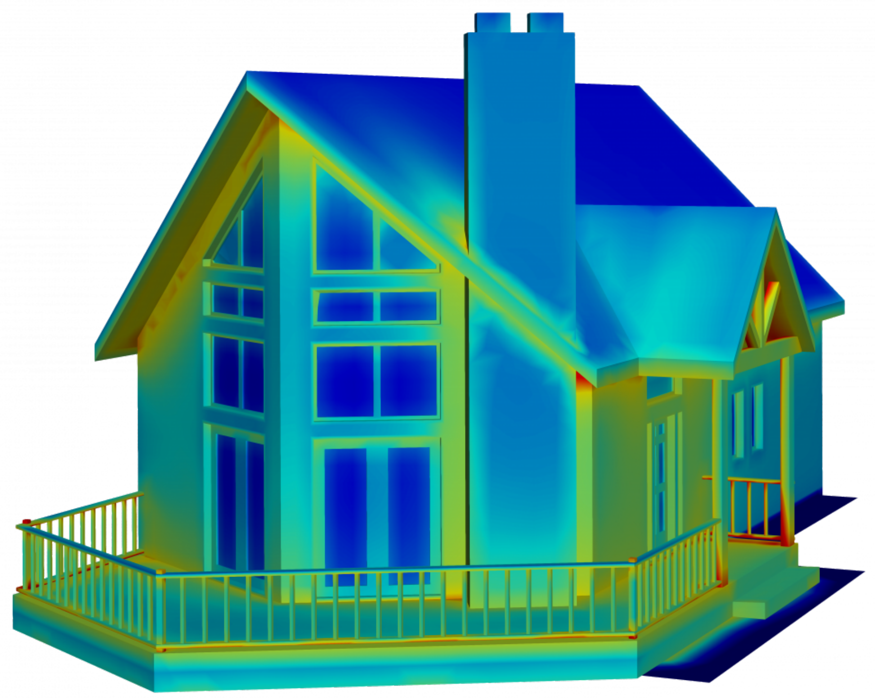
Ordinary Differential Equations

Thermal Models

Let's assume we want to model the thermal behavior of an object

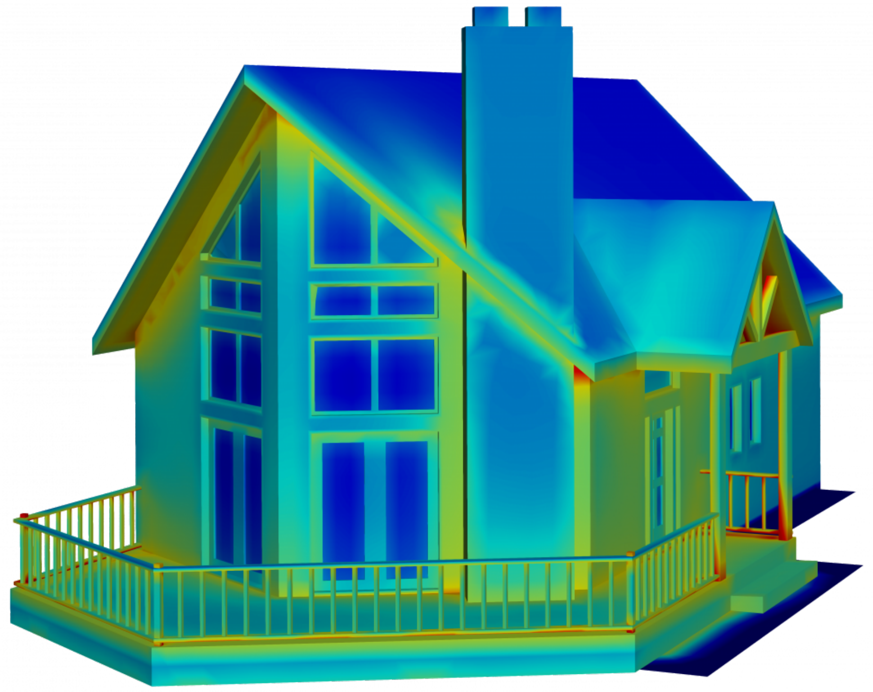


Temperature obeys well-defined physical laws

- These are described by differential equations
- ...And can be used to build powerful computer simulators
- If we assigning values to the model parameters, we can then study its behavior

Thermal Models

Let's assume we want to model the thermal behavior of an object



But what if we don't know the parameters?

