i, \lambda)$ and uniform variance (unary in this case)

As a consequence, we put the same effort in approximating all examples

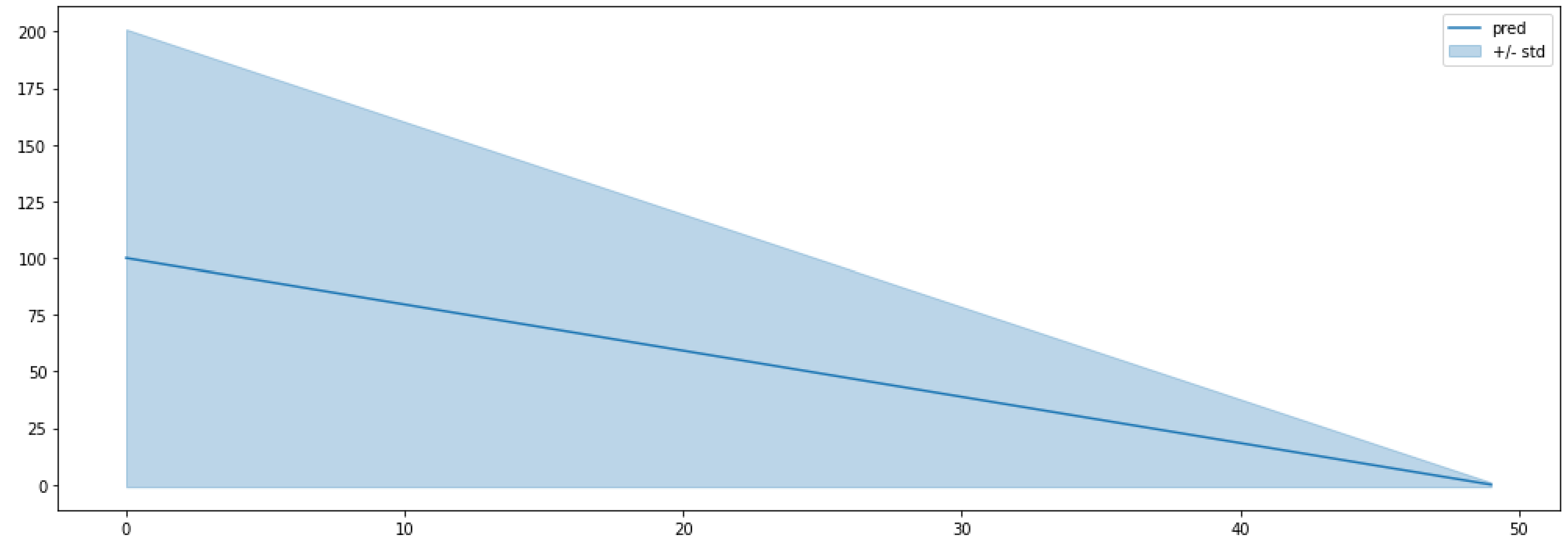
- But when the RUL is larger, even with a poorer approximation
- ...There will be still a high chance that our threshold condition is false

We do not want to put the same effort in all example

Same Stop Chance

For example, assuming perfect predictions and $\sigma_i = 1 + \hat{y}_i$

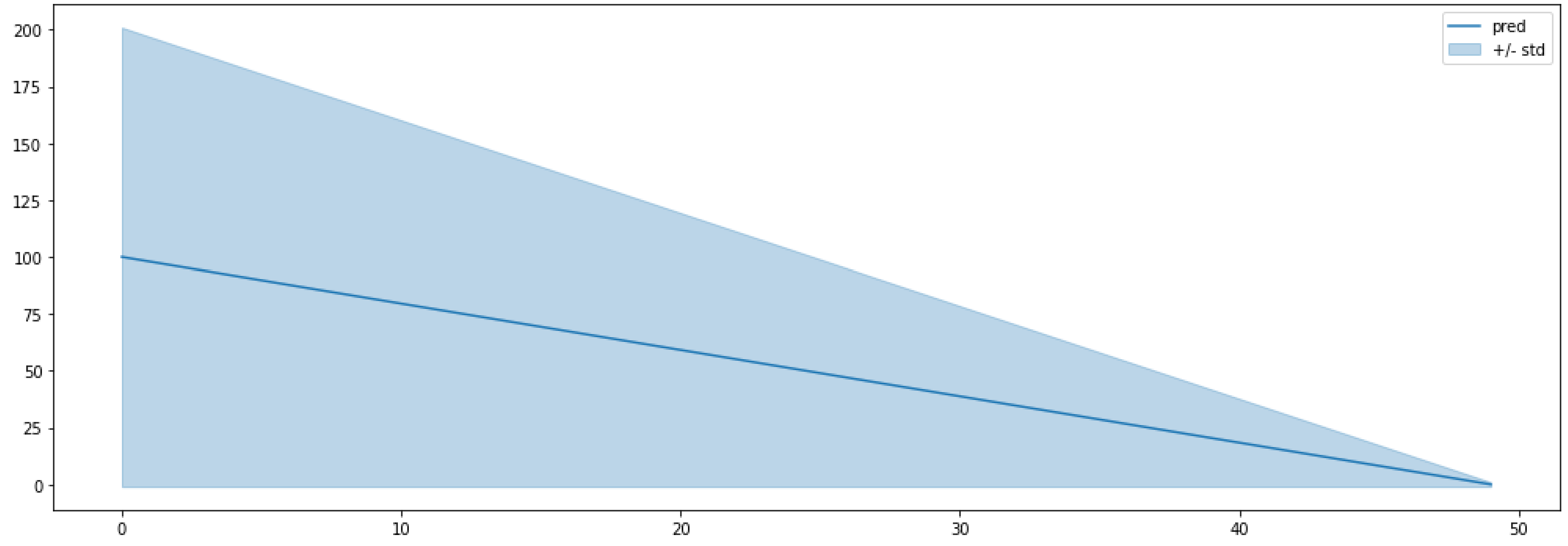
```
In [3]: t = np.linspace(0, 100)
        y, sigma = t[::-1], 1+t[::-1]
        cmapss.plot_rul(pred=y, stddev=sigma, figsize=figsize)
```



Same Stop Chance

For example, assuming perfect predictions and $\sigma_i = 1 + \hat{y}_i$

```
In [3]: t = np.linspace(0, 100)
        y, sigma = t[::-1], 1+t[::-1]
        cmapss.plot_rul(pred=y, stddev=sigma, figsize=figsize)
```



- The lower quantiles are constant!

Same Stop Chance

So, we can train for this behavior by minimizing:

$$\operatorname{argmax}_{\lambda} \prod_{i=1}^{n} \frac{1}{\sigma_i} \phi\left(\frac{f(\hat{x}_i, \lambda) - \hat{y}_i}{\sigma_i}\right)$$

And we will choose $\sigma_i = 1 + \hat{y}_i$. By algebraic manipulation we get:

$$\operatorname{argmin}_{\lambda} - \sum_{i=1}^{n} \log \frac{1}{\sigma_i} - \sum_{i=1}^{n} \log \phi\left(\frac{f(\hat{x}_i, \lambda) - \hat{y}_i}{\sigma_i}\right) =$$

$$\operatorname{argmin}_{\lambda} - \sum_{i=1}^{n} \log \frac{1}{\sigma_i} - \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}} - \frac{1}{\sigma_i^2}\left(f(\hat{x}_i, \lambda) - \hat{y}_i\right)^2 =$$

$$\operatorname{argmin}_{\lambda} \sum_{i=1}^{n} \frac{1}{\sigma_i^2}\left(f(\hat{x}_i, \lambda) - \hat{y}_i\right)^2$$

Same Stop Chance

We have just established that:

$$\text{argmax}_\lambda \prod_{i=1}^{n} \frac{1}{\sigma_i} \phi\left(\frac{f(\hat{x}_i, \lambda) - \hat{y}_i}{\sigma_i}\right) = \text{argmin}_\lambda \sum_{i=1}^{n} \frac{1}{\sigma_i^2} (f(\hat{x}_i, \lambda) - \hat{y}_i)^2$$

- I.e. training a normally distributed predictor with per-sample variance σ_i^2
- Is equivalent to MSE training with sample weights $w_i = 1/\sigma_i^2$

This is suprising simple!

