Predicting the future is something you do all the time. In this chapter, we will discuss recurrent neural networks (RNNs)—a class of nets that can analyze time series data, e.g.,

- the number of daily active users on your website,
- the hourly temperature in your city,
- your home's daily power consumption,
- the trajectories of nearby cars,
- **...** ...



More generally, RNNs can work on sequences of arbitrary lengths, rather than on fixed-sized inputs. For example, they can take sentences, documents, or audio samples as input, making them extremely useful for natural language processing applications such as automatic translation or speech-to-text.

Plan:

- the fundamental concepts underlying RNNs;
- train RNN using backpropagation through time;
- compare with ARMA models;
- two main difficulties that RNNs face:
 - unstable gradients which can be alleviated using various techniques, including recurrent dropout and recurrent layer normalization.
 - limited short-term memory, which can be extended using LSTM and GRU cells.
- handle sequential data with other types of neural networks.



Feed Forward Neural Network: the activations flow only in one direction, from the input layer to the outputlayer.

Recurrent Neural Network: similar to a feed forward neural network, except it also has connections pointing backward.



Simple example: one neuron

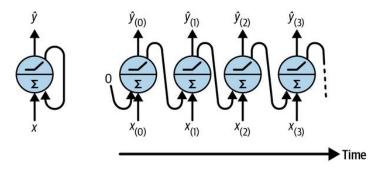


Figure: A recurrent neuron (left) unrolled through time (right)

create a layer of recurrent neurons

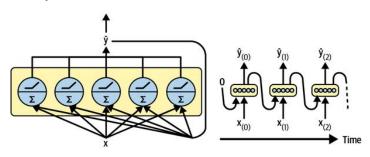


Figure: A layer of recurrent neurons (left) unrolled through time (right)

Each recurrent neuron has two sets of weights: one for the inputs $\boldsymbol{x}_(t)$ and the other for the outputs of the previous time step, $\hat{\boldsymbol{y}}_{(t-1)}$. If we consider the whole recurrent layer instead of just one recurrent neuron, we can place all the weight vectors in two weight matrices: $\boldsymbol{W}_{\boldsymbol{x}}$ and $\boldsymbol{W}_{\hat{\boldsymbol{y}}}$.

$$\hat{\boldsymbol{y}}_{(t)} = \phi(\boldsymbol{W}_{\boldsymbol{x}}\boldsymbol{x}_{(t)} + \boldsymbol{W}_{\hat{\boldsymbol{y}}}\hat{\boldsymbol{y}}_{(t-1)} + \boldsymbol{b})$$



Memory Cell

Since the output of a recurrent neuron at time step t is a function of all the inputs from previous time steps, you could say it has a form of memory. A part of a neural network that preserves some state across time steps is called a memory cell (or simply a cell).

Memory Cell

A cell's state at time step t, denoted $\boldsymbol{h}_{(t)}$ (the " \boldsymbol{h} " stands for "hidden"), is a function of some inputs at that time step and its state at the previous time step: $\boldsymbol{h}_{(t)} = f(\boldsymbol{x}_{(t)}, \boldsymbol{h}_{(t-1)})$.

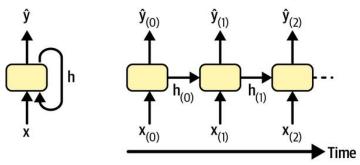
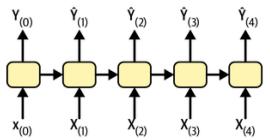


Figure: A cell's hidden state and its output may be different

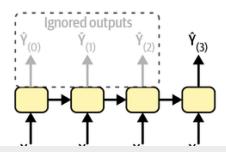


An RNN simultaneously take a sequence of inputs and produce a sequence of outputs. This type of sequence-to-sequence network is useful to forecast time series, such as your home's daily power consumption: you feed it the data over the last N days, and you train it to output the power consumption shifted by one day into the future.