- Then we have an estimation problem
- We can solve it using Machine Learning
- Provided our model is consistent with the physical laws of the simulator

Ordinary Differential Equations

An Ordinary Differential Equation is any equation in the form:

$$\dot{y} = f(y, t)$$

- Where y is the state variable
- ...And f is a function, providing the gradient of the state variable

The peculiarities:

- y is actually a function or the t variable
- The t variable typically (but not always) represents time
- ...Hence $y(t)$ is the state at time t
- The gradient f depends on both the current state and current time

Ordinary = does not feature partial derivatives

Initial Value Problem

An Initial Value Problem consists of an ODE and a initial condition

$$\dot{y} = f(y, t)$$
$$y(0) = y_0$$

- This can be interpreted as running a simulation
- Given that the initial state $y(0)$ is y_0, how will the state unfold?

Initial values problems can be solved (integrated):

...Exactly, using symbolic approaches, e.g.

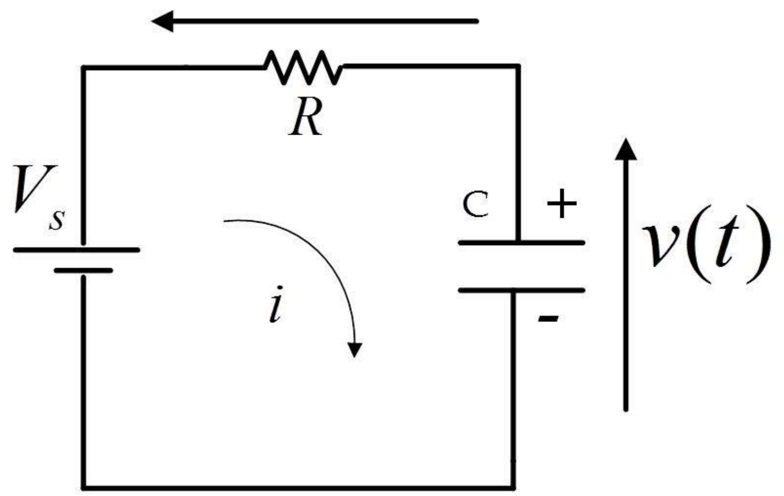
$$\dot{y} = a,\ y(0) = b \quad \Rightarrow \quad y(t) = ay + b$$

- This is the method considered in typical calculus courses

...Or approximately, via numerical approaches

An Example

As an example, let's consider a simple RC circuit



It's dynamic behavior is described by the ODE:

$$\dot{V} = \frac{1}{\tau}(V_s - V)$$

- Where $\tau = RC$

Euler Method

The simplest numerical approach for ODEs is called Euler Method

This is obtained by:

- Considering a fixed sequence of evaluation points $\{t_k\}_{k=0}^n$
- Using a linear approximation for $y(t)$ within each interval $[t_k, t_{k+1}]$
- Approximating the slope with the gradient f at time t_k

The pseudo code of the method consists of a single loop

```
for $k = 1..n$:
    $y_k = y_{k-1} + (t_k - t_{k-1}) f(y_{k-1}, t_{k-1})$
```

- The output is a sequence $\{y_k\}_{i=0}^n$, where y_k is the state at time t_k
- y_0 is also an input for the algorithm

Euler Method for the RC Circuit

A typical Initial Value Problem solver API requires to define

The function that characterizes the equation, i.e. $f(y, t)$:

```
In [2]: tau, Vs = 8, 12
        f = lambda y, t: 1./tau * (Vs - y)
```

The initial state y_0 and the evaluation points $\{t_i\}_{i=0}^n$

```
In [3]: y0 = (0,) # We start from an empty capacitor
        t = np.linspace(0, 40, 12)
```