So, let's define the sample weights

```
In [4]: sample_weight = 1/((1+tr_s['rul'].values)**2)
```

- We use the rule $\sigma_i = 1 + \hat{y}_i$ to have identical stop chances

Training

Let's train our MLP architecture with this modification

```
In [5]: nn1 = build_regressor(hidden=[32, 32])
        nn1.compile(optimizer='Adam', loss='mse')
        history1 = nn1.fit(tr_s[dt_in], tr_s['rul'], validation_split=0.2,
                         sample_weight=sample_weight,
                         callbacks=cb, batch_size=32, epochs=20, verbose=1)
```

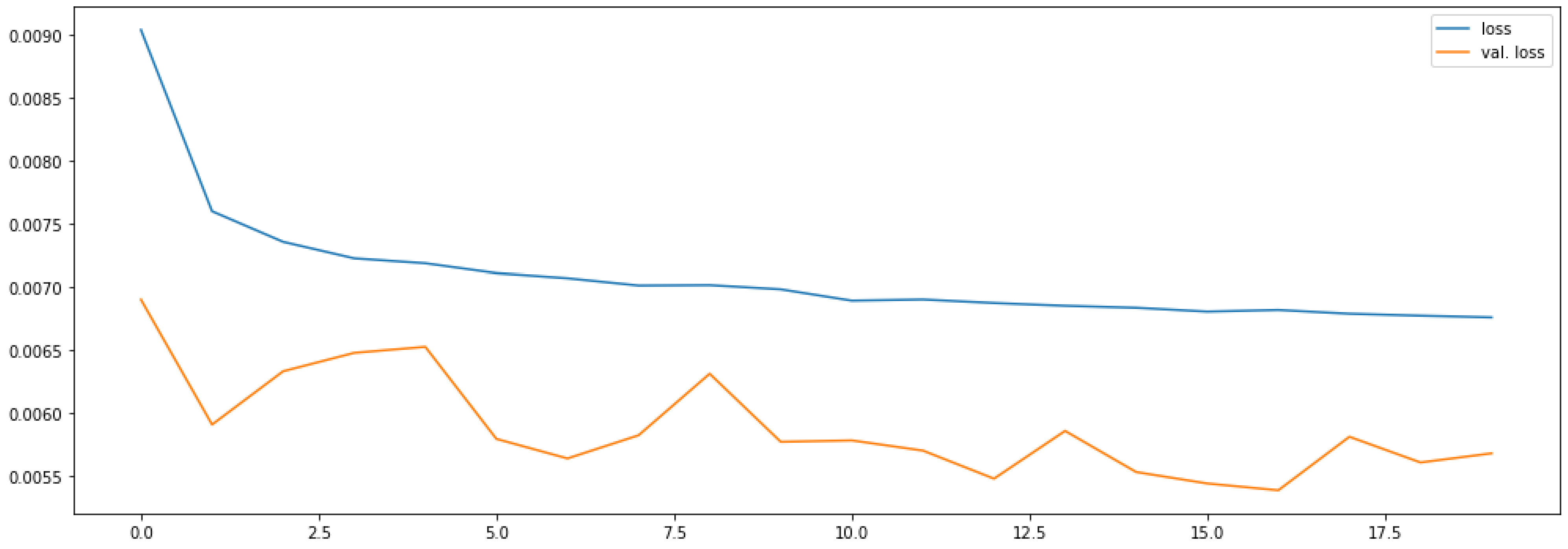
```
Epoch 1/20
1135/1135 [==============================] - 2s 1ms/step - loss: 0.0090 - val_loss: 0.0069
Epoch 2/20
1135/1135 [==============================] - 1s 531us/step - loss: 0.0076 - val_loss: 0.0059
Epoch 3/20
1135/1135 [==============================] - 1s 532us/step - loss: 0.0074 - val_loss: 0.0063
Epoch 4/20
1135/1135 [==============================] - 1s 536us/step - loss: 0.0072 - val_loss: 0.0065
Epoch 5/20
1135/1135 [==============================] - 1s 536us/step - loss: 0.0072 - val_loss: 0.0065
Epoch 6/20
1135/1135 [==============================] - 1s 624us/step - loss: 0.0071 - val_loss: 0.0058
Epoch 7/20
1135/1135 [==============================] - 1s 627us/step - loss: 0.0071 - val_loss: 0.0056
Epoch 8/20
1135/1135 [==============================] - 1s 626us/step - loss: 0.0070 - val_loss: 0.0058
Epoch 9/20
1135/1135 [==============================] - 1s 634us/step - loss: 0.0070 - val_loss: 0.0063
Epoch 10/20
1135/1135 [==============================] - 1s 628us/step - loss: 0.0070 - val_loss: 0.0058
Epoch 11/20
```

Training

Let's check the loss evolution over time and its final value

In [6]:
```
cmapss.plot_training_history(history1, figsize=figsize)
tr1, vl1 = history1.history["loss"][-1], np.min(history1.history["val_loss"])
print(f'Loss: {tr1:.4f} (training, final), {vl1:.4f} (validation, best)')
```

```
Loss: 0.0068 (training, final), 0.0054 (validation, best)
```

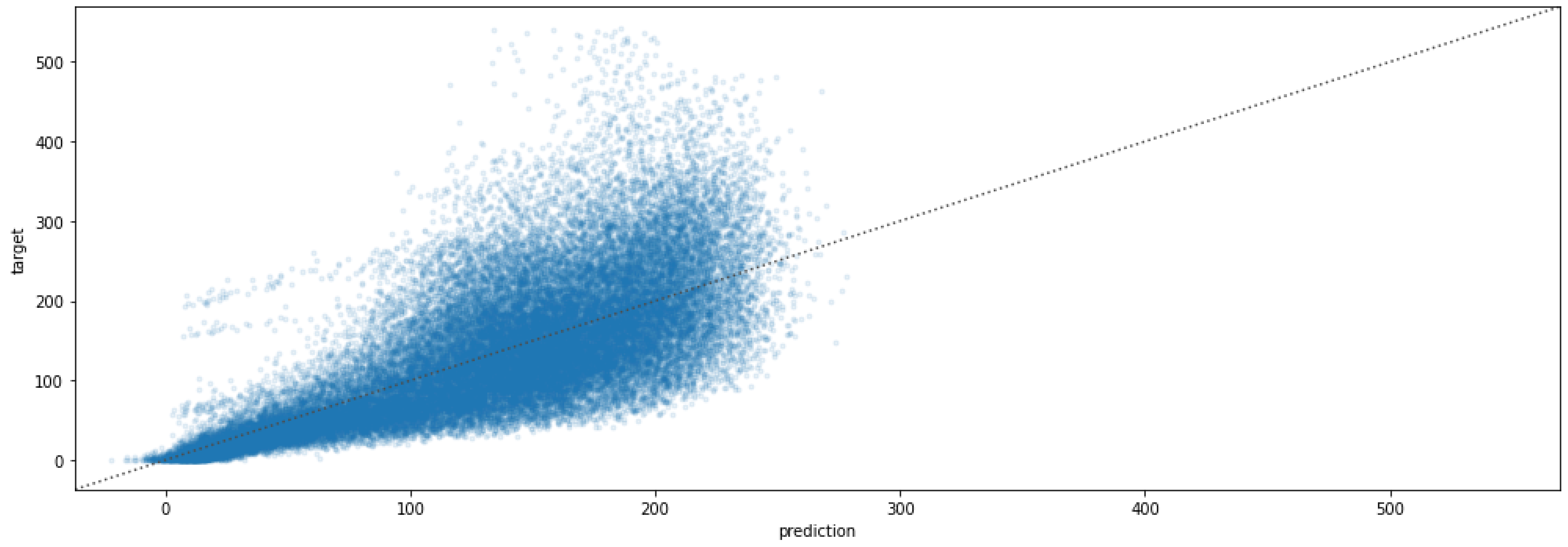


Predictions

The predictions should be (slightly) worse than before in terms of accuracy

```
In [7]: tr_pred1 = nn1.predict(tr_s[dt_in]).ravel() * trmaxrul
        cmapss.plot_pred_scatter(tr_pred1, tr['rul'], figsize=figsize)
        print(f'R2 score: {r2_score(tr["rul"], tr_pred1)}')
```