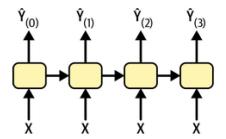
Alternatively, you could feed the network a sequence of inputs and ignore all outputs except for the last one. This is a sequence-to-vector network. For example, you could feed the network a sequence of words corresponding to a movie review, and the network would output a sentiment score (e.g., positive or negative).





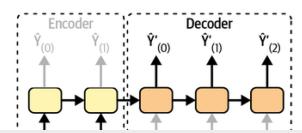
Conversely, you could feed the network the same input vector over and over again at each time step and let it output a sequence.

This is a vector-to-sequence network. For example, the input could be an image (or the output of a CNN), and the output could be a caption for that image.





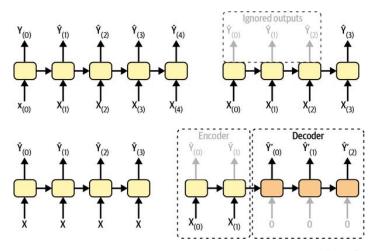
Lastly, you could have a sequence-to-vector network, called an **encoder**, followed by a vector-to-sequence network, called a **decoder**. For example, this could be used for translating a sentence from one language to another. You would feed the network a sentence in one language, the encoder would convert this sentence into a single vector representation, and then the decoder would decode this vector into a sentence in another language.





This two-step model, called an encoder-decoder, works much better than trying to translate on the fly with a single sequence-to-sequence RNN: the last words of a sentence can affect the first words of the translation, so you need to wait until you have seen the whole sentence before translating it.





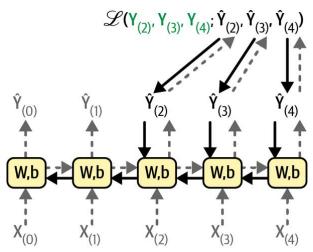
Training RNN

To train an RNN, the trick is to unroll it through time and then use regular backpropagation. This strategy is called backpropagation through time (BPTT).

- a first forward pass through the unrolled network;
- output sequence is evaluated using a loss function;
- compute the gradients of that loss through the unrolled network;
- a gradient descent step to update the parameters.



Training RNN



Training RNN

Note that this loss function may ignore some outputs. For example, in a sequence-to-vector RNN, all outputs are ignored except for the very last one. In this example, since the outputs $\hat{Y}_{(0)}$ and $\hat{Y}_{(1)}$ are not used to compute the loss, the gradients do not flow backward through them; they only flow through $\hat{Y}_{(2)}$, $\hat{Y}_{(3)}$, and $\hat{Y}_{(4)}$. Moreover, since the same parameters \boldsymbol{W} and \boldsymbol{b} are used at each time step, their gradients will be tweaked multiple times during backprop.



Your task is to build a model capable of forecasting the number of passengers that will ride on bus and rail the next day. You have access to daily ridership data since 2001.

The raw data is

	Α	В	С	D	E
1	service_date	day_type	bus	rail_boarding	total_rides
2	01/01/2001	U	297192	126455	423647
3	01/02/2001	W	780827	501952	1282779
4	01/03/2001	W	824923	536432	1361355
5	01/04/2001	W	870021	550011	1420032
6	01/05/2001	W	890426	557917	1448343

We start by loading and cleaning up the data:

```
In [7]: import pandas as pd
from pathlib import Path

path = Path("datasets/ridership/CTA_-_Ridership__Daily_Boarding_Totals.csv")
df = pd.read_csv(path, parse_dates=["service_date"])
df.columns = ["date", "day_type", "bus", "rail", "total"] # shorter names
df = df.sort_values("date").set_index("date")
df = df.drop("total", axis=1) # no need for total, it's just bus + rail
df = df.drop_duplicates() # remove duplicated months (2011-10 and 2014-07)
```

Let's check what the first few rows look like:

	df.head()					
Out[8]:		day_type	bus	rail		
	date					
	2001-01-01	U	297192	126455		
	2001-01-02	W	780827	501952		
	2001-01-03	W	824923	536432		
	2001-01-04	W	870021	550011		
	2001-01-05	W	890426	557917		

On January 1st, 2001, 297,192 people boarded a bus, and 126,455 boarded a train. The day_type column contains $\bf W$ for Week-days, $\bf A$ for Saturdays, and $\bf U$ for Sundays or holidays.

