Better Learning for ODEs

Decomposing Sequences

We can address the first two issues using a reformulation

Let's consider the sequence of measurements $\{\hat{y}_k\}_{k=0}^n$

- We can view it as a sequence of pairs $\{(\hat{y}_{-1}, \hat{y}_k\}_{k=1}^n$
- ...Each referring to a distinct ODE, i.e. $\dot{y}_k = f(y_k, t, \omega)$
- ...With all ODEs sharing the same parameter vector ω

With this approach, we can reformulate the training problem as:

$$\text{argmin}_\omega \sum_{k=1}^n L(y_k(\hat{t}_k), \hat{y}_k)$$

$$\text{subject to: } \dot{y}_k = f(y_k, t, \omega) \qquad \forall k = 1..n$$

$$y_k(\hat{t}_{k-1}) = \hat{y}_{k-1} \qquad \forall k = 1..n$$

- In practice, we assume we are dealing with multiple initial value problems

Decomposing Sequences

Let's examine again the new training problem:

$$\text{argmin}_\omega \sum_{k=1}^{n} L(y_k(\hat{t}_k), \hat{y}_k)$$

$$\text{subject to: } \dot{y}_k = f(y_k, t, \omega) \qquad \forall k = 1..n$$

$$y_k(\hat{t}_{k-1}) = \hat{y}_{k-1} \qquad \forall k = 1..n$$

There a few things to keep in mind:

- The approach is viable only if we have measurements for the full state
- ...And we are also assuming that the original loss is separable
- Finally, the new training problem is not exactly equivalent to the old one
- ...Since by re-starting at each step we are disregarding compound errors

Preparing the Data

Our implementation can naturally deal with the reformulation

We just need to properly prepare the data

- Each ODE can be seen as a different example

```
In [2]: ns = len(data.index)-1
```

- The sequence for each example contains only two measurements
- ...Corresponding to consecutive evaluation points

```
In [3]: tr_T = np.vstack((data.index[:-1], data.index[1:])).T
        print(tr_T[:3])
```

```
[[0. 1.]
 [1. 2.]
 [2. 3.]]
```

Preparing the Data

Our implementation can naturally deal with the reformulation

We just need to properly prepare the data

- The first measurement represents the initial state

```
In [4]: tr_y0 = np.array(data.iloc[:-1]).reshape(-1, 1)
        print(tr_y0[:2])
```

```
[[0.        ]
 [1.41003718]]
```

- The second to the final state, which we need for defining a target tensor

```
In [6]: tr_y = np.full((ns, 2, 1), np.nan)
        tr_y[:, 1, :] = data.iloc[1:]
        print(tr_y[:2])
```

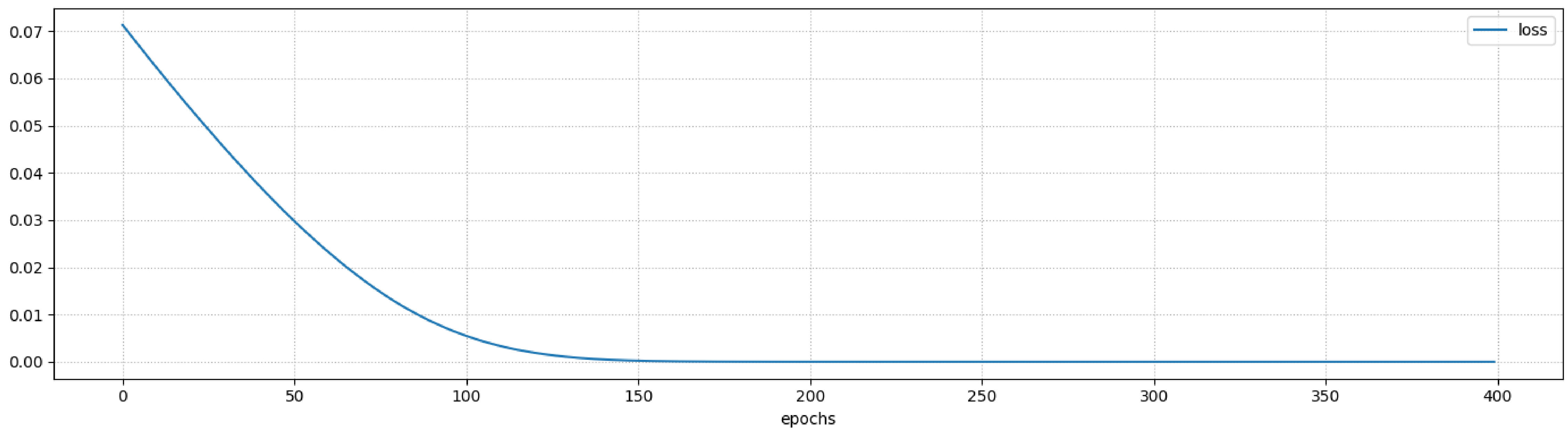
```
[[[       nan]
  [1.41003718]]

 [[       nan]
  [2.6543906 ]]]
```