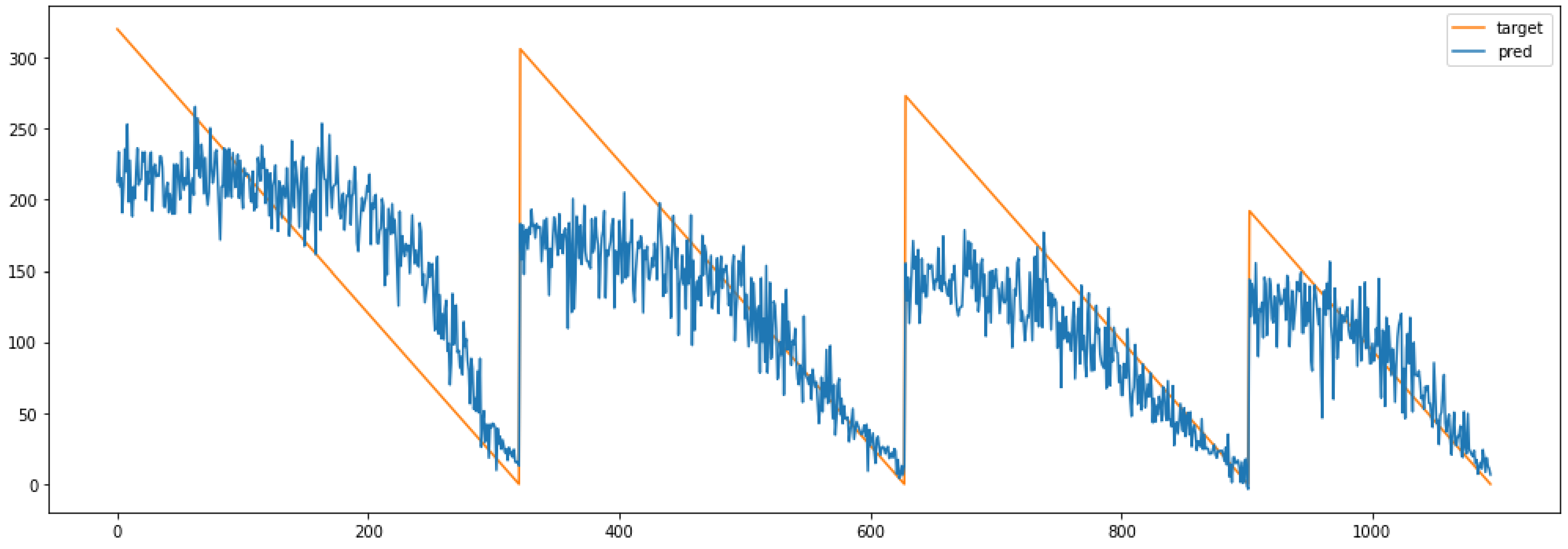
```
R2 score: 0.5389392096077179
```



Predictions

Let's have a look at the predictions over time (on the training set)

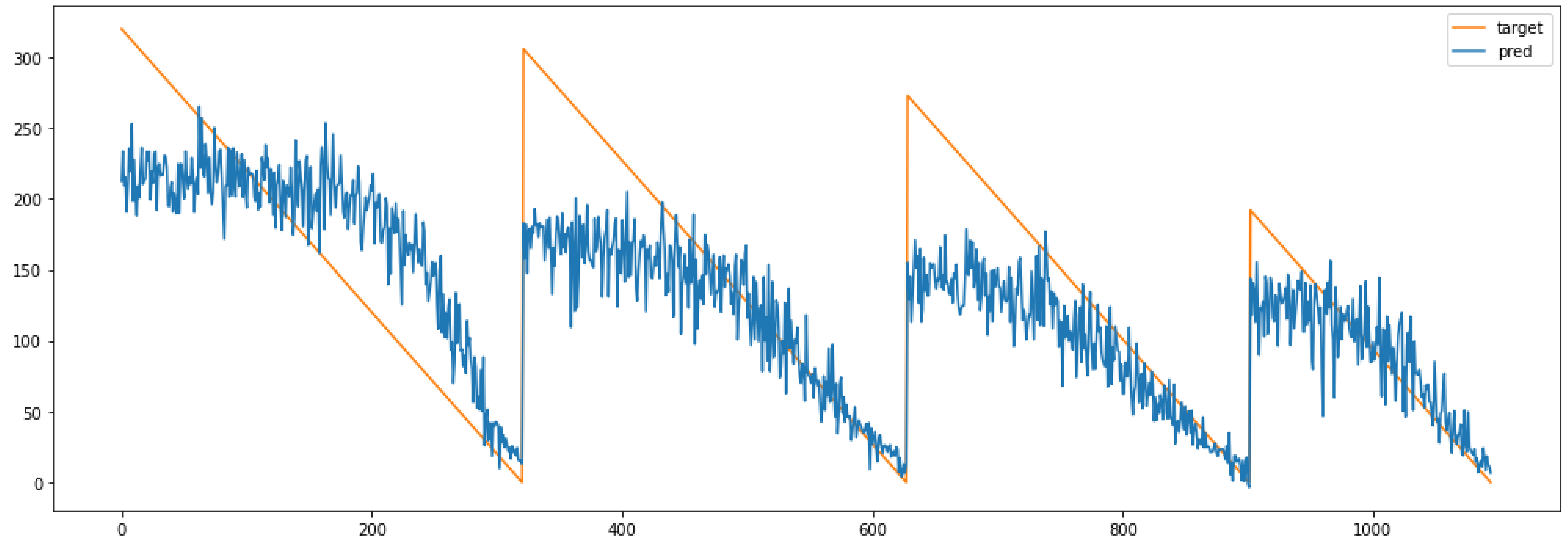
```
In [10]: stop = 1095
         cmapss.plot_rul(tr_pred1[:stop], tr['rul'][:stop], figsize=figsize)
```



Predictions

Let's have a look at the predictions over time (on the training set)

```
In [10]: stop = 1095
         cmapss.plot_rul(tr_pred1[:stop], tr['rul'][:stop], figsize=figsize)
```



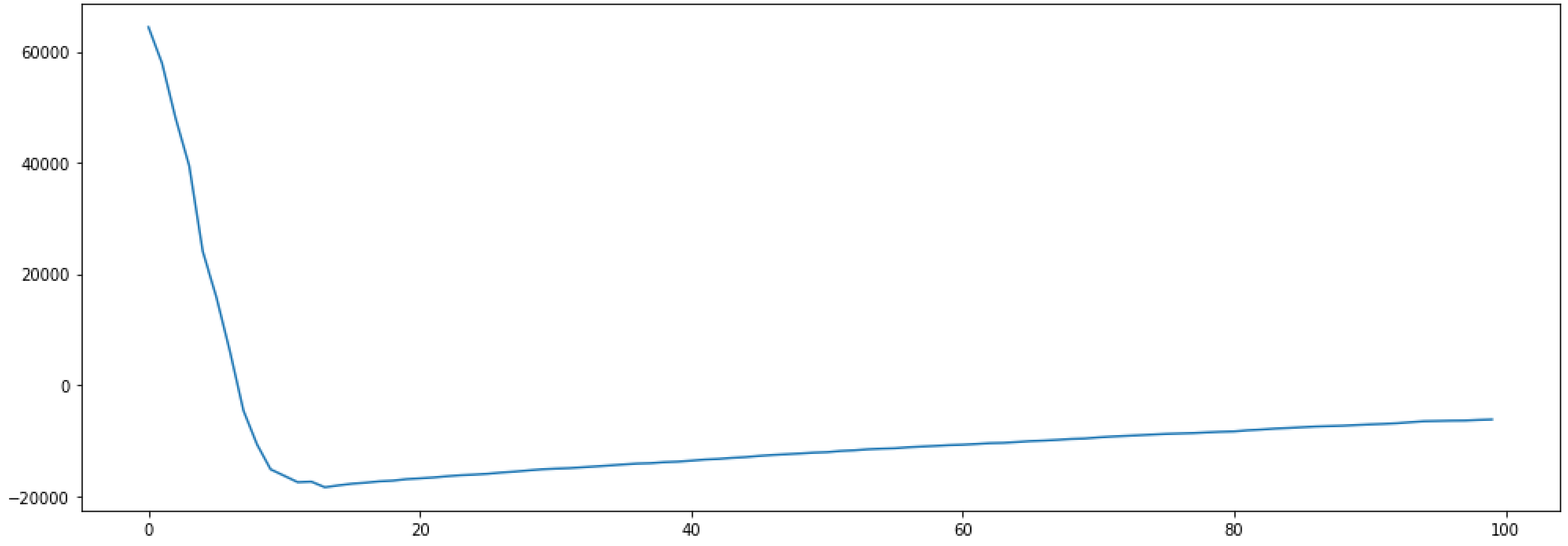
- Notice how they are noisier in the high-RUL section

Threshold Optimization

Now we need to optimize the threshold as usual

```
In [11]: th_range = np.arange(0, 100)
         tr_thr1 = cmapss.opt_threshold_and_plot(tr['machine'].values, tr_pred1, th_range, cmodel, figsiz
         print(f'Optimal threshold for the training set: {tr_thr1}')
```

```
Optimal threshold for the training set: 13
```



Evaluation

Let's see how it fares in terms of cost

```
In [12]: ts_pred1 = nn1.predict(ts_s[dt_in]).ravel() * trmaxrul
         tr_c1, tr_f1, tr_s1 = cmodel.cost(tr['machine'].values, tr_pred1, tr_thr1, return_margin=True)
         ts_c1, ts_f1, ts_s1 = cmodel.cost(ts['machine'].values, ts_pred1, tr_thr1, return_margin=True)
         print(f'Cost: {tr_c1} (training), {ts_c1} (test)')
         print(f'Avg. fails: {tr_f1/len(tr_mcn)} (training), {ts_f1/len(ts_mcn)} (test)')
         print(f'Avg. slack: {tr_s1/len(tr_mcn):.2f} (training), {ts_s1/len(ts_mcn):.2f} (test)')

         Cost: -18425 (training), -6819 (test)
         Avg. fails: 0.0 (training), 0.0 (test)
         Avg. slack: 17.12 (training), 15.57 (test)
```

- The results should be on par than the MLP
    - ...Depending on training randomness
- The number of fails may be slightly larger
    - Forcing equal stop chances tends to lead to slightly more risky models

We did not gain much, but this is a useful trick to know!

