AI in Biomedical Data

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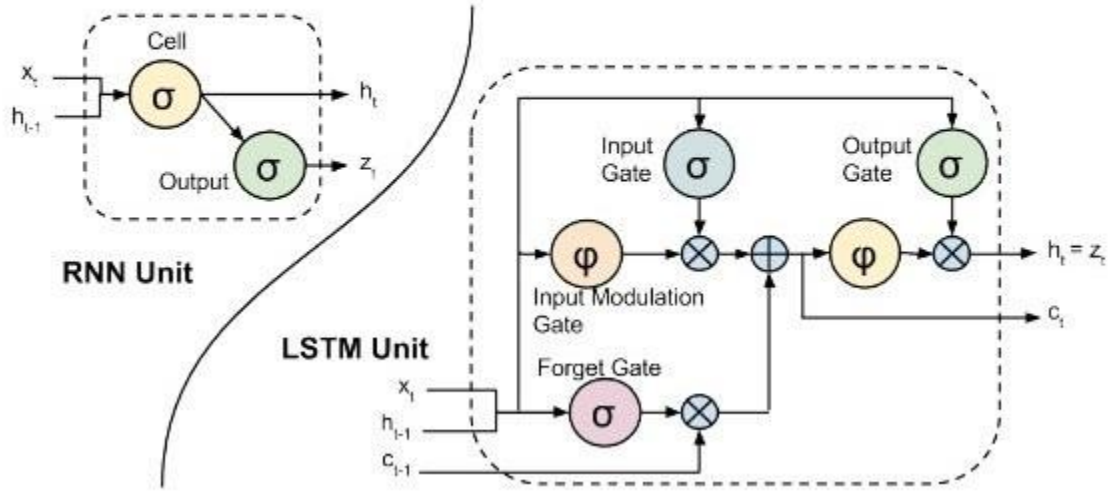
github.com/mbkhodabakhshi/AI_in_BiomedicalData

Sequence Learning



یادگیری ماشین در زیست پزشکی

Chapter 15. Processing Sequences Using RNNs and CNNs

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In this chapter we will discuss recurrent neural networks (RNNs), a class of nets that can predict the future (well, up to a point, of course). They can analyze time series data such as stock prices, and tell you when to buy or sell. In autonomous driving systems, they can anticipate car trajectories and help avoid accidents. More generally, they can work on sequences of arbitrary lengths, rather than on fixed-sized inputs like all the nets we have considered so far. 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.

In this chapter we will first look at the fundamental concepts underlying RNNs and how to train them using backpropagation through time, then we will use them to forecast a time series. After that we'll explore the two main difficulties that RNNs face:

- Unstable gradients (discussed in Chapter 11), which can be alleviated using various techniques, including recurrent dropout and recurrent layer normalization
- A (very) limited short-term memory, which can be extended using LSTM and GRU cells

Recurrent Neurons and Layer

Up to now we have focused on feedforward neural networks, where the activations flow only in one direction, from the input layer to the output layer (a few exceptions are discussed in Appendix E). A recurrent neural network looks very much like a feedforward neural network, except it also has connections pointing backward. Let's look at the simplest possible RNN, composed of one neuron receiving inputs, producing an output, and sending that output back to itself, as shown in Figure 15-1 (left). At each *time step t* (also called a *frame*), this *recurrent neuron* receives the inputs $\mathbf{x}_{(t)}$ as well as its own output from the previous time step, $y_{(t-1)}$. Since there is no previous output at the first time step, it is generally set to 0. We can represent this tiny network against the time axis, as shown in Figure 15-1 (right). This is called *unrolling the network through time* (it's the same recurrent neuron represented once per time step).

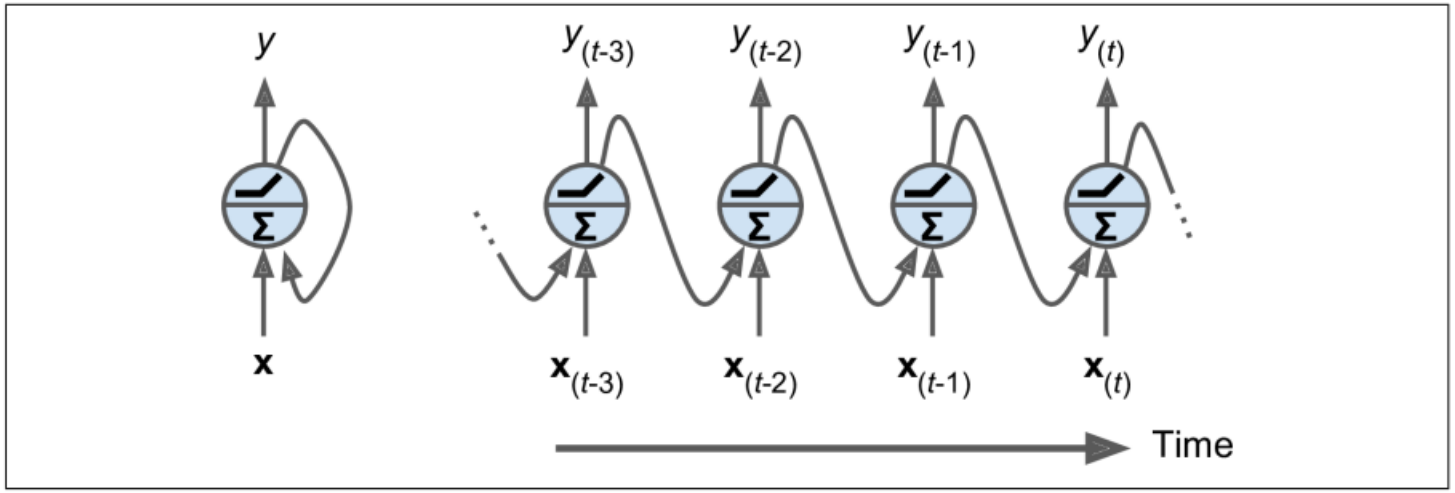


Figure 15-1. A recurrent neuron (left) unrolled through time (right)

You can easily create a layer of recurrent neurons. At each time step t, every neuron receives both the input vector $\mathbf{x}_{(t)}$ and the output vector from the previous time step $\mathbf{y}_{(t-1)}$, as shown in Figure 15-2. Note that both the inputs and outputs are vectors now (when there was just a single neuron, the output was a scalar).