Training

Then we can perform training as usual

In [8]:
```
%%time
dRC = util.RCNablaLayer(tau_ref=10, vs_ref=10)
euler = util.ODEEulerModel(dRC)
history = util.train_nn_model(euler, [tr_y0, tr_T], tr_y, loss='mse', validation_split=0.0, epoc
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.0000 (training)
CPU times: user 1.48 s, sys: 308 ms, total: 1.79 s
Wall time: 1.26 s
```

Training

The results are the same as before (including estimation problems)

In [9]:
```
print(f'tau: {tau:.2f} (real), {dRC.get_tau().numpy()[0]:.2f} (estimated)')
print(f'Vs: {Vs:.2f} (real), {dRC.get_vs().numpy()[0]:.2f} (estimated)')
```

```
tau: 8.00 (real), 8.51 (estimated)
Vs: 12.00 (real), 12.00 (estimated)
```

...But there are significant computational advantages

Since we are using a shallow compute graph rather than a deep one...

- The training time is much lower
- Potential vanishing/exploding gradient problems are absent

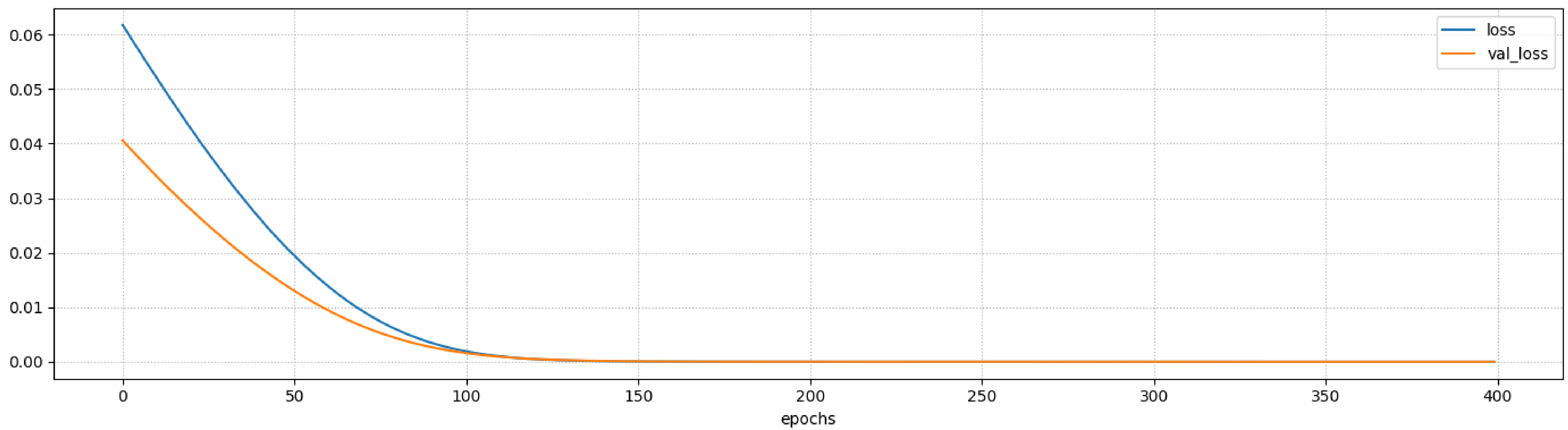
Since we now have multiple examples...