Negative-Binomial Model

Negative Binomial Distribution

The negative binomial distribution

- ...Models the probability to have a number "failures"
- ...Before a given number of "successes" is achieved
- ...Assuming a constant success probability p

It's probability mass function is given by:

$$f(k, r, p) = \binom{k + r - 1}{r - 1} (1 - p)^k p^r$$

- k is the number of failures
- r is the number of successes
- The binomial coefficient yields the number of combinations of $r - 1$ successes
- ...Over $k + r - 1$ trials

RUL and NB Distribution

There is a connection between the NB distribution and our process

We can view a "success" as the end of the run, a "failure" as an operating step

- So, if we assume a constant $\boldsymbol{p}$ for all future steps...
- ...The RUL follows a negative binomial distribution, i.e.:

$$y \sim NB(1, p)$$

- The first distribution parameter is $\boldsymbol{r}$
- We have $\boldsymbol{r} = 1$ since after a single "success" the run is over

We can use a neural model to estimate p based on the observed data, i.e.:

$$y \sim NB(1, p(\hat{x}_i, \lambda))$$

- By doing so, we effectively obtain a hybrid neural-probabilistic model

Training a Neural-Probabilistic Model

We can train our hybrid model for maximum likelihood

Or, better, for minimum negative log likelihood:

$$\text{argmin}_\lambda - \sum_{i=1}^{n} \log f(\hat{y}_i, 1, p(\hat{x}_i, \lambda))$$

- Where f is the probability mass function for the NB distribution
- $\hat{y}_i$ is the RUL value (i.e. the number of "failures"...
- ...1 is the number of successes (end of the run)
- ...$p(\hat{x}_i, \lambda)$ is the "success" probability estimated by the neural model

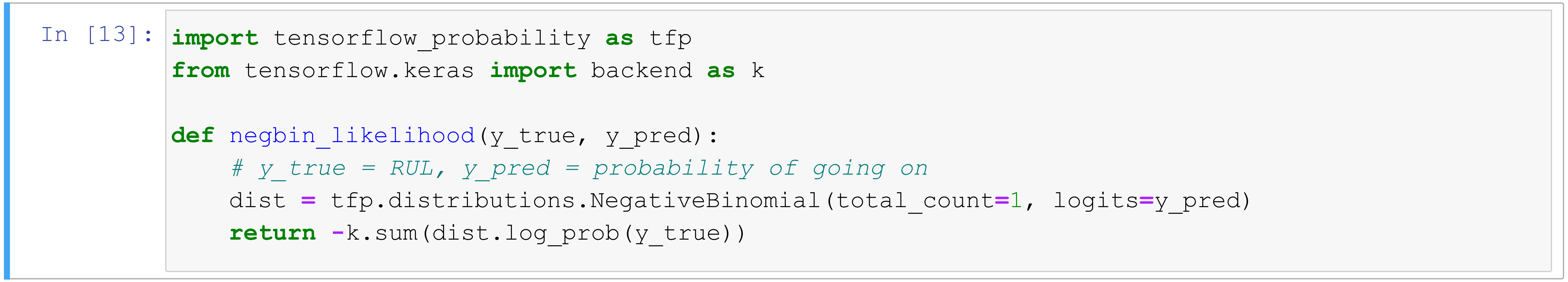
At inference time:

- The distribution mean will provide a RUL estimate
- We will be able to access a variance, quantiles, and confidence intervals!

Building the Probabilistic Model

We will build the probabilistic model using `tensorflow_probability`

In particular, we will build a custom loss function for keras:



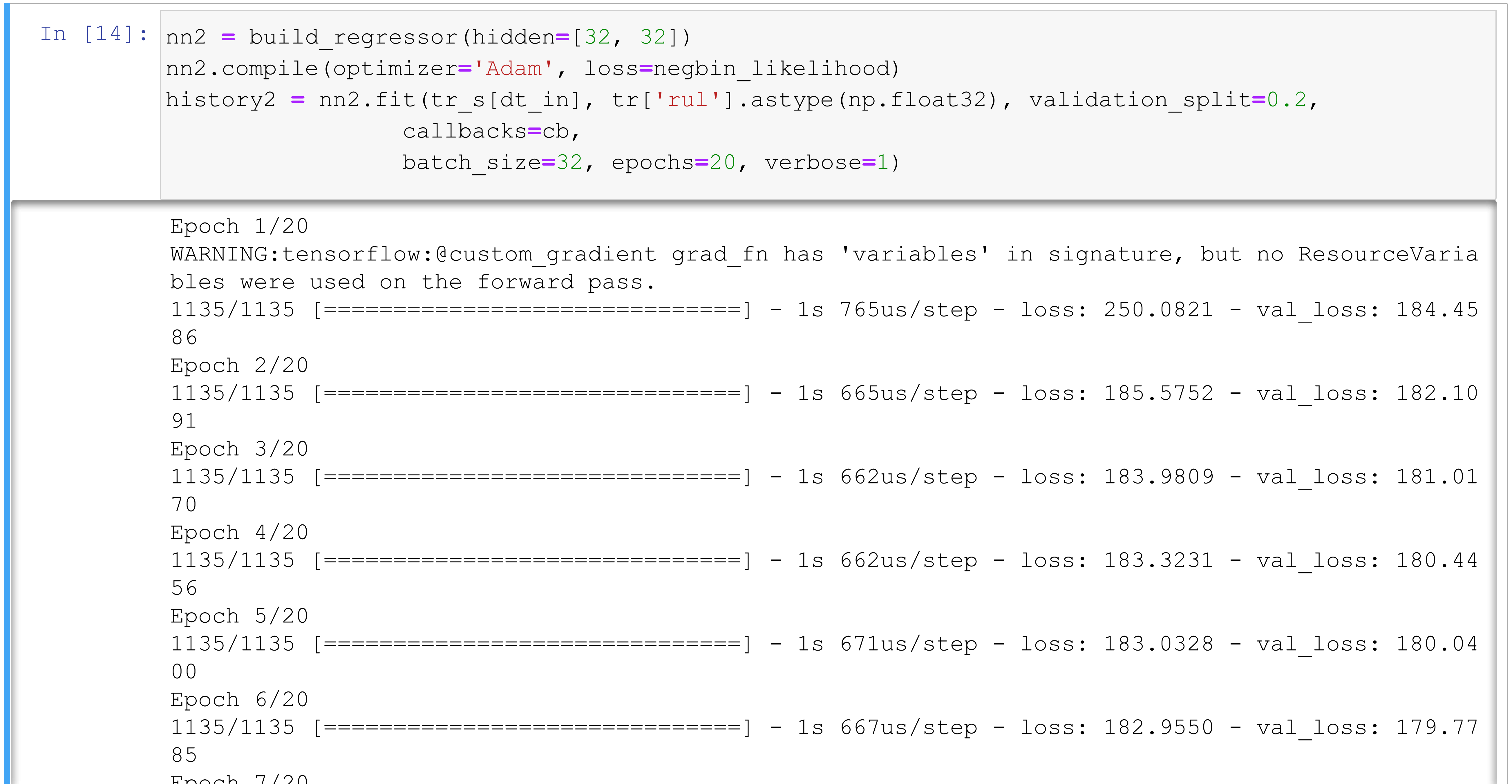
In [13]:
```python
import tensorflow_probability as tfp
from tensorflow.keras import backend as k

def negbin_likelihood(y_true, y_pred):
    # y_true = RUL, y_pred = probability of going on
    dist = tfp.distributions.NegativeBinomial(total_count=1, logits=y_pred)
    return -k.sum(dist.log_prob(y_true))
```

- The `NegativeBinomial` class swaps the roles of "success" and "failure"
- In particular, it is designed to work with the "failure" probability (i.e. moving on)
- It supports logit input, in which case a sigmoid is applied to obtain a probability
- ...And it allows the easy computation of log probabilities

Training the Hybrid Model

We can use our MLP architecture to estimate the NB logit



```
In [14]: nn2 = build_regressor(hidden=[32, 32])
         nn2.compile(optimizer='Adam', loss=negbin_likelihood)
         history2 = nn2.fit(tr_s[dt_in], tr['rul'].astype(np.float32), validation_split=0.2,
                            callbacks=cb,
                            batch_size=32, epochs=20, verbose=1)
```