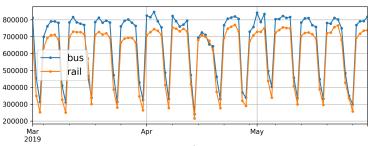


Let's plot the bus and rail ridership figures over a few months in 2019:

```
In [10]: import matplotlib.pyplot as plt

df["2019-03":"2019-05"].plot(grid=True, marker=".", figsize=(8, 3.5))

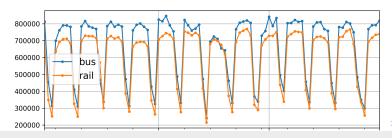
save_fig("daily_ridership_plot") # extra code - saves the figure for the book
plt.show()
```



- This is a time series: data with values at different time steps, usually at regular intervals.
- Since there are multiple values per time step, this is called a multivariate time series.
- ► If we only looked at the bus column, it would be a univariate time series, with a single value per time step.
- Predicting future values (i.e., forecasting) is the most typical task when dealing with time series.



We can see that a similar pattern is clearly repeated every week. This is called a weekly seasonality. In fact, it's so strong in this case that forecasting tomorrow's ridership by just copying the values from a week earlier will yield reasonably good results. This is called naive forecasting: simply copying a past value to make our forecast. Naive fore-casting is often a great baseline, and it can even be tricky to beat in some cases.

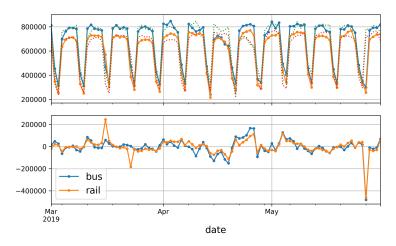




To visualize these naive forecasts, let's overlay the two time series (for bus and rail) as well as the same time series lagged by one week using dotted lines. We'll also plot the difference between the two (i.e., the value at time t minus the value at time t - 7); this is called differencing.

```
In [12]: diff_7 = df[["bus", "rail"]].diff(7)["2019-03":"2019-05"]

fig, axs = plt.subplots(2, l, sharex=True, figsize=(8, 5))
df.plot(ax=axs[0], legend=False, marker=".") # original time series
df.shift(7).plot(ax=axs[0], grid=True, legend=False, linestyle=":") # lagged
diff_7.plot(ax=axs[1], grid=True, marker=".") # 7-day difference time series
axs[0].set_ylim([170_000, 900_000]) # extra code - beautifies the plot
save_fig("differencing_plot") # extra code - saves the figure
plt.show()
```



Notice how closely the lagged time series track the actual time series. When a time series is correlated with a lagged version of itself, we say that the time series is autocorrelated. As you can see, most of the differences are fairly small, except at the end of May. Maybe there was a holiday at that time?

```
In [13]: list(df.loc["2019-05-25":"2019-05-27"]["day_type"])
Out[13]: ['A', 'U', 'U']
```



Let's just measure the mean absolute error (MAE) over the three-month period:

It's hard to tell at a glance how good or bad this is:

Figure: mean absolute percentage error (MAPE)



Note. The MAE, MAPE, and MSE are among the most common metrics you can use to evaluate your forecasts. As always, choosing the right metric depends on the task. For example, if your project suffers quadratically more from large errors than from small ones, then the MSE may be preferable, as it strongly penalizes large errors.