- We can benefit from stochastic gradient descent
- We can use a validation set

Training

Just keep in mind that using a validation set will slow down the process

In [10]:
```
%%time
dRC = util.RCNablaLayer(tau_ref=10, vs_ref=10)
euler = util.ODEEulerModel(dRC)
history = util.train_nn_model(euler, [tr_y0, tr_T], tr_y, loss='mse', validation_split=0.2, epoc
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.0000 (training), 0.0000 (validation)
CPU times: user 7.02 s, sys: 624 ms, total: 7.65 s
Wall time: 6.69 s
```

Accuracy Issues

We are now ready to tackle our estimation issues

- We know we have trouble estimating the τ parameter
- Intuitively, that should translate in trouble estimating the dynamic behavior

Let's try to replicate integration using our model

- We prepare data structures to replicate our original run

In [12]:
```python
run_y0 = data.iloc[0].values.reshape(1, -1)
run_T = np.array([data.index])
print('y0:', run_y0)
print('T:', run_T)
```

```
y0: [[0.]]
T: [[ 0.  1.  2.  3.  4.  5.  6.  7.  8.  9. 10. 11. 12. 13. 14. 15. 16. 17.
  18. 19. 20. 21. 22. 23. 24. 25. 26. 27. 28. 29. 30. 31. 32. 33. 34. 35.
  36. 37. 38. 39. 40. 41. 42. 43. 44. 45. 46. 47. 48. 49. 50. 51. 52. 53.
  54. 55. 56. 57. 58. 59. 60.]]
```

Accuracy Issues

Then we can run Euler method directly using our model

As a side benefit, this will naturally use the estimate parameters

In [14]:
```
run_y = euler.predict([run_y0, run_T], verbose=0)
```

Next, let's build a dataset with the original data and the predictions:

In [15]:
```
data_euler = data.copy()
data_euler['euler'] = run_y[0]
data_euler.head()
```

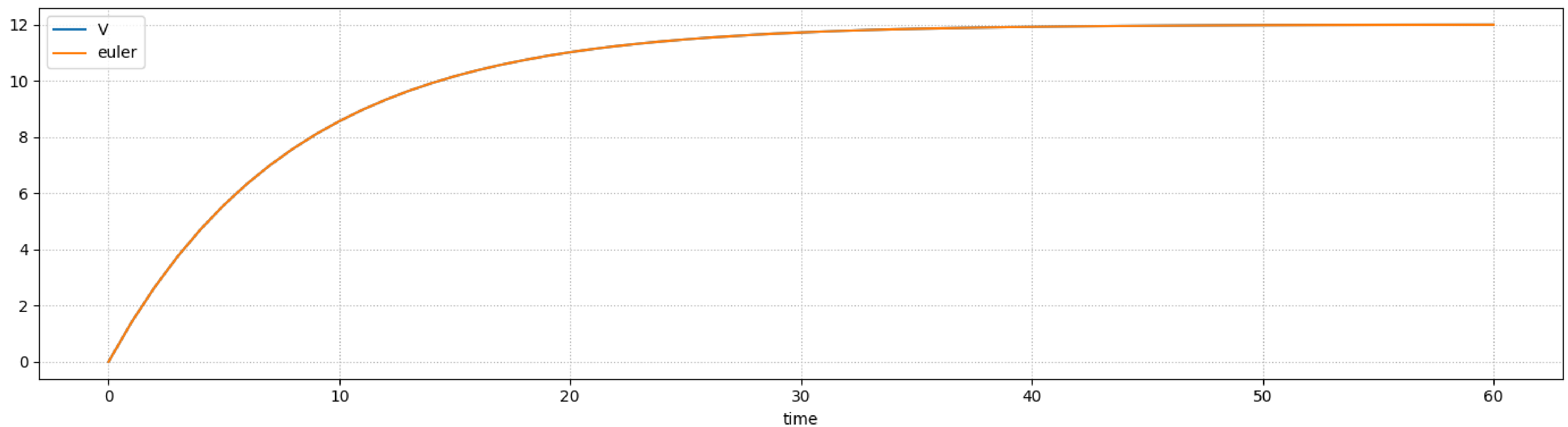
Out[15]:

	V	euler
time		
0.0	0.000000	0.000000
1.0	1.410037	1.410401
2.0	2.654391	2.655018
3.0	3.752529	3.753339
4.0	4.721632	4.722559

Accuracy Issues

Finally, we can plot the two curves

In [16]:
```
util.plot_df_cols(data_euler, figsize=figsize)
```



We have a very good match!

What is going on?

Accuracy Issues?

We formulated the training problem in terms of curve fitting

- I.e. we optimized τ and V_s so as to obtain a close fitting curve
- ...Constructed using Euler method

The problem is that Euler method is inaccurate

- If using wrong parameters will lead to a better fitting curve
- ...Our approach will not hesitate to do just that

Accuracy Issues?

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Is this a problem?