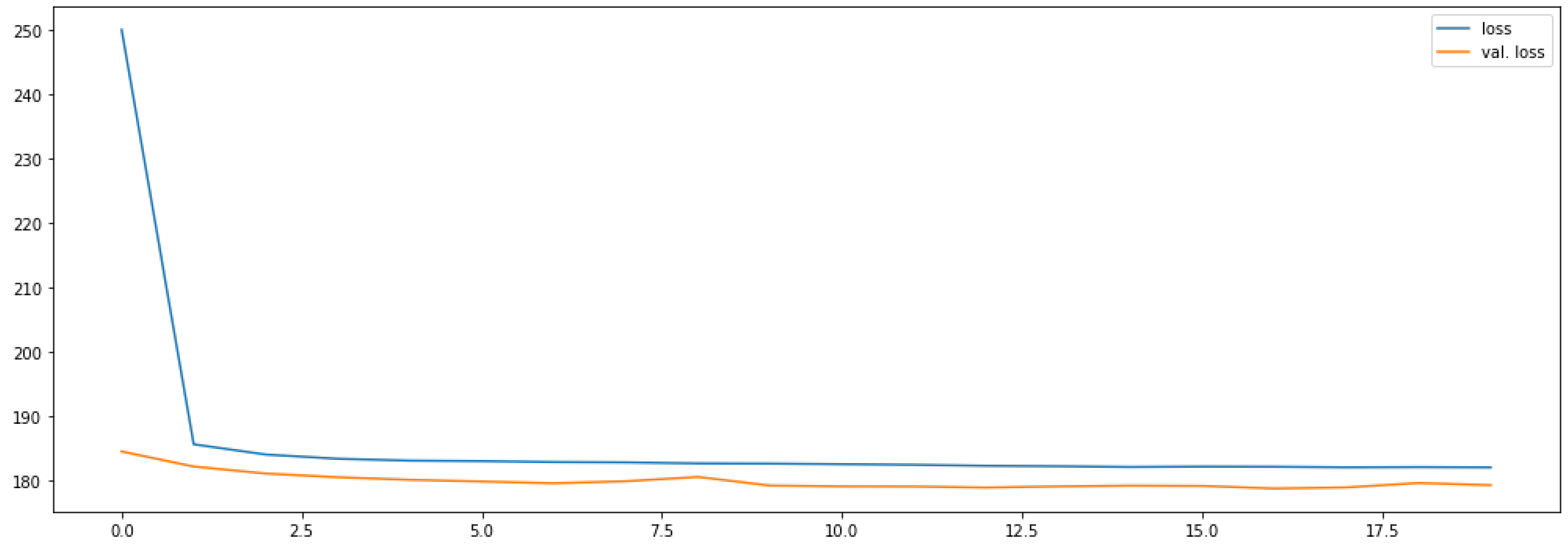
```
Epoch 1/20
WARNING:tensorflow:@custom_gradient grad_fn has 'variables' in signature, but no ResourceVaria
bles were used on the forward pass.
1135/1135 [==============================] - 1s 765us/step - loss: 250.0821 - val_loss: 184.45
86
Epoch 2/20
1135/1135 [==============================] - 1s 665us/step - loss: 185.5752 - val_loss: 182.10
91
Epoch 3/20
1135/1135 [==============================] - 1s 662us/step - loss: 183.9809 - val_loss: 181.01
70
Epoch 4/20
1135/1135 [==============================] - 1s 662us/step - loss: 183.3231 - val_loss: 180.44
56
Epoch 5/20
1135/1135 [==============================] - 1s 671us/step - loss: 183.0328 - val_loss: 180.04
00
Epoch 6/20
1135/1135 [==============================] - 1s 667us/step - loss: 182.9550 - val_loss: 179.77
85
Epoch 7/20
```

Training the Hybrid Model

Let's check the loss behavior over time

```
In [15]: cmapss.plot_training_history(history2, figsize=figsize)
         tr2, vl2 = history2.history["loss"][-1], np.min(history2.history["val_loss"])
         print(f'Loss: {tr2:.4f} (training, final), {vl2:.4f} (validation, best)')
```

```
Loss: 181.9762 (training, final), 178.6933 (validation, best)
```



Obtaining the Predictions

The hybrid model prediction corresponds to the mean of the NB distribution

First, we need to obtain the estimated probabilities:

```
In [16]: from scipy.special import expit

         tr_logits = nn2.predict(tr_s[dt_in]).ravel()
         tr_p = expit(tr_logits)

         ts_logits = nn2.predict(ts_s[dt_in]).ravel()
         ts_p = expit(ts_logits)
```

- `expit` is just the sigmoid function (i.e. reverse of logit)

Obtaining the Predictions

The hybrid model prediction corresponds to the mean of the NB distribution

Second, we need to build NB distribution objects

```
In [17]: from scipy.stats import nbinom

         tr_dist = nbinom(1, 1-tr_p)
         ts_dist = nbinom(1, 1-ts_p)
```

The scipy NB implementation goes by the textbook definition

- Hence, it is parameterized with the probability of a "success"
- ...I.e. the complement of what tensorflow does

That's why we use `1-tr_p` and `1 - ts_p`

Obtaining the Predictions

The hybrid model prediction corresponds to the mean of the NB distribution

Third, we can obtain the means:

```
In [18]: tr_pred2 = tr_dist.mean()
         ts_pred2 = ts_dist.mean()
```

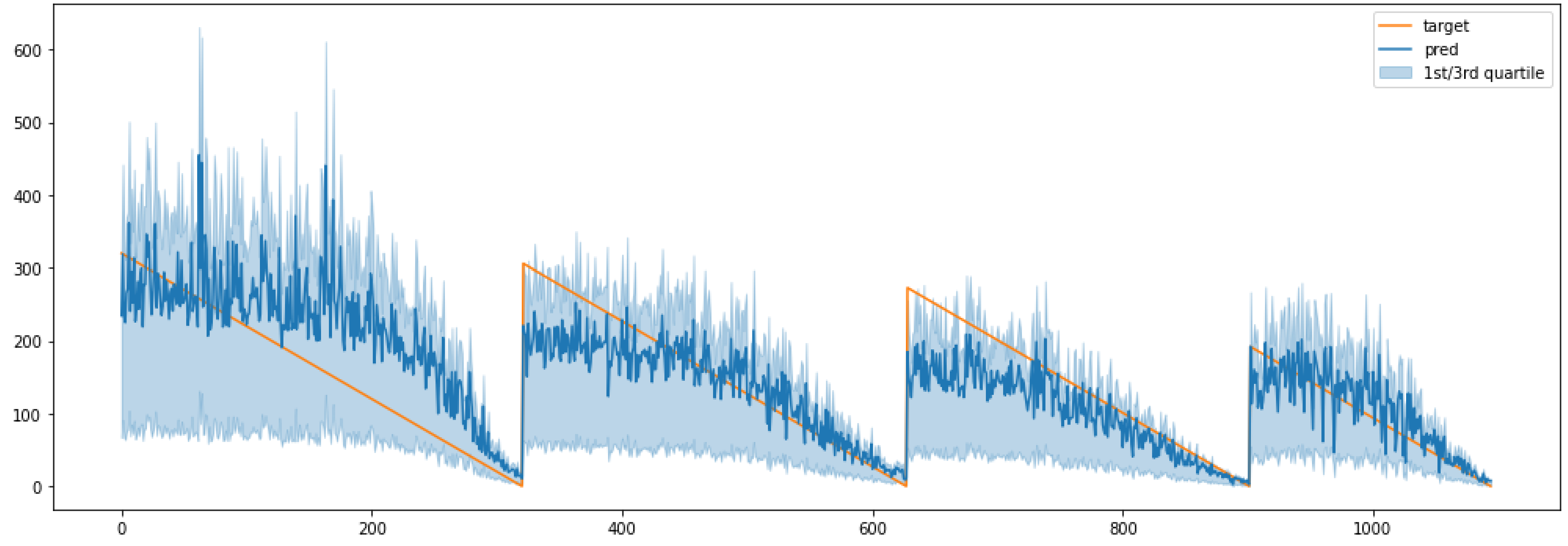
But we are not limited to that! We can obtain variances, quantiles, etc.

```
In [19]: tr_q1 = tr_dist.ppf(0.25)
         tr_q3 = tr_dist.ppf(0.75)
         ts_q1 = ts_dist.ppf(0.25)
         ts_q3 = ts_dist.ppf(0.75)
```