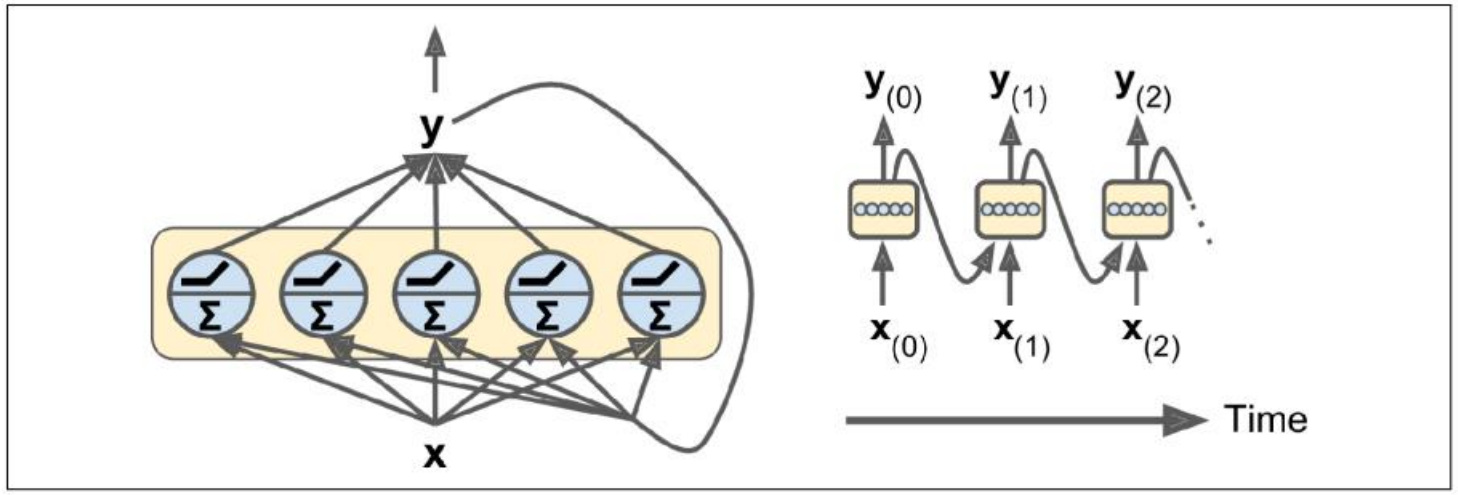


Figure 15-2. A layer of recurrent neurons (left) unrolled through time (right)

Each recurrent neuron has two sets of weights: one for the inputs $\mathbf{x}_{(t)}$ and the other for the outputs of the previous time step, $\mathbf{y}_{(t-1)}$. Let's call these weight vectors $\mathbf{w}_x$ and $\mathbf{w}_y$. If we consider the whole recurrent layer instead of just one recurrent neuron, we can place all the weight vectors in two weight matrices, $\mathbf{W}_x$ and $\mathbf{W}_y$. The output vector of the whole recurrent layer can then be computed pretty much as you might expect, as shown in Equation 15-1 ($\mathbf{b}$ is the bias vector and $\phi(\cdot)$ is the activation function (e.g., ReLU[1]).

Equation 15-1. Output of a recurrent layer for a single instance

$$\mathbf{y}_{(t)} = \phi\left(\mathbf{W}_x{}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_y{}^{\top}\mathbf{y}_{(t-1)} + \mathbf{b}\right)$$

Just as with feedforward neural networks, we can compute a recurrent layer's output in one shot for a whole mini-batch by placing all the inputs at time step t in an input matrix $\mathbf{X}_{(t)}$ (see Equation 15-2).

$$\mathbf{Y}_{(t)} = \phi\left(\mathbf{X}_{(t)}\mathbf{W}_x + \mathbf{Y}_{(t-1)}\mathbf{W}_y + \mathbf{b}\right)$$
$$= \phi\left(\left[\mathbf{X}_{(t)} \quad \mathbf{Y}_{(t-1)}\right]\mathbf{W} + \mathbf{b}\right) \text{ with } \mathbf{W} = \begin{bmatrix}\mathbf{W}_x \\ \mathbf{W}_y\end{bmatrix}$$

In this equation:

- $\mathbf{Y}_{(t)}$ is an $m \times n_{\text{neurons}}$ matrix containing the layer's outputs at time step t for each instance in the mini-batch (m is the number of instances in the mini-batch and n_{neurons} is the number of neurons).
- $\mathbf{X}_{(t)}$ is an $m \times n_{\text{inputs}}$ matrix containing the inputs for all instances (n_{inputs} is the number of input features).
- $\mathbf{W}_x$ is an $n_{\text{inputs}} \times n_{\text{neurons}}$ matrix containing the connection weights for the inputs of the current time step.
- $\mathbf{W}_y$ is an $n_{\text{neurons}} \times n_{\text{neurons}}$ matrix containing the connection weights for the outputs of the previous time step.
- $\mathbf{b}$ is a vector of size n_{neurons} containing each neuron's bias term.
- The weight matrices $\mathbf{W}_x$ and $\mathbf{W}_y$ are often concatenated vertically into a single weight matrix $\mathbf{W}$ of shape $(n_{\text{inputs}} + n_{\text{neurons}}) \times n_{\text{neurons}}$ (see the second line of Equation 15-2).
- The notation $[\mathbf{X}_{(t)}\ \mathbf{Y}_{(t-1)}]$ represents the horizontal concatenation of the matrices $\mathbf{X}_{(t)}$ and $\mathbf{Y}_{(t-1)}$.

Memory Cells

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*). A single recurrent neuron, or a layer of recurrent neurons, is a very basic cell, capable of learning only short patterns (typically about 10 steps long, but this varies depending on the task). Later in this chapter, we will look at some more complex and powerful types of cells capable of learning longer patterns (roughly 10 times longer, but again, this depends on the task).

In general a cell's state at time step t, denoted $\mathbf{h}_{(t)}$ (the "h" stands for "hidden"), is a function of some inputs at that time step and its state at the previous time step: $\mathbf{h}_{(t)} = f(\mathbf{h}_{(t-1)}, \mathbf{x}_{(t)})$. Its output at time step t, denoted $\mathbf{y}_{(t)}$, is also a function of the previous state and the current inputs. In the case of the basic cells we have discussed so far, the output is simply equal to the state, but in more complex cells this is not always the case, as shown in Figure 15-3.

In the case of the basic cells we have discussed so far, the output is simply equal to the state, but in more complex cells this is not always the case, as shown in Figure 15-3.