Looking at the time series, there does not appear to be any significant monthly seasonality, but let's check whether there's any yearly seasonality.

```
In [16]: period = slice("2001", "2019")

df_monthly = df.resample("M').mean() # compute the mean for each month rolling_average_12_months = df_monthly[period].rolling(window=12).mean()

fig, ax = plt.subplots(figsize=(8, 4))

df_monthly[period].plot(ax=ax, marker=".")

rolling_average_12_months.plot(ax=ax, grid=True, legend=False)

save_fig("long_term_ridership_plot") # extra code - saves the figure plt.show()
```

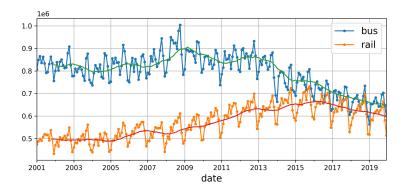
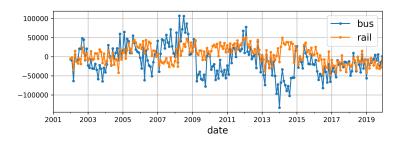


Figure: There's definitely some yearly seasonality as well, although it is noisier than the weekly seasonality and more visible for the rail series than the bus series.



Let's check what we get if we plot the 12-month difference

```
In [17]: df_monthly.diff(12)[period].plot(grid=True, marker=".", figsize=(8, 3))
    save_fig("yearly_diff_plot") # extra code - saves the figure
    plt.show()
```



- ▶ Notice how differencing not only removed the yearly seasonality but also removed the long-term trends. For example, the linear downward trend present in the time series from 2016 to 2019 became a roughly constant negative value in the differenced time series.
- Differencing is a common technique used to remove trend and seasonality from a time series: it's easier to study a stationary time series, meaning one whose statistical properties remain constant over time, without any seasonality or trends.
- Once you're able to make accurate forecasts on the differenced time series, it's easy to turn them into forecasts for the actual time series by just adding back the past values that were previously subtracted.



Recall

Important concepts in time series analysis:

- seasonality;
- trend;
- differencing;
- moving average.

ARMA Model

We start with the autoregressive moving average (ARMA) model: it computes its forecasts using a simple weighted sum of lagged values and corrects these forecasts by adding a moving average.

$$\hat{\boldsymbol{y}}_{(t)} = \sum_{i=1}^{p} \alpha_i \boldsymbol{y}_{(t-i)} + \sum_{i=1}^{q} \theta_i \epsilon_{(t-i)}$$

with
$$\epsilon_{(t)} = \boldsymbol{y}_{(t)} - \hat{\boldsymbol{y}}_{(t)}$$
.



- ► This model assumes that the time series is stationary. If it is not, then differencing may help.
- Using differencing over a single time step will produce an approximation of the derivative of the time series: indeed, it will give the slope of the series at each time step.
- This means that it will eliminate any linear trend, transforming it into a constant value. For example, if you apply one-step differencing to the series [3,5,7,9,11], you get the differenced series [2,2,2,2].



- ▶ If the original time series has a quadratic trend instead of a linear trend, then a single round of differencing will not be enough. For example, the series [1,4,9,16,25,36] becomes [3,5,7,9,11] after one round of differencing.
- ▶ But if you run differencing for a second round, then you get [2, 2, 2, 2]. So, running two rounds of differencing will eliminate quadratic trends.
- More generally, running d consecutive rounds of differencing computes an approximation of the d-th order derivative of the time series, so it will eliminate polynomial trends up to degree d.
- ightharpoonup This hyperparameter d is called the order of integration.



Differencing is the central contribution of the autoregressive integrated moving average (ARIMA) model that runs d rounds of differencing to make the time series more stationary, then it applies a regular ARMA model. When making forecasts, it uses this ARMA model, then it adds back the terms that were subtracted by differencing.



- One last member of the ARMA family is the seasonal ARIMA (SARIMA) model: it models the time series in the same way as ARIMA, but it additionally models a seasonal component for a given frequency (e.g., weekly), using the exact same ARIMA approach.
- It has a total of seven hyperparameters: the same $p,\ d$, and q hyperparameters as ARIMA, plus additional $P,\ D$, and Q hyperparameters to model the seasonal pattern, and lastly the period of the seasonal pattern, noted s.
- ▶ The hyperparameters P, D, and Q are just like p, d, and q, but they are used to model the time series at t-s, t-2s, t-3s, etc.



We pretend today is the last day of May 2019, and we want to forecast the rail ridership for "tomorrow", the 1st of June, 2019.