Predictions

We can plot the predictions and the 1s/3rd quartiles

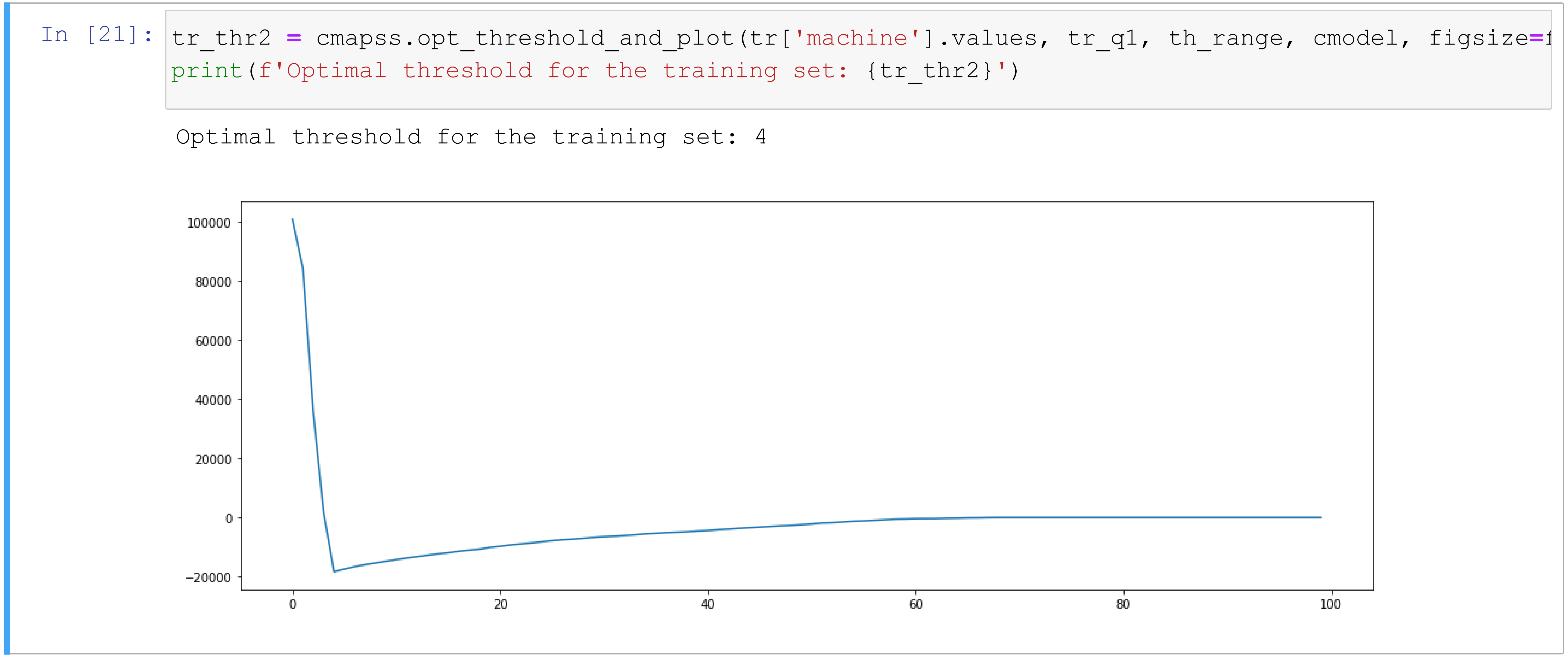
```
In [20]: stop = 1095
         cmapss.plot_rul(tr_pred2[:stop], tr['rul'][:stop], q1_3=(tr_q1[:stop], tr_q3[:stop]), figsize=fi
```



Threshold Optimization

We can perform threshold optimization using quantiles

- E.g. using the 1st quartile we have can choose θ so that we stop...
- ...Once the estimated probability of $f(\hat{x}_i, \lambda) \geq \theta$ drops below 25%

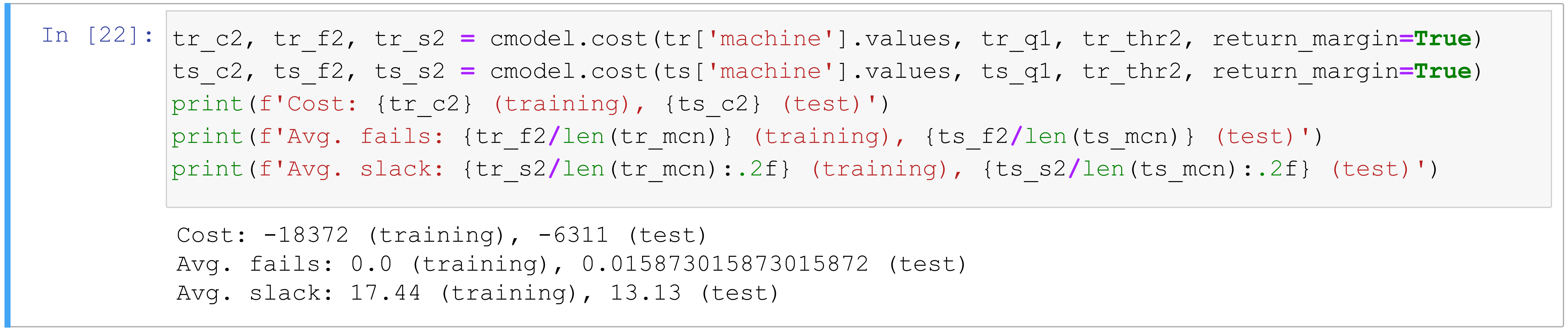


```
In [21]: tr_thr2 = cmapss.opt_threshold_and_plot(tr['machine'].values, tr_q1, th_range, cmodel, figsize=f
         print(f'Optimal threshold for the training set: {tr_thr2}')

Optimal threshold for the training set: 4
```

Evaluation

Let's see how it fares in terms of cost



```
In [22]: tr_c2, tr_f2, tr_s2 = cmodel.cost(tr['machine'].values, tr_q1, tr_thr2, return_margin=True)
         ts_c2, ts_f2, ts_s2 = cmodel.cost(ts['machine'].values, ts_q1, tr_thr2, return_margin=True)
         print(f'Cost: {tr_c2} (training), {ts_c2} (test)')
         print(f'Avg. fails: {tr_f2/len(tr_mcn)} (training), {ts_f2/len(ts_mcn)} (test)')
         print(f'Avg. slack: {tr_s2/len(tr_mcn):.2f} (training), {ts_s2/len(ts_mcn):.2f} (test)')
```

```
Cost: -18372 (training), -6311 (test)
Avg. fails: 0.0 (training), 0.015873015873015872 (test)
Avg. slack: 17.44 (training), 13.13 (test)
```

- The results are again on par with the best approaches
- ...But we have a clearer interpretations and confidence intervals!

Normal Distribution Model

Normal Distribution Model

The NB distribution fits naturally our process, but has a few drawbacks

In particular, the distribution variance is tied to its mean:

$$mean = \frac{pr}{1-p} \qquad variance = \frac{pr}{(1-p)^2}$$

- We may want to let the model free to adjust its confidence (variance)
- ...Independently on the prediction (mean)

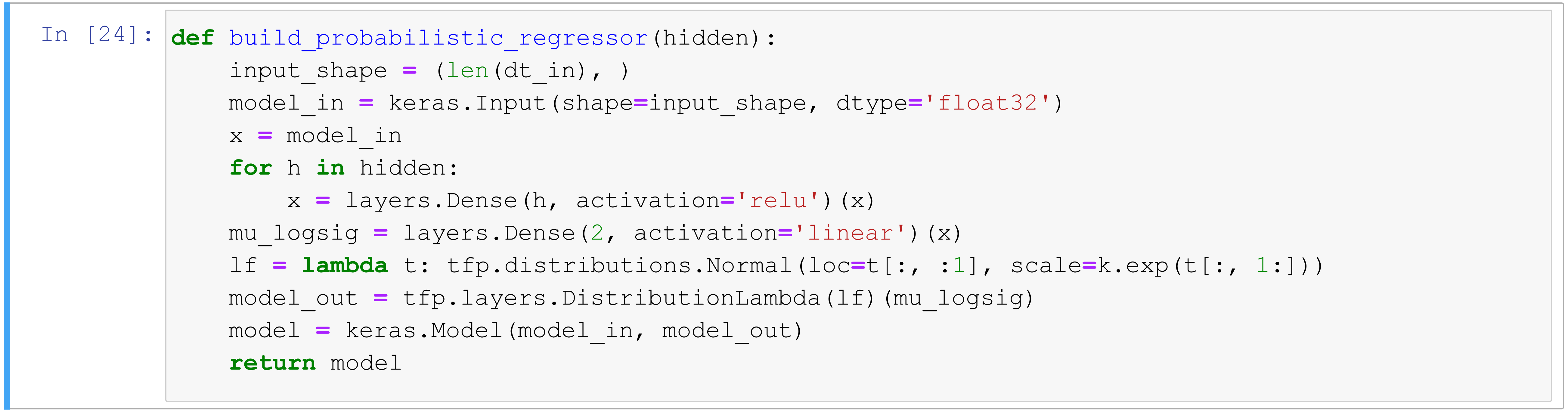
This can be done via a hybrid neural-probabilistic model

- We need a distribution with (at least two) parameters (e.g. the Normal one)
- ...And then we need neural models to estimate both. E.g.:

$$y \sim \mathcal{N}(\mu(\hat{x}, \lambda), \sigma(\hat{x}, \lambda))$$

Building the Architecture

First, we define a function to build the architecture



In [24]:
```python
def build_probabilistic_regressor(hidden):
    input_shape = (len(dt_in), )
    model_in = keras.Input(shape=input_shape, dtype='float32')
    x = model_in
    for h in hidden:
        x = layers.Dense(h, activation='relu')(x)
    mu_logsig = layers.Dense(2, activation='linear')(x)
    lf = lambda t: tfp.distributions.Normal(loc=t[:, :1], scale=k.exp(t[:, 1:]))
    model_out = tfp.layers.DistributionLambda(lf)(mu_logsig)
    model = keras.Model(model_in, model_out)
    return model
```

- This time we have chosen to rely on the `DistributionLambda`
  - `DistributionLambda` wraps a probability distribution into a layer
- We pass means and (log) standard deviations in a single tensor
  - Therefore the need to unpack them (i.e. `t[:, :1]` and `t[:, 1:]`)

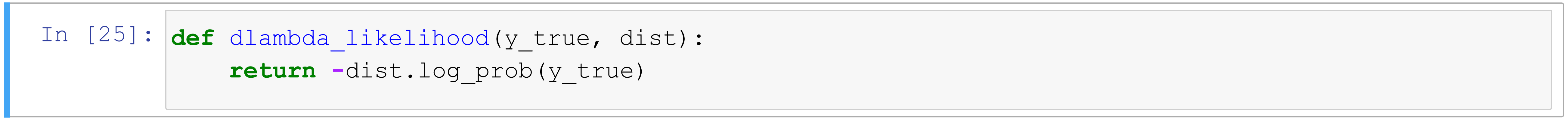
Loss Function

Our loss function will be the negative log likelihood

How can that be implemented?