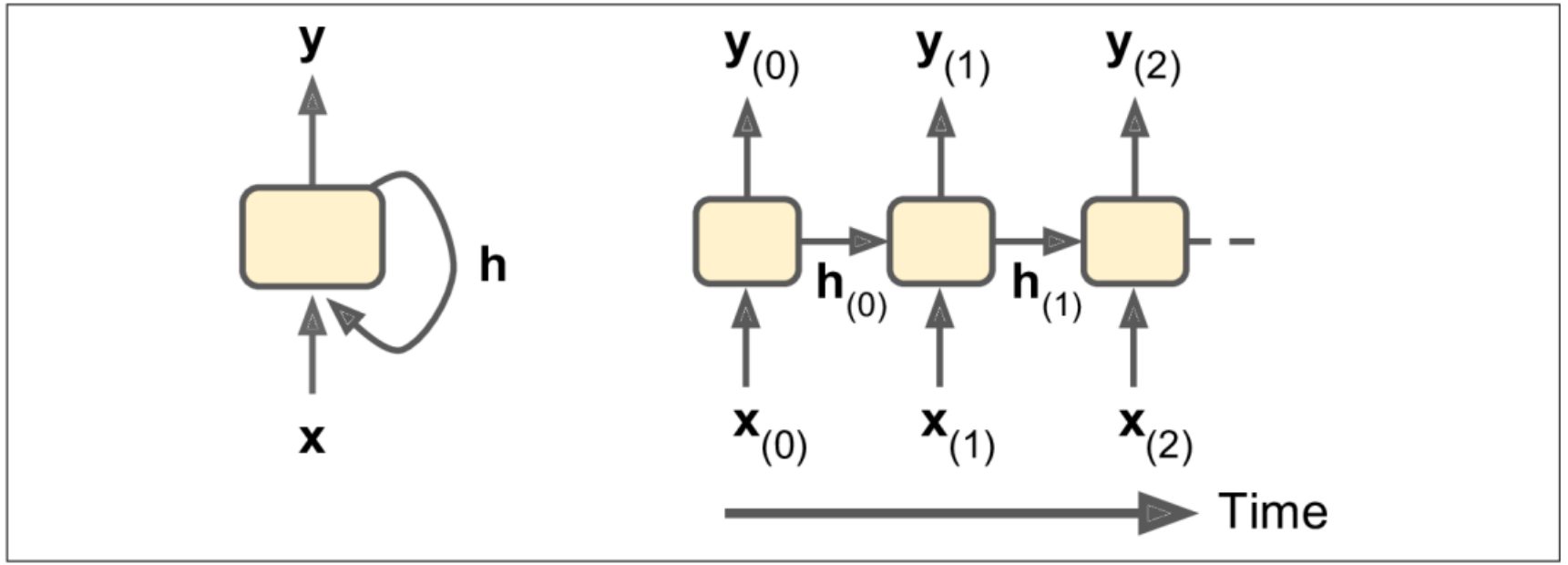
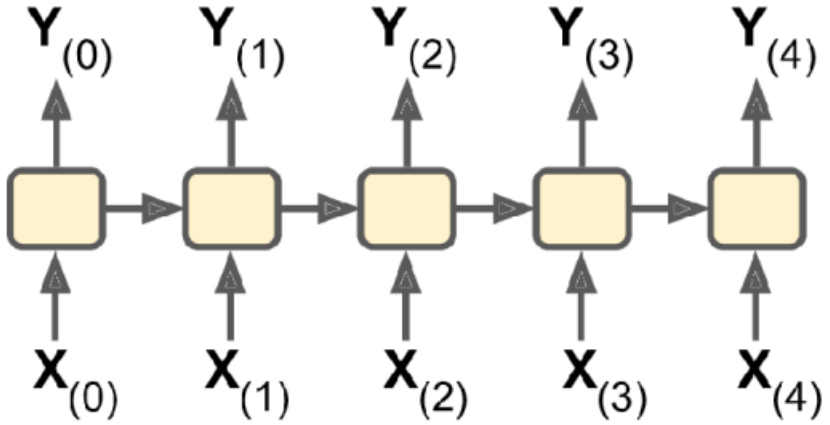
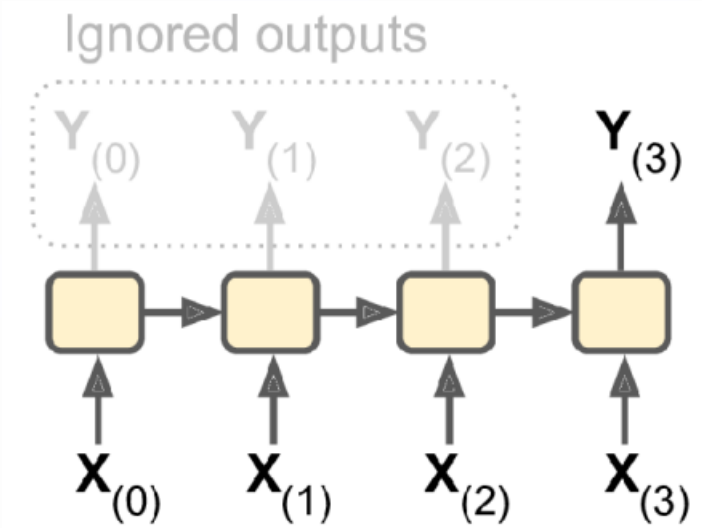


Figure 15-3. A cell's hidden state and its output may be different

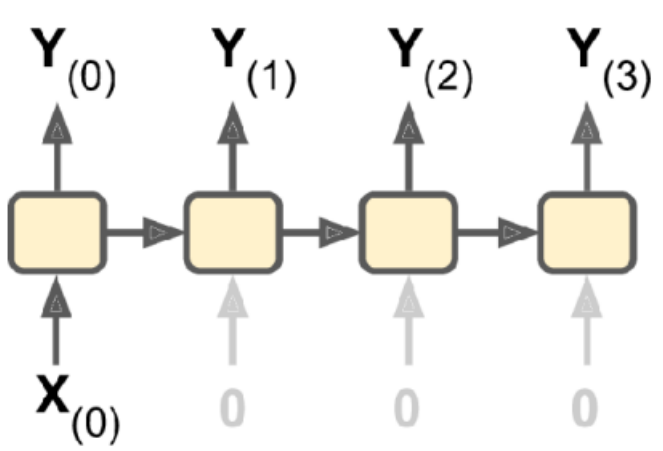
An RNN can simultaneously take a sequence of inputs and produce a sequence of outputs (see the top-left network in Figure 15-4). This type of *sequence-to-sequence network* is useful for predicting time series such as stock prices: you feed it the prices over the last N days, and it must output the prices shifted by one day into the future (i.e., from $N - 1$ days ago to tomorrow).



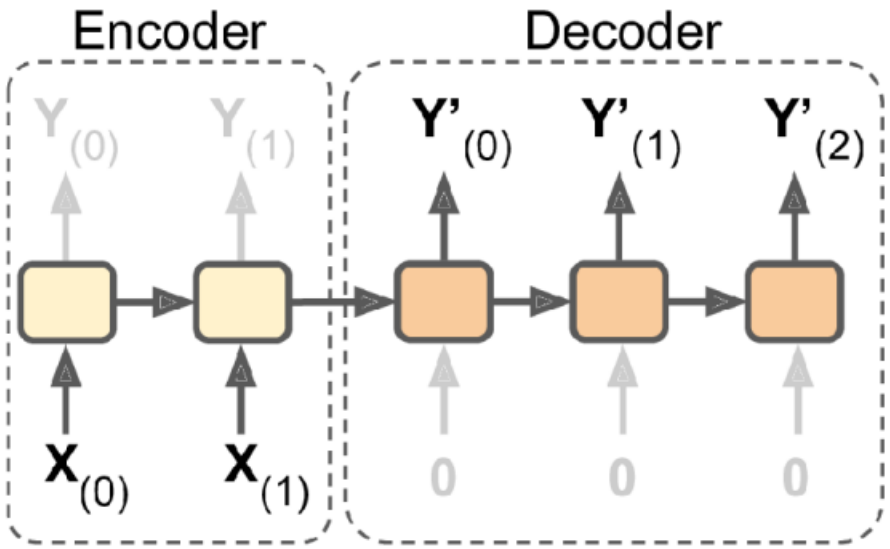
Alternatively, you could feed the network a sequence of inputs and ignore all outputs except for the last one (see the top-right network in Figure 15-4). In other words, this is a *sequence-to-vector network*. For example, you could feed the network a sequence of words corresponding to a movie review, and the network would output a sentiment score (e.g., from –1 [hate] to +1 [love]).