- asfreq("D") sets the time series' frequency to daily;
- order = (1,0,0) means that p = 1, d = 0, q = 0;
- ▶ seasonal_order = (0,1,1,7) means that P=0, D=1, Q=1, and s=7.



Pretty bad. Perhaps we were just unlucky that day.

```
In [25]: y_pred[0] # ARIMA forecast
Out[25]: 427758.62630005495

In [26]: df["rai1"].loc["2019-06-01"] # target value
Out[26]: 379044

In [27]: df["rai1"].loc["2019-05-25"] # naive forecast out[27]: 426932
```

We run the same code in a loop to make forecasts for every day in March, April, and May, and compute the MAE over that period.

```
In [28]:

origin, start_date, end_date = "2019-01-01", "2019-03-01", "2019-05-31" time_period = pd.date_range(start_date, end_date) rail_series = df.loc[origin:end_date]["rail"].asfreq("D") y_preds = []

for today in time_period.shift(-1):

model = ARIMA(rail_series[origin:today], # train on data up to "today" order=(1, 0, 0), seasonal_order=(0, 1, 1, 7))

model = model.fit() # note that we retrain the model every day! y_pred = model.forecast()[0]

y_preds.append(y_pred)

y_preds = pd.Series(y_preds, index=time_period)

mae = (y_preds - rail_series[time_period]).abs().mean() # returns 32,040.7

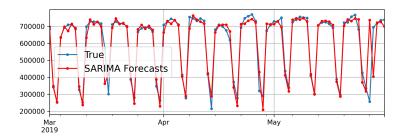
In [29]: mae

Out[29]: 32040.720106810877
```

The MAE is about 32,041, which is significantly lower than the MAE we got with naive forecasting (42,143).

Displays the SARIMA forecasts

```
In [30]: fig, ax = plt.subplots(figsize=(8, 3))
    rail_series.loc[time_period].plot(label="True", ax=ax, marker=".", grid=True)
    ax.plot(y_preds, color="r", marker=".", label="SARIMA Forecasts")
    plt.legend()
    plt.show()
```



At this point, you may be wondering how to pick good hyperparameters for the SARIMA model. There are several methods, but the simplest to understand and to get started with is the brute-force approach: just run a grid search. For each model you want to evaluate (i.e., each hyperparameter combination), you can run the preceding code example, changing only the hyperparameter values.

The model with the lowest MAE wins. Of course, you can replace the MAE with another metric if it better matches your business objective.



Preparing the Data

Now we have two baselines: naive forecasting and SARIMA. Let's try to use machine learning models to forecast this time series, starting with a basic linear model. Our goal will be to forecast tomorrow's ridership based on the ridership of the past 8 weeks of data (56 days).

But what will we use as training data? Well, that's the trick: we will use every 56-day window from the past as training data, and the target for each window will be the value immediately following it.

Preparing the Data

The windows are [0, 1, 2], [1, 2, 3], and [2, 3, 4], and their respective targets are 3, 4, and 5.



Preparing the Data

We split the data into a training period, a validation period, and a test period. We focus on the rail ridership and scale it down by a factor of one million, to ensure the values are near the 0-1 range.

```
In [9]: rail_train = df["rail"]["2016-01": "2018-12"] / le6
   rail_valid = df["rail"]["2019-01": "2019-06"] / le6
   rail_test = df["rail"]["2019-06":] / le6
```

Now we are ready to build and train any model.

```
In [10]:

seq_length = 56

tf.random_set_seed(42)  # extra code - ensures reproducibility

train_ds = tf.keras.utils.timeseries_dataset_from_array(
    rail_train.to_numpy(),
    targets=rail_train[seq_length:],
    sequence_length=seq_length,
    batch_size=32,
    shuffle=True,
    seed=42

)

valid_ds = tf.keras.utils.timeseries_dataset_from_array(
    rail_valid.to_numpy(),
    targets=rail_valid.seq_length:],
    sequence_length=seq_length,
    batch_size=32
)
```