- At training time, keras repeatedly "calls" the model
- I.e. it literally invokes the `__call__` method
- For `DistributionLambda`, calling returns a distribution object

Therefore we can formulate the log likelihood as follows:



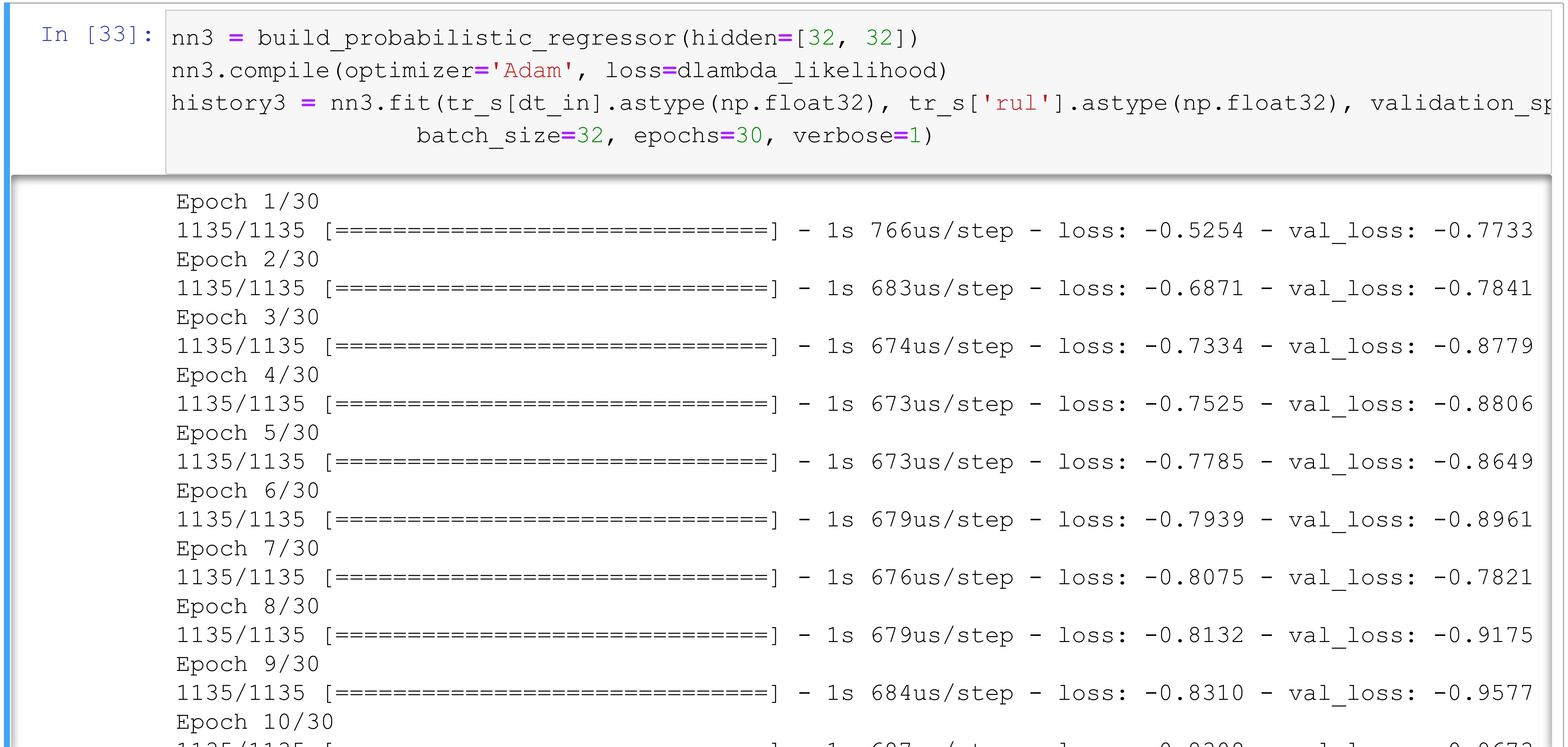
```
In [25]: def dlambda_likelihood(y_true, dist):
             return -dist.log_prob(y_true)
```

- This is very similar to our previous customized loss
- ...Except that we are returning negative log likelihoods for individual examples
- keras will aggregate by default via a sum, taking into account sample weights
- Our previous formulation couldn't do this

Training

Finally we can train our model

These type of models often needs to be trained for more epochs



```
In [33]: nn3 = build_probabilistic_regressor(hidden=[32, 32])
         nn3.compile(optimizer='Adam', loss=dlambda_likelihood)
         history3 = nn3.fit(tr_s[dt_in].astype(np.float32), tr_s['rul'].astype(np.float32), validation_sp
                                  batch_size=32, epochs=30, verbose=1)
```

```
Epoch 1/30
1135/1135 [==============================] - 1s 766us/step - loss: -0.5254 - val_loss: -0.7733
Epoch 2/30
1135/1135 [==============================] - 1s 683us/step - loss: -0.6871 - val_loss: -0.7841
Epoch 3/30
1135/1135 [==============================] - 1s 674us/step - loss: -0.7334 - val_loss: -0.8779
Epoch 4/30
1135/1135 [==============================] - 1s 673us/step - loss: -0.7525 - val_loss: -0.8806
Epoch 5/30
1135/1135 [==============================] - 1s 673us/step - loss: -0.7785 - val_loss: -0.8649
Epoch 6/30
1135/1135 [==============================] - 1s 679us/step - loss: -0.7939 - val_loss: -0.8961
Epoch 7/30
1135/1135 [==============================] - 1s 676us/step - loss: -0.8075 - val_loss: -0.7821
Epoch 8/30
1135/1135 [==============================] - 1s 679us/step - loss: -0.8132 - val_loss: -0.9175
Epoch 9/30
1135/1135 [==============================] - 1s 684us/step - loss: -0.8310 - val_loss: -0.9577
Epoch 10/30
```

Obtaining the Predictions

We are interested both in the predicted mean and standard deviation

- Therefore, we cannot simply call `predict`
- Instead, we call the model to obtain distribution objects

```
In [34]: tr_prob_pred = nn3(tr_s[dt_in].values)
         ts_prob_pred = nn3(ts_s[dt_in].values)
```

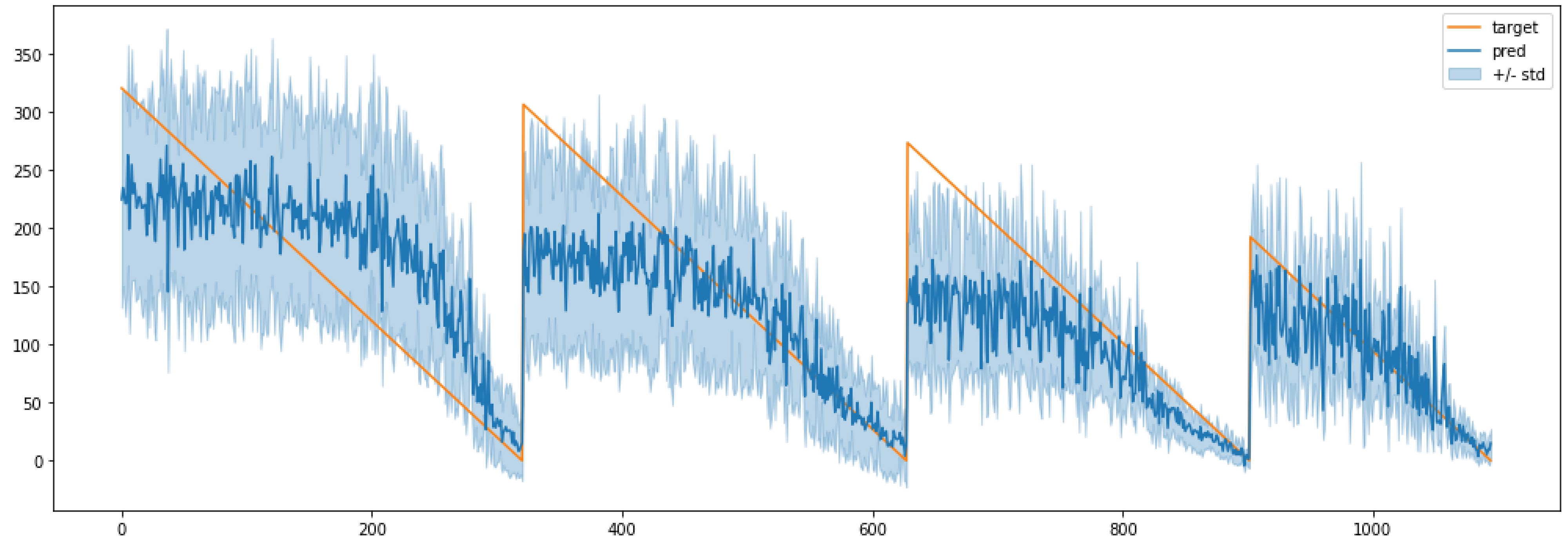
From these, we can obtain means and standard deviations:

```
In [35]: tr_pred3 = tr_prob_pred.mean().numpy().ravel() * trmaxrul
         tr_std3 = tr_prob_pred.stddev().numpy().ravel() * trmaxrul
         ts_pred3 = ts_prob_pred.mean().numpy().ravel() * trmaxrul
         ts_std3 = ts_prob_pred.stddev().numpy().ravel() * trmaxrul
```