Conversely, you could feed the network the same input vector over and over again at each time step and let it output a sequence (see the bottom-left network of Figure 15-4). 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* (see the bottom-right network of Figure 15-4). 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 (like the one represented at the top left): 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. We will see how to implement an Encoder–Decoder in Chapter 16 (as we will see, it is a bit more complex than in Figure 15-4 suggests).



Training RNNs

To train an RNN, the trick is to unroll it through time (like we just did) and then simply use regular backpropagation (see Figure 15-5). This strategy is called *backpropagation through time* (BPTT).

Just like in regular backpropagation, there is a first forward pass through the unrolled network (represented by the dashed arrows). Then the output sequence is evaluated using a cost function $C(\mathbf{Y}_{(0)}, \mathbf{Y}_{(1)}, \ldots \mathbf{Y}_{(T)})$ (where T is the max time step). Note that this cost function may ignore some outputs, as shown in Figure 15-5 (for example, in a sequence-to-vector RNN, all outputs are ignored except for the very last one). The gradients of that cost function are then propagated backward through the unrolled network (represented by the solid arrows). Finally the model parameters are updated using the gradients computed during BPTT. Note that the gradients flow backward through all the outputs used by the cost function, not just through the final output (for example, in Figure 15-5 the cost function is computed using the last three outputs of the network, $\mathbf{Y}_{(2)}$, $\mathbf{Y}_{(3)}$, and $\mathbf{Y}_{(4)}$, so gradients flow through these three outputs, but not through $\mathbf{Y}_{(0)}$ and $\mathbf{Y}_{(1)}$). Moreover, since the same parameters $\mathbf{W}$ and $\mathbf{b}$ are used at each time step, backpropagation will do the right thing and sum over all time steps.

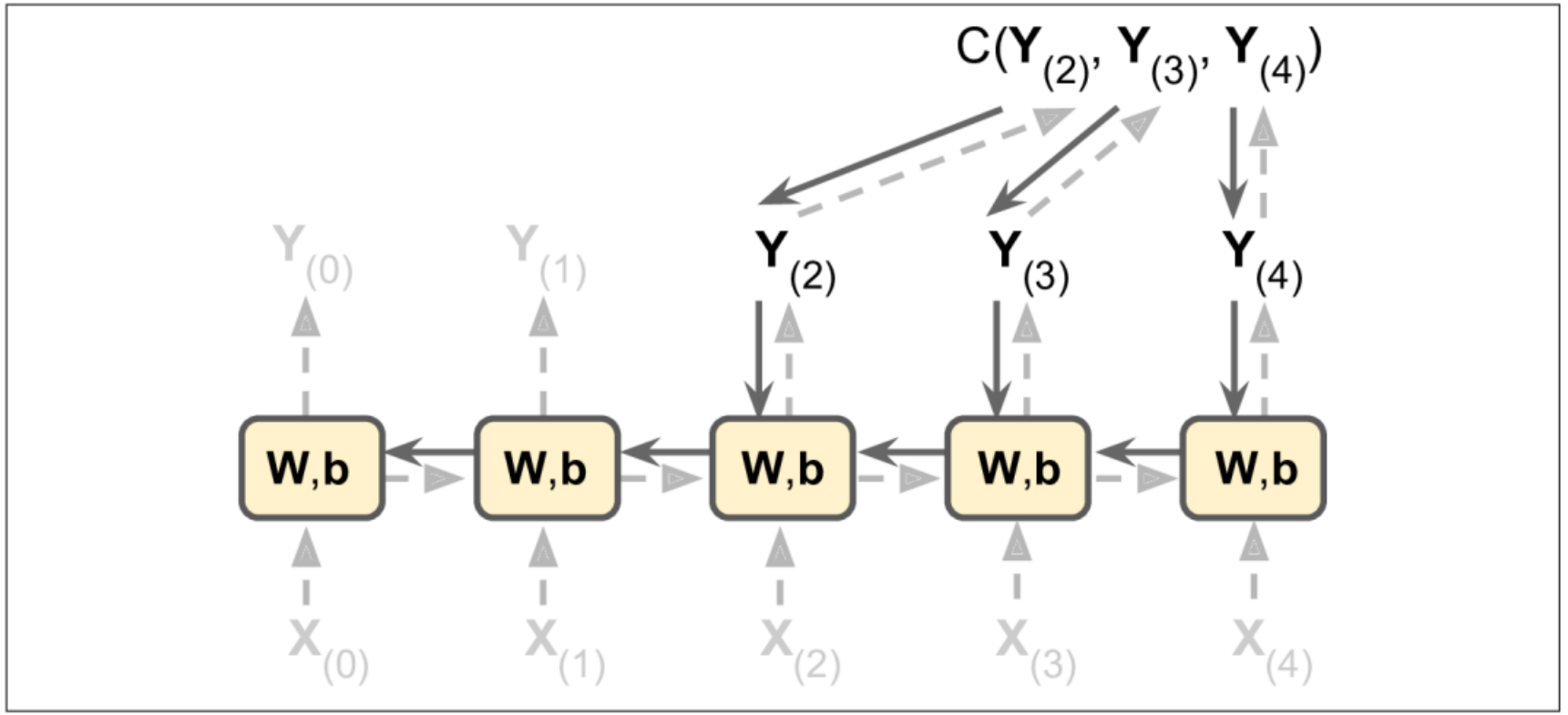


Figure 15-5. Backpropagation through time

- Suppose you are studying the number of active users per hour on your website, or the daily temperature in your city, or your company's financial health, measured quarterly using multiple metrics. In all these cases, the data will be a sequence of one or more values per time step. This is called a *time series*.
- In the first two examples there is a single value per time step, so these are *univariate time series*, while in the financial example there are multiple values per time step (e.g., the company's revenue, debt, and so on), so it is a *multivariate time series*.
- A typical task is to predict future values, which is called *forecasting*.
- Another common task is to fill in the blanks: to predict (or rather "postdict") missing values from the past. This is called *imputation*. For example, Figure 15-6 shows 3 univariate time series, each of them 50 time steps long, and the goal here is to forecast the value at the next time step (represented by the X) for ea