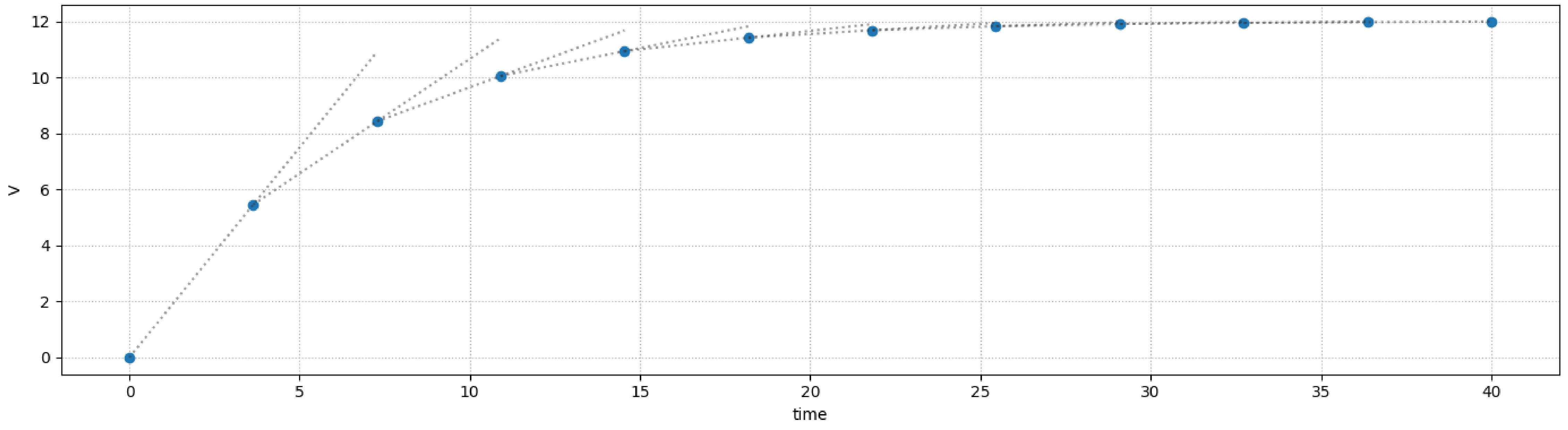
Then we can call the solver itself (the code is in the `util` module)

```
In [5]: y, dy = util.euler_method(f, y0, t, return_gradients=True)
```

Euler Method for the RC Circuit

Visually, the method works as follows:

```
In [8]: util.plot_euler_method(y, t, dy=dy, xlabel='time', ylabel='V', figsize=figsize)
```



- The dots represent evaluated states
- The slope of the lines corresponds to the gradient at each step

ODE Integration Methods

The Euler method is the simplest ODE integration approach

...But also one of the worst in terms of accuracy

- This is due to errors in the local approximation
- ...And forces to use very small steps to obtain high-quality results

There are many alternative integration methods, e.g.:

- Backward Euler method
  - Like Euler method, but we use the gradient at the next state
  - In practice it requires to solve a (typically non-linear) equation
- Runge-Kutta methods
  - It's a family of method (Euler method is the simplest version)
  - They combine multiple gradients to obtain a local slope

"Learning" ODEs

"Learning" ODEs

The parameters of an ODE can be estimated from data

Formally, this "training" problem amounts to solving:

$$\text{argmin}_\theta \left\{ L(y(\hat{t}), \hat{y}) \mid \dot{y} = f(y, t, \theta), y(0) = \hat{y}_0 \right\}$$

Where:

- $\{\hat{t}_k\}_{k=0}^n$ is a sequence of points for which measurements are available
- $\{\hat{y}_k\}_{k=0}^n$ are the corresponding state measurements
- f is a parameterized gradient function
- L is a loss function (e.g. the classical MSE)

Intuitively, we require the integrated ODE to be close to the real one

- The goal is to choose the parameters (e.g. τ, V_s) so as to achieve this

How can we deal with that?

"Learning" ODEs

We start from observing that every step in the Euler method is differentiable

...If we assume f to be differentiable (which is often the case):

$$y_k = y_{k-1} + (t_k - t_{k-1})f(y_{k-1}, t_{k-1})$$

- This is actually true for the whole Runge-Kutta family
- ...And for more advanced methods as well

Therefore, a viable approach is to discretize, then optimize

- We choose one automatic differentiation engine
- ...And we use it to solve the initial value problem using a numerical method
- Then, we compute the loss L
- ...And we update the parameters using (e.g.) gradient descent

Building Ground Truth for an Example

We'll see an example using our simple RC circuit

Let's start by building a high-quality ground truth sequence

- We will use the `odeint` solver from scikit learn for this
- The code can be found in the `simulate_RC` function

```
In [12]: V0, tau, Vs, tmax = 0, tau, Vs, 60
         data = util.simulate_RC(V0, tau, Vs, tmax, steps_per_unit=1)
         data.head()
```