If we just care about the curve, not at all

- It can actually be an advantage, if properly exploited

If we care about estimating parameters, then yes

- ...But it also suggests an easy fix (using a more accurate integration method)

Improving Parameter Estimation

For sake of simplicity, we will keep using Euler method

...And we will just increase the number of steps to improve its accuracy

- First, we introduce more evaluation points for each measurement pair

In [19]:
```
nsteps = 11
tr_T2 = np.vstack(np.linspace(data.index[:-1], data.index[1:], nsteps)).T
print(tr_T2[:2])
```

```
[[0.  0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1. ]
 [1.  1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2. ]]
```

- Second, we update the target sequences to match the size

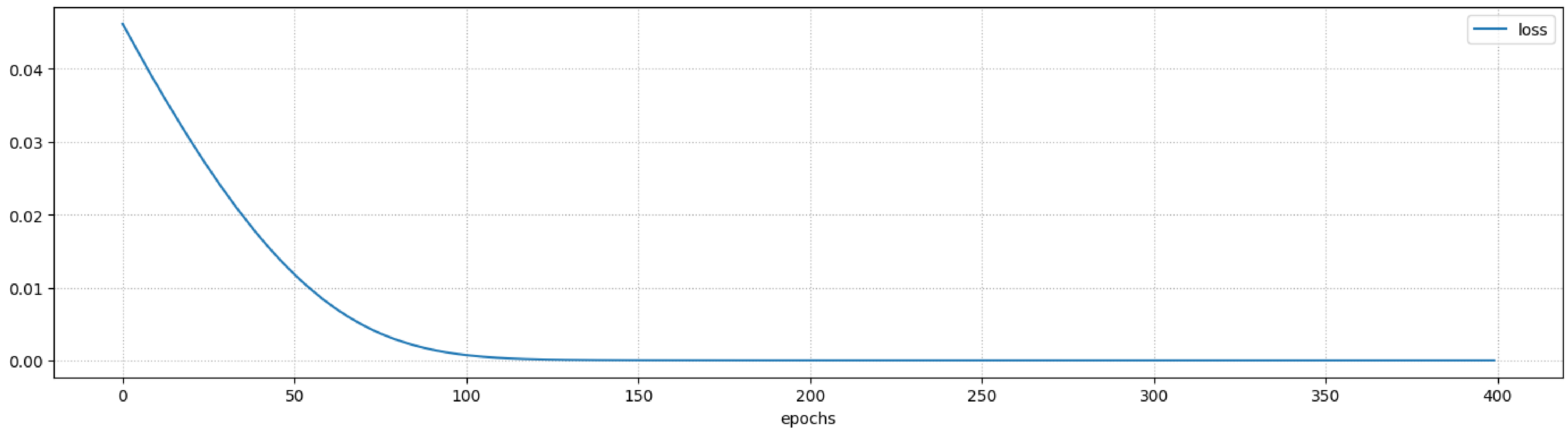
In [20]:
```
tr_y2 = np.full((ns, nsteps, 1), np.nan)
tr_y2[:, -1, :] = data.iloc[1:]
print(str(tr_y2[:2]).replace('\n', ', ').replace(' ', '').replace(',,', '\n'))
```

```
[[[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[1.41003718]]
[[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[nan],[2.6543906]]]
```

Improving Parameter Estimation

Then, we can train as usual

In [21]:
```
%%time
dRC2 = util.RCNablaLayer(tau_ref=10, vs_ref=10)
euler2 = util.ODEEulerModel(dRC2)
history = util.train_nn_model(euler2, [tr_y0, tr_T2], tr_y2, loss='mse', validation_split=0.0, e
util.plot_training_history(history, figsize=figsize)
```




```
Final loss: 0.0000 (training)
CPU times: user 2.36 s, sys: 266 ms, total: 2.63 s
Wall time: 1.99 s
```

Improving Parameter Estimation

This approach leads to considerably better estimates

```
In [22]: print(f'tau: {tau:.2f} (real), {dRC2.get_tau().numpy()[0]:.2f} (estimated)')
         print(f'Vs: {Vs:.2f} (real), {dRC2.get_vs().numpy()[0]:.2f} (estimated)')

         tau: 8.00 (real), 8.05 (estimated)
         Vs: 12.00 (real), 12.00 (estimated)
```

- The results can be improved by using additional steps
- ...Or by switching to a different method (e.g. RK4, adjoint state...)

Overall, when using this appraoch...

...It's important to be aware that integration methods are approximate

- This can easily lead to incorrectly estimated parameters
- Which may or may not be a problem, depending on your priorities