Linear Model

This model reaches a validation MAE of about 37591. That's better than naive forecasting but worse than the SARIMA model.

```
In [12]: # extra code - evaluates the model valid_loss, valid_mae = model.evaluate(valid_ds) valid_mae * le6

3/3 [=======] - 0s 43ms/step - loss: 0.0021 - mae: 0.0376

Out[12]: 37591.252475976944
```

Simple RNN

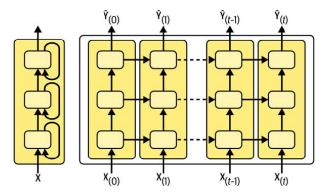
It's no good at all: its validation MAE is greater than 100,000! (102784.6559882164)

That's the best model we've trained so far (30813.174322247505), and it even beats the SARIMA model



Deep RNN

Just stack recurrent layers!



Deep RNN

It reaches an MAE of about 30422.

Multivariate Time Series

A great quality of neural networks is their flexibility: in particular, they can deal with multivariate time series with almost no change to their architecture.

```
In [20]: df_mulvar = df[["bus", "rail"]] / le6 # use both bus & rail series as input
          df_mulvar["next_day_type"] = df["day_type"].shift(-1) # we know tomorrow's type
          df mulvar = pd, get dummies(df mulvar) # one-hot encode the day type
In [21]: mulvar train = df mulvar["2016-01":"2018-12"]
          mulvar valid = df mulvar["2019-01":"2019-05"]
          mulvar_test = df_mulvar["2019-06":]
In [22]: tf. random, set seed (42) # extra code - ensures reproducibility
          train mulvar ds = tf. keras, utils, timeseries dataset from arrav(
              mulvar_train.to_numpy(), # use all 5 columns as input
              targets=mulvar train["rail"][see length:], # forecast only the rail series
              sequence length=seq length.
              batch size=32.
              shuffle=True.
              seed=42
          valid_mulvar_ds = tf. keras. utils. timeseries_dataset_from_array(
              mulvar valid to numpy().
              targets=mulvar_valid["rail"][seq length:].
              sequence length=seq length.
              batab siza-22
```



Deep RNN

```
In [23]:
tf.random.set_seed(42) # extra code - ensures reproducibility
mulvar_model = tf.keras.Sequential([
    tf.keras.layers.SimpleRNN(32, input_shape=[None, 5]),
    tf.keras.layers.Dense(1)
])
```

At each time step, the model now receives five inputs instead of one. This model reaches a validation MAE of 23537.

Deep RNN

It's not too hard to make the RNN forecast for both the bus and rail ridership.

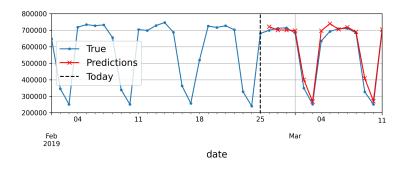
```
In [56]: # extra code - build and train a multitask RNN that forecasts both bus and rail
          tf. random. set seed (42)
          seq length = 56
          train multask ds = tf. keras. utils. timeseries dataset from array(
               mulvar train. to numpy(),
              targets=mulvar_train[["bus", "rail"]][seq_length:], # 2 targets per day
              sequence_length=seq_length,
              batch size=32.
              shuffle=True
               seed=42
          valid multask ds = tf. keras, utils, timeseries dataset from array(
              mulvar valid to numpy(),
              targets=mulvar_valid[["bus", "rail"]][seq_length:],
               sequence_length=seq_length,
              batch size=32
          tf. random. set seed(42)
          multask model = tf.keras.Sequential([
               tf. keras. layers. SimpleRNN(32, input_shape=[None, 5]),
              tf. keras, lavers, Dense (2)
```

It reaches a validation MAE of 25,330 for rail and 26,369for bus, which is pretty good.