Out[12]:

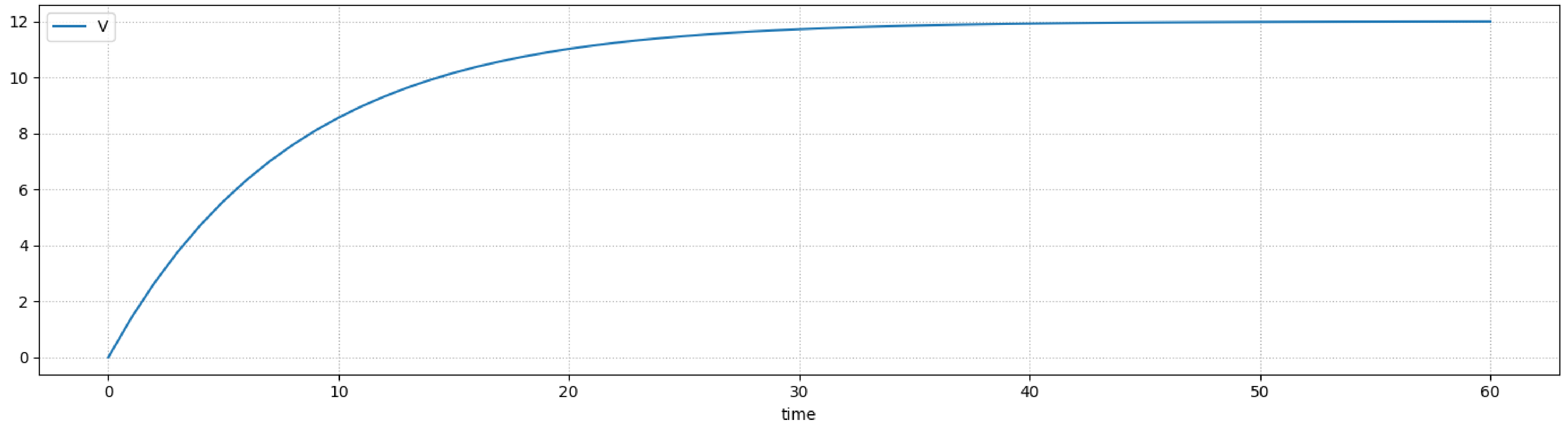
	V
time	
0.0	0.000000
1.0	1.410037
2.0	2.654391
3.0	3.752529
4.0	4.721632

- `steps_per_unit` defines how many evaluations to perform per unit of time

Building Ground Truth for an Example

Let' check (visually) that the result is smooth enough

```
In [15]: util.plot_df_cols(data, figsize=figsize)
```



- We need to ensure the data quality is high enough
- ...Since we'll treat it as our ground truth

Outline of the Approach

We will build a relatively simple, but quite general approach

- We will view the (parameterized) gradient function $f(y, t, \theta)$ as a layer type
- ...And we will use a `keras.Model` to encode Euler method, i.e.

$$y(\hat{t}_k) = y(\hat{t}_{k-1}) + (\hat{t}_k - \hat{t}_{k-1}) f(y(\hat{t}_{k-1}), \hat{t}_{k-1}, \theta)$$