Predictions

We can now plot the predictions for the training set

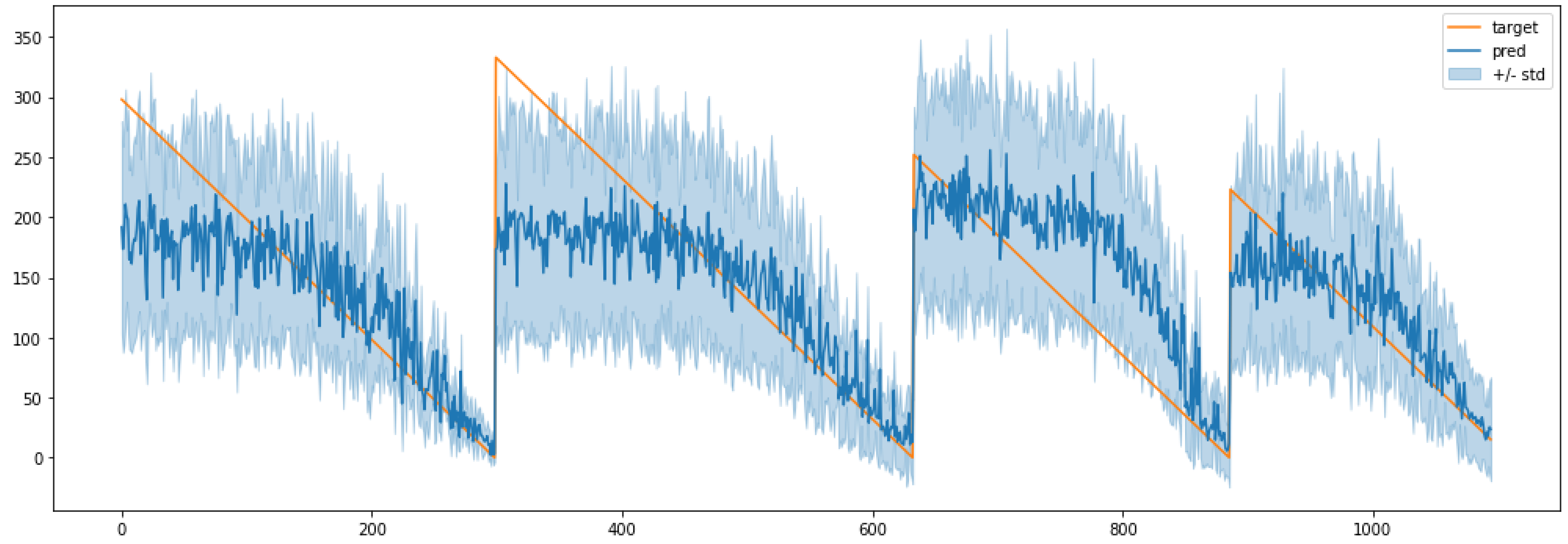
```
In [36]: cmapss.plot_rul(tr_pred3[:stop], tr['rul'][:stop], stddev=tr_std3[:stop], figsize=figsize)
```



Predictions

...And for the test set

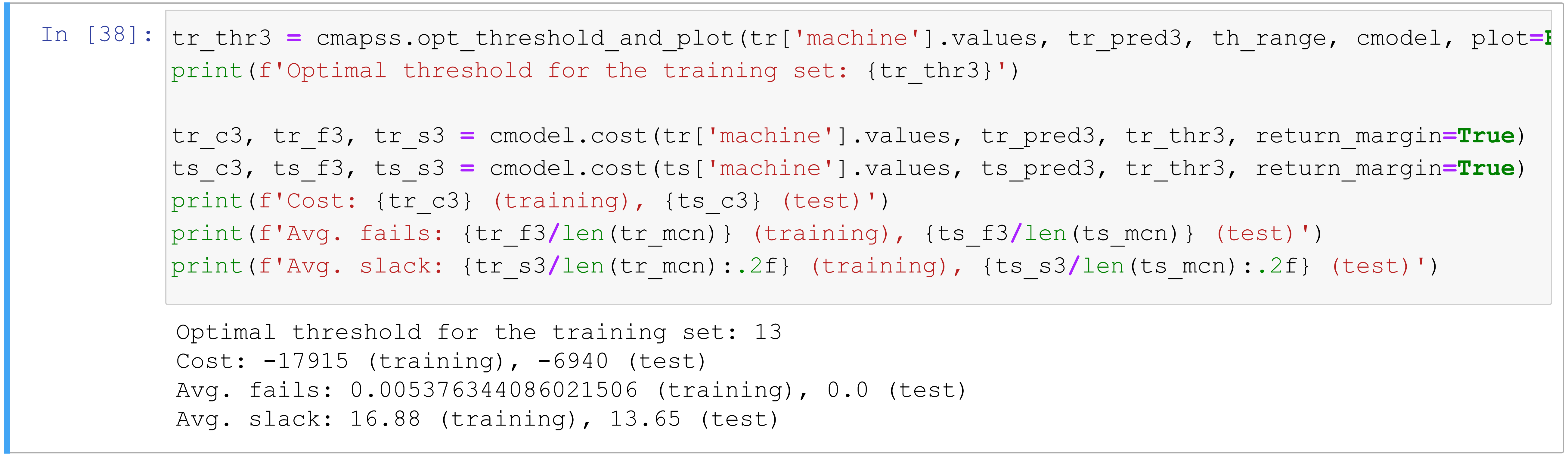
```
In [37]: cmapss.plot_rul(ts_pred3[:stop], ts['rul'][:stop], stddev=ts_std3[:stop], figsize=figsize)
```



Evaluation

We can perform threshold optimization and evaluation

We can use either the means or some quantile



```
In [38]: tr_thr3 = cmapss.opt_threshold_and_plot(tr['machine'].values, tr_pred3, th_range, cmodel, plot=
         print(f'Optimal threshold for the training set: {tr_thr3}')

         tr_c3, tr_f3, tr_s3 = cmodel.cost(tr['machine'].values, tr_pred3, tr_thr3, return_margin=True)
         ts_c3, ts_f3, ts_s3 = cmodel.cost(ts['machine'].values, ts_pred3, tr_thr3, return_margin=True)
         print(f'Cost: {tr_c3} (training), {ts_c3} (test)')
         print(f'Avg. fails: {tr_f3/len(tr_mcn)} (training), {ts_f3/len(ts_mcn)} (test)')
         print(f'Avg. slack: {tr_s3/len(tr_mcn):.2f} (training), {ts_s3/len(ts_mcn):.2f} (test)')

         Optimal threshold for the training set: 13
         Cost: -17915 (training), -6940 (test)
         Avg. fails: 0.005376344086021506 (training), 0.0 (test)
         Avg. slack: 16.88 (training), 13.65 (test)
```

- The results are once again on par with the best approaches
- As in the previous case, we have a clearer interpretation...
- ...But also more flexible confidence intervals!

Considerations

Why going for hybrid probabilistic models?

- They are typically harder to train than traditional ML models
- ...But the provide confidence quantiles and standard deviations!
- Never underestimate how useful a confidence interval can be

Probabilistic models enable reasoning

- We can choose thresholds based on probabilistic considerations
  - E.g. I want the estimated chance that RUL <= 1 to be lower than 0.10
  - This is very handy when data is scarce
  - ...And cost optimization becomes therefore impossible
- It is possible to define probabilistic cost models
  - E.g. expected financial cost of maintenance policy
  - They are often the key to build end-to-end cost optimization approaches