The first option is to take the univar_model RNN we trained earlier for the rail time series, make it predict the next value, and add that value to the inputs, acting as if the predicted value had actually occurred; we would then use the model again to predict the following value, and so on.

```
In [36]: import numpy as np

X = rail_valid.to_numpy()[np.newaxis, :seq_length, np.newaxis]
for step_ahead in range(14):
    y_pred_one = univar_model.predict(X)
    X = np.concatenate([X, y_pred_one.reshape(1, 1, 1)], axis=1)
```



The second option is to train an RNN to predict the next 14 values in one shot. We can still use a sequence-to-vector model, but it will output 14 values instead of 1.

```
[38]: tf.random.set_seed(42) # extra code - ensures reproducibility
       def split inputs and targets(mulvar series, ahead=14, target col=1):
            return mulvar series[:, :-ahead], mulvar series[:, -ahead:, target col]
       ahead_train_ds = tf. keras. utils. timeseries_dataset_from_array(
            mulvar train, to numpy().
           targets=None.
           sequence length=seq length + 14.
           batch size=32.
            shuffle=True.
            seed=42
       ).map(split_inputs_and_targets)
       ahead valid ds = tf. keras, utils, timeseries dataset from arrav(
            mulvar valid to numpy().
           targets=None.
           sequence length=seq length + 14.
            batch size=32
        ), map(split inputs and targets)
```

It reaches a prediction MAE of 34203.

This approach works quite well. Its forecasts for the next day are obviously better than its forecasts for 14 days into the future, but it doesn't accumulate errors as the previous approach did.

Instead of training the model to forecast the next 14 values only at the very last time step, we can train it to forecast the next 14 values at each and every time step. In other words, we can turn this sequence-to-vector RNN into a sequence-to-sequence RNN.



At time step 0 the model will output a vector containing the forecasts for time steps 1 to 14, then at time step 1 the model will forecast time steps 2 to 15, and so on. In other words, the targets are sequences of consecutive windows, shifted by one-time step at each time step. The target is not a vector any more, but a sequence of the same length as the inputs, containing a 14-dimensional vector at each step.

Preparing the datasets is not trivial. For example, let's turn the series of numbers 0 to 6 into a dataset containing sequences of 4 consecutive windows, each of length 3:

Now we can use the map() method to split these windows of windows into inputs and targets:

```
In [45]: 

def to_seq2seq_dataset(series, seq_length=56, ahead=14, target_col=1, batch_size=32, shuffle=False, seed=None):

ds = to_windows(tf. data.Dataset.from_tensor_slices(series), ahead + 1)

ds = to_windows(ds, seq_length).map(lambda S: (S[:, 0], S[:, 1:, 1]))

if shuffle:

ds = ds. shuffle(8 * batch_size, seed=seed)

return ds. batch(batch_size)

In [46]: 
seq2seq_train = to_seq2seq_dataset(mulvar_train, shuffle=True, seed=42)

seq2seq_valid = to_seq2seq_dataset(mulvar_valid)

In [47]: 
tf. random.set_seed(42) # extra code - ensures reproducibility

seq2seq_model = tf. keras. Sequential([
    tf. keras. layers. SimpleRNN(32, return_sequences=True, input_shape=[None, 5]),
    tf. keras. layers.Dense(14)

# equivalent: tf. keras. layers. TimeDistributed(tf. keras. layers.Dense(14))

# also equivalent: tf. keras. layers. Conv1D(14, kernel_size=1)

])
```

```
In [50]: Y pred valid = seq2seq model.predict(seq2seq valid)
          for ahead in range (14):
             preds = pd. Series(Y_pred_valid[:-1, -1, ahead],
                               index=mulvar valid, index[56 + ahead : -14 + ahead])
             mae = (preds - mulvar_valid["rail"]).abs().mean() * 1e6
             print(f"MAE for +{ahead + 1}: {mae:..0f}")
          3/3 [======] - Os 5ms/step
         MAE for +1: 24,501
         MAE for +2: 27,870
         MAE for +3: 29,396
         MAE for +4: 32,048
         MAE for +5: 32,972
         MAE for +6: 34, 170
         MAE for +7: 35,778
         MAE for +8: 36,076
         MAE for +9: 33,626
         MAE for +10: 32,891
         MAE for +11: 38,944
         MAE for +12: 38,702
         MAE for +13: 37,223
         MAE for +14: 35.361
```