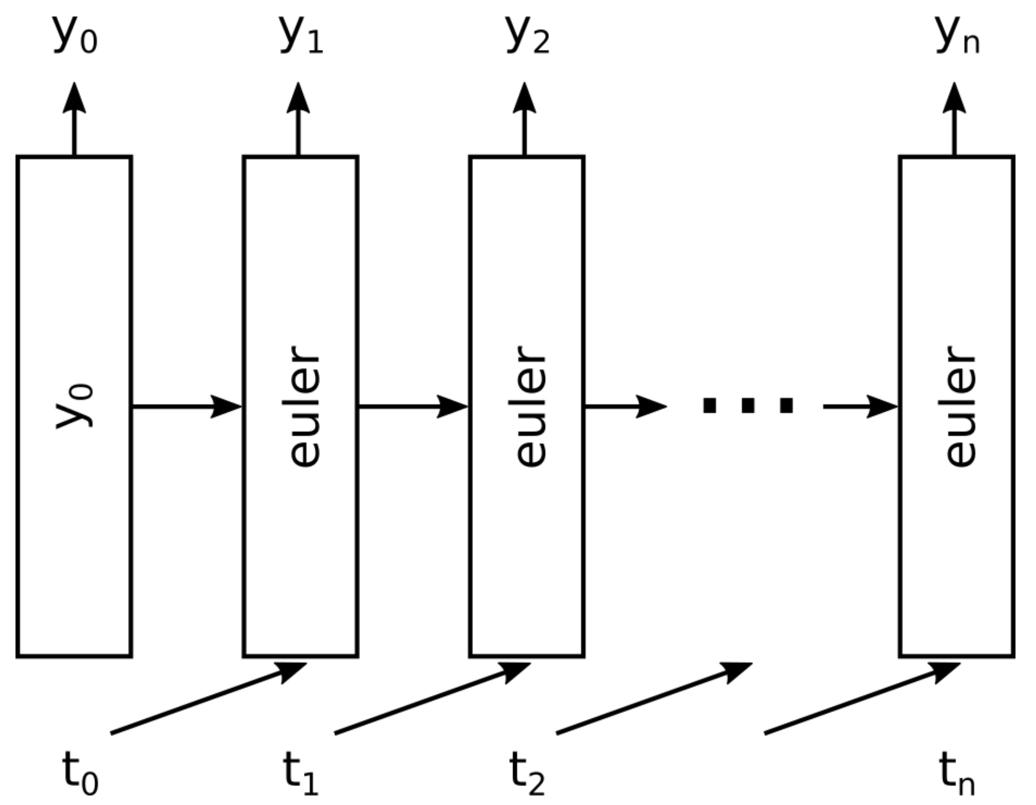
- Each step of the method can be viewed as layer instance
- ...And all instances share the same weights

In terms of input/output:

- The initial state corresponds to the input
- ...And a secondary input is given by the sequence $\{\hat{t}_k\}_{k=0}^n$
- The output is the state for each evaluation step

Outline of the Approach

Overall, our "architecture" looks like this:

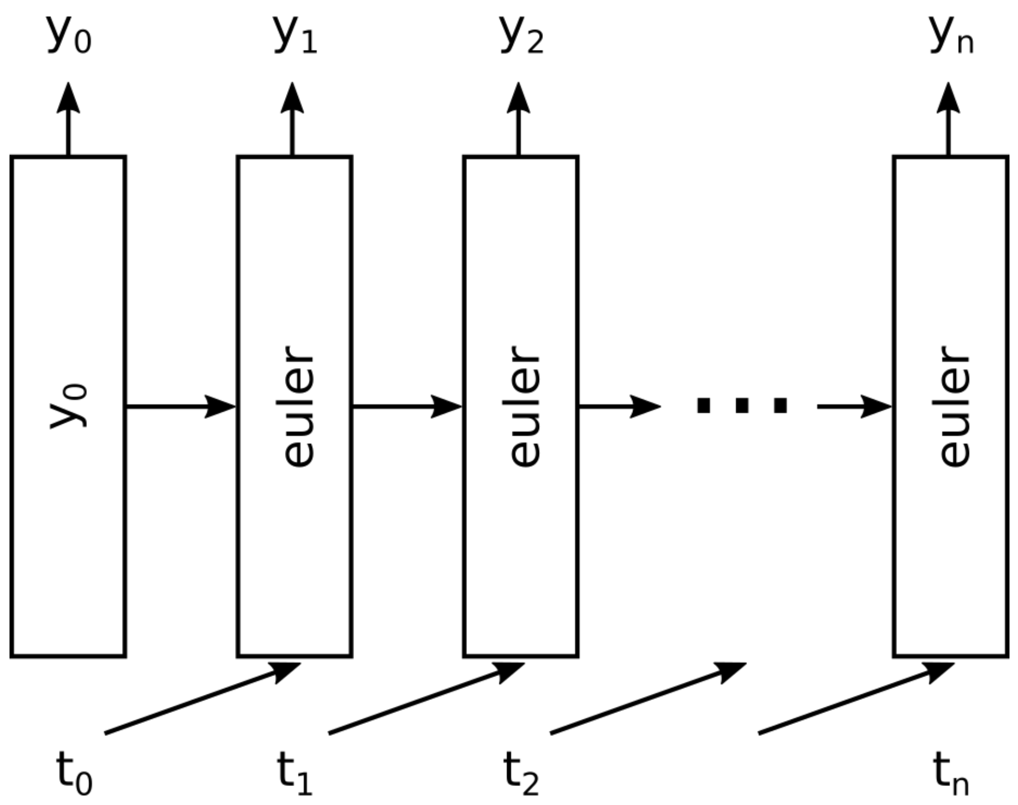


- The input includes the initial state y_0 and the evaluation points $\{\hat{t}_k\}_{k=0}^n$
- The output consists of the sequence of state evaluations $\{y_k\}_{k=0}^n$

Overall, the signature is analogous to that of an ODE solver

Outline of the Approach

Overall, our "architecture" looks like this:



- Each example corresponds to an initial value problem solution for the same system
- ...And the architecture is very similar to a recurrent NN
- In particular, the "depth" grows with the number of evaluation points

Details Matter

In our RC circuit case, we have:

$$\operatorname{argmin}_{\tau, V_s} \; L(y(\hat{t}), \hat{y})$$
$$\text{subject to } \dot{y} = \frac{1}{\tau}(V_s - y)$$
$$y(0) = y_0$$

- Where the parameters to be learned are τ and V_s

There are a few details we need to account for

- For both parameters, negative values make no sense
- Moreover, since we plan to use gradient descent for training
- ...We need to make sure that our initial guesses are reasonable

Details Matter

We can meet both conditions by adopting the reformulation:

$$\tau = \sigma_\tau e^{\theta_\tau}$$
$$V_s = \sigma_{V_s} e^{\theta_{V_s}}$$

Where the parameters to be learned are now $\boldsymbol{\theta_\tau}$ and $\boldsymbol{\theta_{V_s}}$

- Using an exponential ensures we get non-negative values
- The scaling factors $\boldsymbol{\sigma_\tau}$ and $\boldsymbol{\sigma_{V_s}}$ are user-provided
- They should lead to reasonable guesses for typical NN weight initiliazers

There are just a few mild downsides:

- The exponential may lead to numerical issues in edge cases
- We need to have a rough idea of the scale of $\boldsymbol{\tau}$ and $\boldsymbol{V_s}$

RC Circuit Layer

The layer for the RC circuit gradient is in the `RCNablaLayer` class

```
class RCNablaLayer(keras.layers.Layer):
    def __init__(self, tau_ref=0.1, vs_ref=0.1):
        self.tau_ref = tau_ref # store scales
        self.vs_ref = vs_ref
        p_init = tf.random_normal_initializer() # weight initializer
        self.logtau = tf.Variable( # init the \omega_\tau param
            initial_value=p_init(shape=(1, ), dtype="float32"),
            trainable=True)
        self.logvs = tf.Variable( # init the \omega_{V_s} param
            initial_value=p_init(shape=(1, ), dtype="float32"),
            trainable=True)

    ...
```

- In the `__init__` method we take care of weight initialization

RC Circuit Layer

The layer for the RC circuit gradient is in the `RCNablaLayer` class

```
class RCNablaLayer(keras.layers.Layer):
    ...

    def get_tau(self):
        return tf.math.exp(self.logtau) * self.tau_ref

    def get_vs(self):
        return tf.math.exp(self.logvs) * self.vs_ref

    def call(self, inputs):
        y, t = inputs # unpack the inputs
        return 1. / self.get_tau() * (self.get_vs() - y)
```

- We use dedicated method to obtain τ and V_s
- In the `call` method we compute the (ODE) gradient

Euler Method Model

The model for the Euler method is in the `ODEEulerModel` class

```
class ODEEulerModel(keras.Model):
    def __init__(self, f, **params): ...

    def call(self, inputs, training=False):
        y, T = inputs # unpack
        res = [y] # initial state
        for i in range(T.shape[1]-1):
            t, nt = T[:, i:i+1], T[:, i+1:i+2] # t_k and t_{k+1}
            dy = self.f([y, t], training=training) # gradient
            y = y + (nt - t) * dy # next state
            res.append(y) # store result
        res = tf.stack(res, axis=1) # concatenate
        return res
```

- The `__call__` method implements the method using tensor operators

Euler Method Model

The model for the Euler method is in the `ODEEulerModel` class

```
class ODEEulerModel(keras.Model):
    ...

    def train_step(self, data):
        (y0, T), yt = data # unpack
        with tf.GradientTape() as tape:
            y = self.call([y0, T], training=True) # ODE integration
            # Loss computation
            mask = ~tf.math.is_nan(yt)
            loss = self.compiled_loss(yt[mask], y[mask])
        ...
```

- The loss is computed as usual on all available measurements
- We can exclude points by setting the corresponding target to NaN

Training Set

We have a single sequence of measurements

...Therefore, just a training set (no validation, no test)

- Our first input is the initial state:

```
In [16]: tr_y0 = np.array(data.iloc[0]).reshape(1, -1); display(tr_y0)

         array([[0.]])
```

- The second is the sequence of evaluation points (time steps)

```
In [18]: tr_T = np.array(data.index).reshape(1, -1); display(tr_T[:, :30])

         array([[ 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.]])
```

Training Set

We have a single sequence of measurements

...Therefore, just a training set (no validation, no test)

- Then we need to prepare our ground truth

```
In [19]: tr_y = np.array(data['V']).reshape(1, -1)
         tr_y[:, 0] = np.nan
         display(tr_y[:, :30])
```

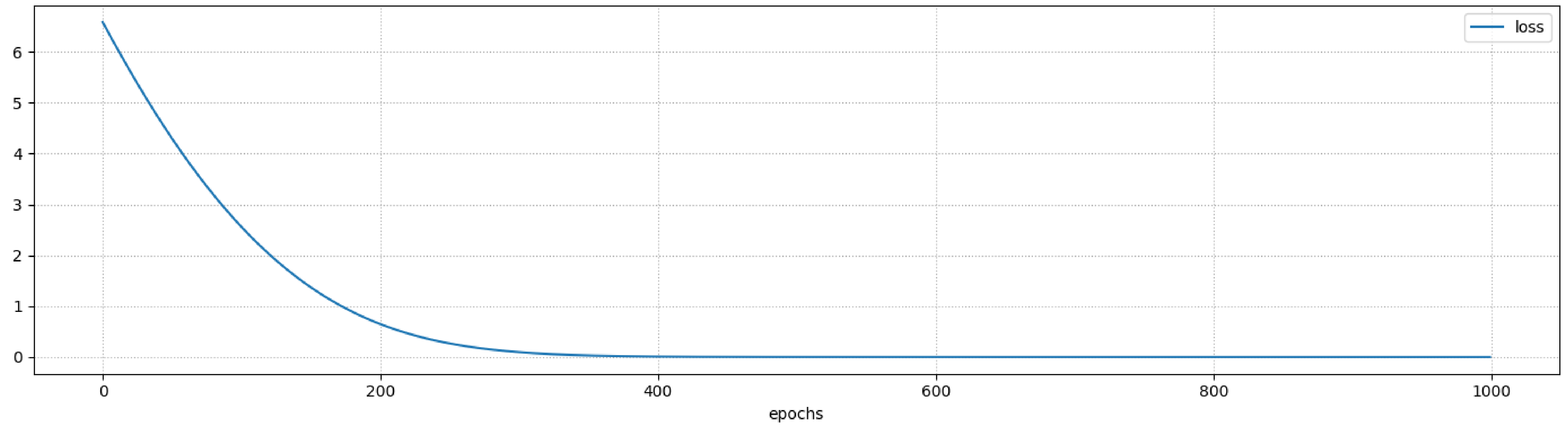
```
array([[        nan,  1.41003718,  2.6543906 ,  3.75252866,  4.7216321 ,
         5.57686288,  6.33160139,  6.99765581,  7.58544676,  8.10417046,
         8.56194251,  8.96592493,  9.32243816,  9.63705999,  9.91471279,
        10.15974045, 10.37597661, 10.56680439, 10.73520931, 10.88382613,
        11.01498002, 11.13072291, 11.23286566, 11.32300631, 11.40255515,
        11.47275676, 11.53470947, 11.58938254, 11.63763136, 11.6802108 ]])
```

- This is the sequence of all measurements, with the first state "masked"

Training Process

We can now build and train the model

```
In [23]: %%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: 0.0001 (training)
CPU times: user 9.1 s, sys: 497 ms, total: 9.6 s
Wall time: 8.23 s
```

Some Considerations

It seems to be working! But there are a few issues

First, the convergence is slow

- Stopping before ~500 epochs leads to less stable results

Second, we cannot use a validation set:

- This is due to the fact that we have a single sequence

Third, we are still not getting the correct parameters:

```
In [24]: 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), 8.56 (estimated)
Vs: 12.00 (real), 12.01 (estimated)
```

In the next section, we will see how to address these issues