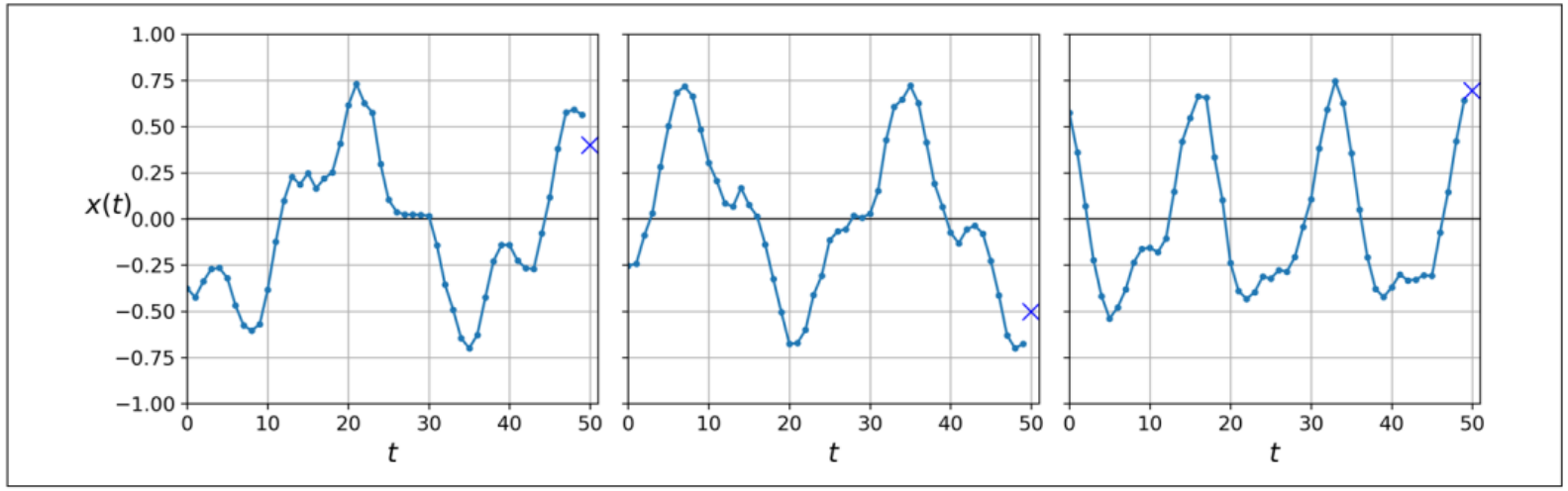


Figure 15-6. Time series forecasting

For simplicity, we are using a time series generated by the `generate_time_series()` function, shown here:

```
def generate_time_series(batch_size, n_steps):
    freq1, freq2, offsets1, offsets2 = np.random.rand(4, batch_size, 1)
    time = np.linspace(0, 1, n_steps)
    series = 0.5 * np.sin((time - offsets1) * (freq1 * 10 + 10))  #   wave 1
    series += 0.2 * np.sin((time - offsets2) * (freq2 * 20 + 20)) # + wave 2
    series += 0.1 * (np.random.rand(batch_size, n_steps) - 0.5)   # + noise
    return series[..., np.newaxis].astype(np.float32)
```

This function creates as many time series as requested (via the `batch_size` argument), each of length `n_steps`, and there is just one value per time step in each series (i.e., all series are univariate). The function returns a NumPy array of shape [*batch size*, *time steps*, 1], where each series is the sum of two sine waves of fixed amplitudes but random frequencies and phases, plus a bit of noise.

When dealing with time series (and other types of sequences such as sentences), the input features are generally represented as 3D arrays of shape [*batch size*, *time steps*, *dimensionality*], where *dimensionality* is 1 for univariate time series and more for multivariate time series.

Now let's create a training set, a validation set, and a test set using this function:

```
n_steps = 50
series = generate_time_series(10000, n_steps + 1)
X_train, y_train = series[:7000, :n_steps], series[:7000, -1]
X_valid, y_valid = series[7000:9000, :n_steps], series[7000:9000, -1]
X_test, y_test = series[9000:, :n_steps], series[9000:, -1]
```

`X_train` contains 7,000 time series (i.e., its shape is [7000, 50, 1]), while `X_valid` contains 2,000 (from the 7,000th time series to the 8,999th) and `X_test` contains 1,000 (from the 9,000th to the 9,999th). Since we want to forecast a single value for each series, the targets are column vectors (e.g., `y_train` has a shape of [7000, 1]).

Baseline Metrics

Before we start using RNNs, it is often a good idea to have a few baseline metrics, or else we may end up thinking our model works great when in fact it is doing worse than basic models. For example, the simplest approach is to predict the last value in each series. This is called *naive forecasting*, and it is sometimes surprisingly difficult to outperform. In this case, it gives us a mean squared error of about 0.020:

```
>>> y_pred = X_valid[:, -1]
>>> np.mean(keras.losses.mean_squared_error(y_valid, y_pred))
0.020211367
```

Another simple approach is to use a fully connected network. Since it expects a flat list of features for each input, we need to add a `Flatten` layer. Let's just use a simple Linear Regression model so that each prediction will be a linear combination of the values in the time series:

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[50, 1]),
    keras.layers.Dense(1)
])
```

If we compile this model using the MSE loss and the default Adam optimizer, then fit it on the training set for 20 epochs and evaluate it on the validation set, we get an MSE of about 0.004. That's much better than the naive approach!

Implementing a Simple RNN

Let's see if we can beat that with a simple RNN:

```
model = keras.models.Sequential([
  keras.layers.SimpleRNN(1, input_shape=[None, 1])
])
```

That's really the simplest RNN you can build. It just contains a single layer, with a single neuron, as we saw in Figure 15-1. We do not need to specify the length of the input sequences (unlike in the previous model), since a recurrent neural network can process any number of time steps (this is why we set the first input dimension to `None`). By default, the `SimpleRNN` layer uses the hyperbolic tangent activation function. It works exactly as we saw earlier: the initial state $h_{(\text{init})}$ is set to 0, and it is passed to a single recurrent neuron, along with the value of the first time step, $x_{(0)}$. The neuron computes a weighted sum of these values and applies the hyperbolic tangent activation function to the result, and this gives the first output, y_0. In a simple RNN, this output is also the new state h_0. This new state is passed to the same recurrent neuron along with the next input value, $x_{(1)}$, and the process is repeated until the last time step. Then the layer just outputs the last value, y_{49}. All of this is performed simultaneously for every time series.

By default, recurrent layers in Keras only return the final output. To make them return one output per time step, you must set `return_sequences=True`, as we will see.

If you compile, fit, and evaluate this model (just like earlier, we train for 20 epochs using Adam), you will find that its MSE reaches only 0.014, so it is better than the naive approach but it does not beat a simple linear model. Note that for each neuron, a linear model has one parameter per input and per time step, plus a bias term (in the simple linear model we used, that's a total of 51 parameters). In contrast, for each recurrent neuron in a simple RNN, there is just one parameter per input and per hidden state dimension (in a simple RNN, that's just the number of recurrent neurons in the layer), plus a bias term. In this simple RNN, that's a total of just three parameters.

Trend and Seasonality

There are many other models to forecast time series, such as *weighted moving average* models or *autoregressive integrated moving average* (ARIMA) models. Some of them require you to first remove the trend and seasonality. For example, if you are studying the number of active users on your website, and it is growing by 10% every month, you would have to remove this trend from the time series. Once the model is trained and starts making predictions, you would have to add the trend back to get the final predictions. Similarly, if you are trying to predict the amount of sunscreen lotion sold every month, you will probably observe strong seasonality: since it sells well every summer, a similar pattern will be repeated every year. You would have to remove this seasonality from the time series, for example by computing the difference between the value at each time step and the value one year earlier (this technique is called *differencing*). Again, after the model is trained and makes predictions, you would have to add the seasonal pattern back to get the final predictions.

When using RNNs, it is generally not necessary to do all this, but it may improve performance in some cases, since the model will not have to learn the trend or the seasonality.

Deep RNNs

It is quite common to stack multiple layers of cells, as shown in Figure 15-7. This gives you a *deep RNN*.

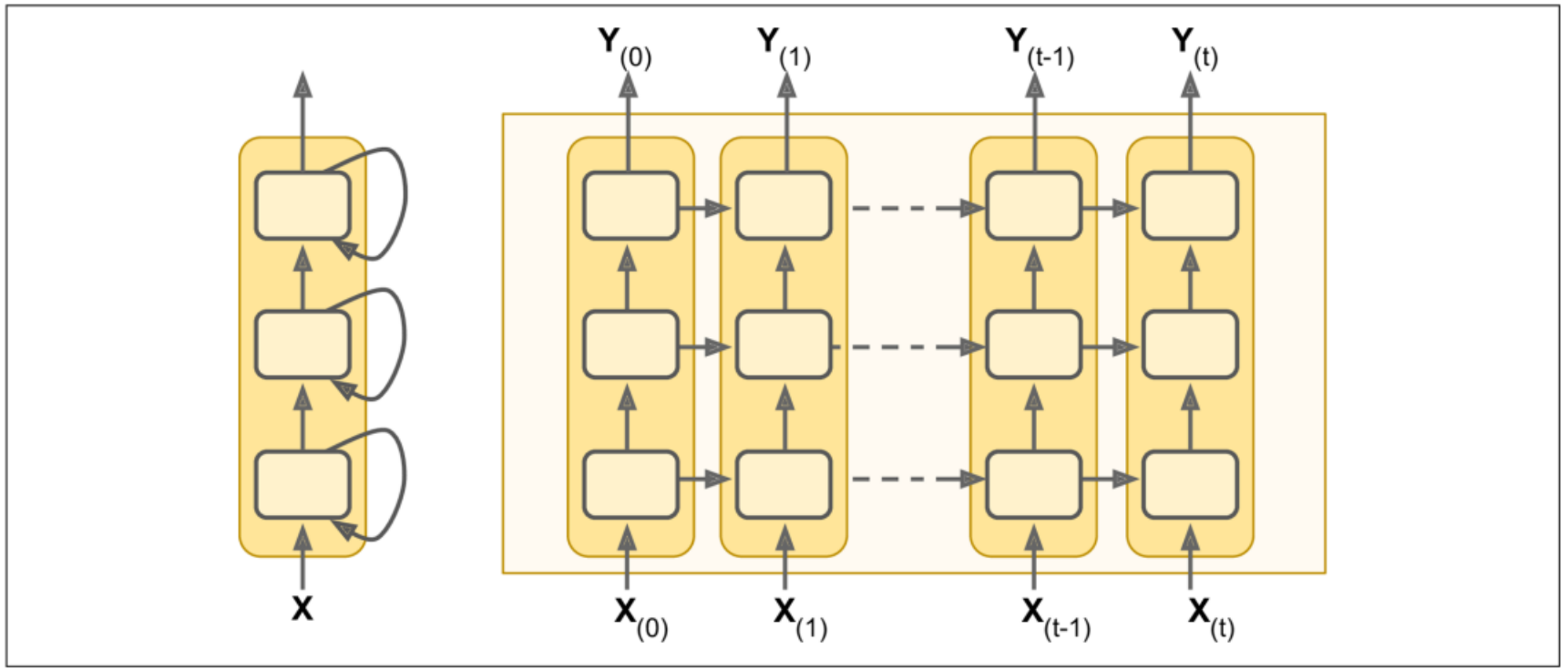


Figure 15-7. Deep RNN (left) unrolled through time (right)

Implementing a deep RNN with tf.keras is quite simple: just stack recurrent layers. In this example, we use three `SimpleRNN` layers (but we could add any other type of recurrent layer, such as an `LSTM` layer or a `GRU` layer, which we will discuss shortly):

```
model = keras.models.Sequential([
    keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.SimpleRNN(20, return_sequences=True),
    keras.layers.SimpleRNN(1)
])
```

Make sure to set `return_sequences=True` for all recurrent layers (except the last one, if you only care about the last output). If you don't, they will output a 2D array (containing only the output of the last time step) instead of a 3D array (containing outputs for all time steps), and the next recurrent layer will complain that you are not feeding it sequences in the expected 3D format.

If you compile, fit, and evaluate this model, you will find that it reaches an MSE of 0.003. We finally managed to beat the linear model!

Note that the last layer is not ideal: it must have a single unit because we want to forecast a univariate time series, and this means we must have a single output value per time step. However, having a single unit means that the hidden state is just a single number. That's really not much, and it's probably not that useful; presumably, the RNN will mostly use the hidden states of the other recurrent layers to carry over all the information it needs from time step to time step, and it will not use the final layer's hidden state very much. Moreover, since a `SimpleRNN` layer uses the tanh activation function by default, the predicted values must lie within the range –1 to 1. But what if you want to use another activation function? For both these reasons, it might be preferable to replace the output layer with a `Dense` layer: it would run slightly faster, the accuracy would be roughly the same, and it would allow us to choose any output activation function we want. If you make this change, also make sure to remove `return_sequences=True` from the second (now last) recurrent layer:

```
model = keras.models.Sequential([
    keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.SimpleRNN(20),
    keras.layers.Dense(1)
])
```

If you train this model, you will see that it converges faster and performs just as well. Plus, you could change the output activation function if you wanted.

Forecasting Several Time Steps Ahead

So far we have only predicted the value at the next time step, but we could just as easily have predicted the value several steps ahead by changing the targets appropriately (e.g., to predict 10 steps ahead, just change the targets to be the value 10 steps ahead instead of 1 step ahead). But what if we want to predict the next 10 values?

The first option is to use the model we already trained, make it predict the next value, then add that value to the inputs (acting as if this predicted value had actually occurred), and use the model again to predict the following value, and so on, as in the following code:

```
series = generate_time_series(1, n_steps + 10)
X_new, Y_new = series[:, :n_steps], series[:, n_steps:]
X = X_new
for step_ahead in range(10):
    y_pred_one = model.predict(X[:, step_ahead:])[:, np.newaxis, :]
    X = np.concatenate([X, y_pred_one], axis=1)

Y_pred = X[:, n_steps:]
```

As you might expect, the prediction for the next step will usually be more accurate than the predictions for later time steps, since the errors might accumulate (as you can see in Figure 15-8). If you evaluate this approach on the validation set, you will find an MSE of about 0.029. This is much higher than the previous models, but it's also a much harder task, so the comparison doesn't mean much. It's much more meaningful to compare this performance with naive predictions (just forecasting that the time series will remain constant for 10 time steps) or with a simple linear model. The naive approach is terrible (it gives an MSE of about 0.223), but the linear model gives an MSE of about 0.0188: it's much better than using our RNN to forecast the future one step at a time, and also much faster to train and run. Still, if you only want to forecast a few time steps ahead, on more complex tasks, this approach may work well.

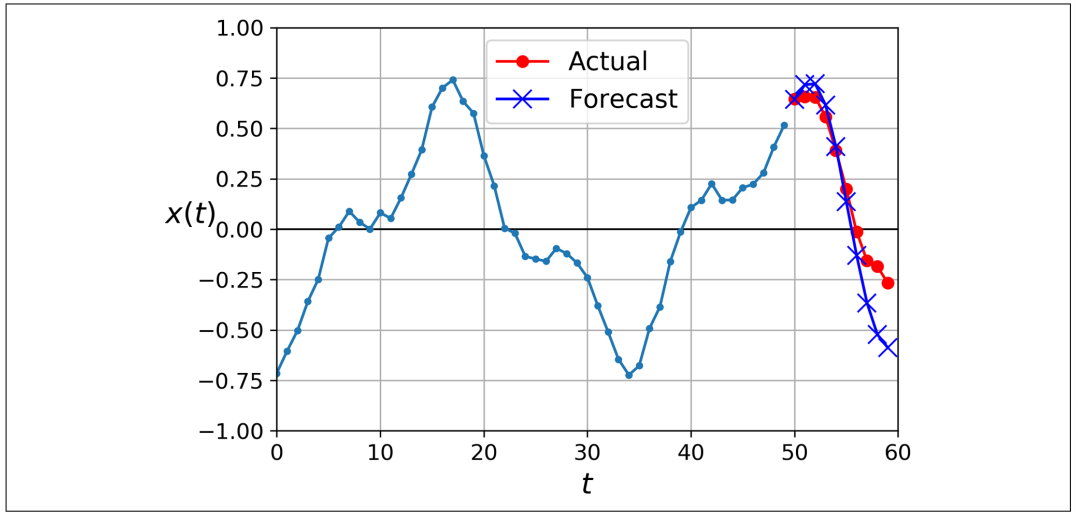


Figure 15-8. Forecasting 10 steps ahead, 1 step at a time

The second option is to train an RNN to predict all 10 next values at once. We can still use a sequence-to-vector model, but it will output 10 values instead of 1. However, we first need to change the targets to be vectors containing the next 10 values:

```
series = generate_time_series(10000, n_steps + 10)
X_train, Y_train = series[:7000, :n_steps], series[:7000, -10:, 0]
X_valid, Y_valid = series[7000:9000, :n_steps], series[7000:9000, -10:, 0]
X_test, Y_test = series[9000:, :n_steps], series[9000:, -10:, 0]
```

Now we just need the output layer to have 10 units instead of 1:

```
model = keras.models.Sequential([
    keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.SimpleRNN(20),
    keras.layers.Dense(10)
])
```

After training this model, you can predict the next 10 values at once very easily:

```
Y_pred = model.predict(X_new)
```

This model works nicely: the MSE for the next 10 time steps is about 0.008. That's much better than the linear model. But we can still do better: indeed, instead of training the model to forecast the next 10 values only at the very last time step, we can train it to forecast the next 10 values at each and every time step. In other words, we can turn this sequence-to-vector RNN into a sequence-to-sequence RNN. The advantage of this technique is that the loss will contain a term for the output of the RNN at each and every time step, not just the output at the last time step. This means there will be many more error gradients flowing through the model, and they won't have to flow only through time; they will also flow from the output of each time step. This will both stabilize and speed up training.

To be clear, at time step 0 the model will output a vector containing the forecasts for time steps 1 to 10, then at time step 1 the model will forecast time steps 2 to 11, and so on. So each target must be a sequence of the same length as the input sequence, containing a 10-dimensional vector at each step. Let's prepare these target sequences:

```
Y = np.empty((10000, n_steps, 10)) # each target is a sequence of 10D vectors
for step_ahead in range(1, 10 + 1):
    Y[:, :, step_ahead - 1] = series[:, step_ahead:step_ahead + n_steps, 0]
Y_train = Y[:7000]
Y_valid = Y[7000:9000]
Y_test = Y[9000:]
```

It may be surprising that the targets will contain values that appear in the inputs (there is a lot of overlap between `X_train` and `Y_train`). Isn't that cheating? Fortunately, not at all: at each time step, the model only knows about past time steps, so it cannot look ahead. It is said to be a *causal* model.

To turn the model into a sequence-to-sequence model, we must set `return_sequences=True` in all recurrent layers (even the last one), and we must apply the output `Dense` layer at every time step. Keras offers a `TimeDistributed` layer for this very purpose: it wraps any layer (e.g., a `Dense` layer) and applies it at every time step of its input sequence. It does this efficiently, by reshaping the inputs so that each time step is treated as a separate instance (i.e., it reshapes the inputs from [*batch size*, *time steps*, *input dimensions*] to [*batch size* × *time steps*, *input dimensions*]; in this example, the number of input dimensions is 20 because the previous `SimpleRNN` layer has 20 units), then it runs the `Dense` layer, and finally it reshapes the outputs back to sequences (i.e., it reshapes the outputs from [*batch size* × *time steps*, *output dimensions*] to [*batch size*, *time steps*, *output dimensions*]; in this example the number of output dimensions is 10, since the `Dense` layer has 10 units).[2] Here is the updated model:

```
model = keras.models.Sequential([
    keras.layers.SimpleRNN(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.SimpleRNN(20, return_sequences=True),
    keras.layers.TimeDistributed(keras.layers.Dense(10))
])
```

The `Dense` layer actually supports sequences as inputs (and even higher-dimensional inputs): it handles them just like `TimeDistributed(Dense(...))`, meaning it is applied to the last input dimension only (independently across all time steps). Thus, we could replace the last layer with just `Dense(10)`. For the sake of clarity, however, we will keep using `TimeDistributed(Dense(10))` because it makes it clear that the `Dense` layer is applied independently at each time step and that the model will output a sequence, not just a single vector.

All outputs are needed during training, but only the output at the last time step is useful for predictions and for evaluation. So although we will rely on the MSE over all the outputs for training, we will use a custom metric for evaluation, to only compute the MSE over the output at the last time step:

```
def last_time_step_mse(Y_true, Y_pred):
    return keras.metrics.mean_squared_error(Y_true[:, -1], Y_pred[:, -1])

optimizer = keras.optimizers.Adam(lr=0.01)
model.compile(loss="mse", optimizer=optimizer, metrics=[last_time_step_mse])
```

We get a validation MSE of about 0.006, which is 25% better than the previous model. You can combine this approach with the first one: just predict the next 10 values using this RNN, then concatenate these values to the input time series and use the model again to predict the next 10 values, and repeat the process as many times as needed. With this approach, you can generate arbitrarily long sequences. It may not be very accurate for long-term predictions, but it may be just fine if your goal is to generate original music or text, as we will see in Chapter 16.

Long Short-Term Memory (LSTM)

LSTM cell as a black box, it can be used very much like a basic cell, except it will perform much better; training will converge faster, and it will detect long-term dependencies in the data. In Keras, you can simply use the `LSTM` layer instead of the `SimpleRNN` layer:

```
model = keras.models.Sequential([
    keras.layers.LSTM(20, return_sequences=True, input_shape=[None, 1]),
    keras.layers.LSTM(20, return_sequences=True),
    keras.layers.TimeDistributed(keras.layers.Dense(10))
])
```

Alternatively, you could use the general-purpose `keras.layers.RNN` layer, giving it an `LSTMCell` as an argument:

```
model = keras.models.Sequential([
    keras.layers.RNN(keras.layers.LSTMCell(20), return_sequences=True,
                     input_shape=[None, 1]),
    keras.layers.RNN(keras.layers.LSTMCell(20), return_sequences=True),
    keras.layers.TimeDistributed(keras.layers.Dense(10))
])
```

However, the `LSTM` layer uses an optimized implementation when running on a GPU (see Chapter 19), so in general it is preferable to use it (the `RNN` layer is mostly useful when you define custom cells, as we did earlier).

If you don't look at what's inside the box, the LSTM cell looks exactly like a regular cell, except that its state is split into two vectors: $\mathbf{h}_{(t)}$ and $\mathbf{c}_{(t)}$ ("c" stands for "cell"). You can think of $\mathbf{h}_{(t)}$ as the short-term state and $\mathbf{c}_{(t)}$ as the long-term state.

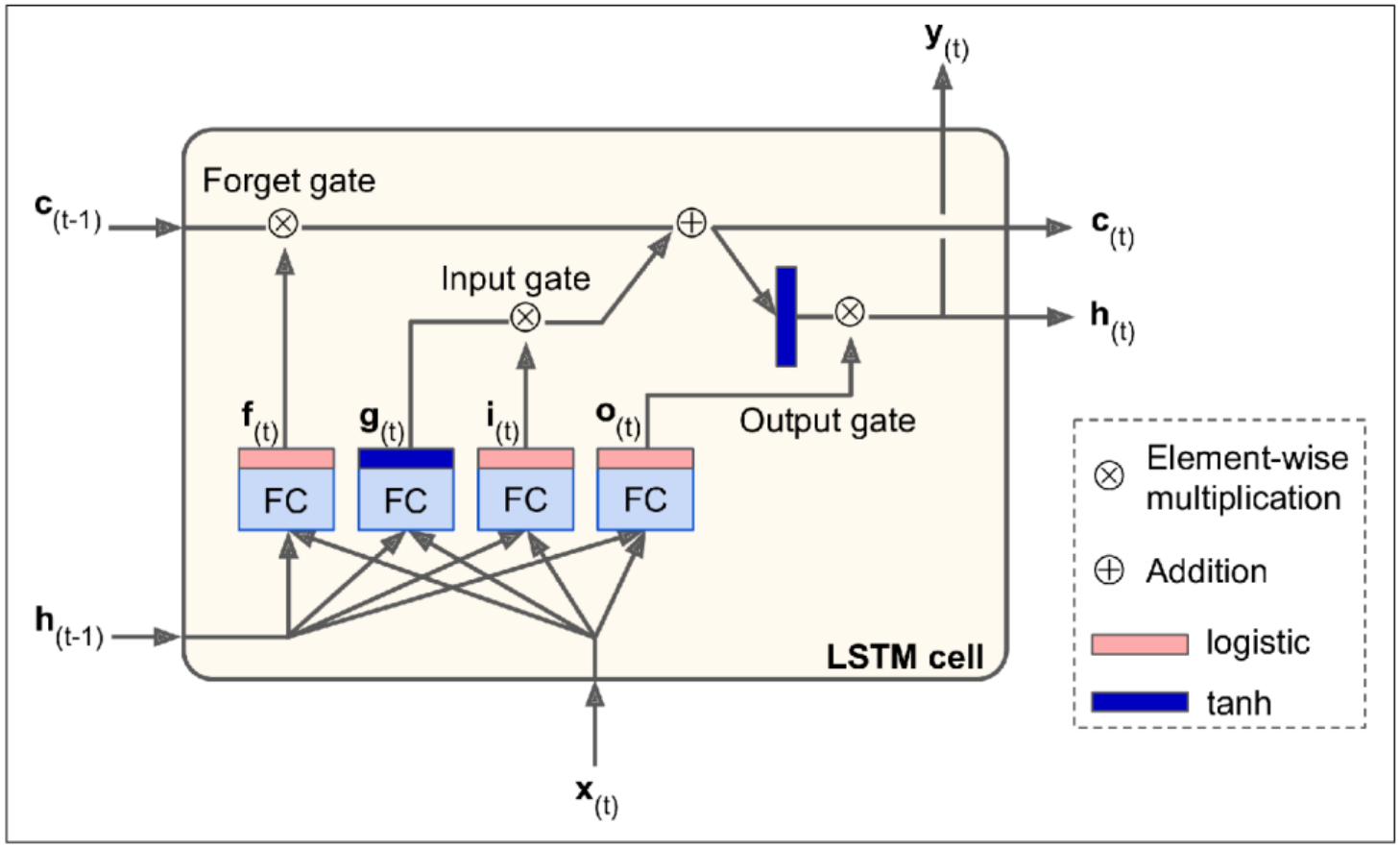


Figure 15-9. LSTM cell

Now let's open the box! The key idea is that the network can learn what to store in the long-term state, what to throw away, and what to read from it. As the long-term state $\mathbf{c}_{(t-1)}$ traverses the network from left to right, you can see that it first goes through a *forget gate*, dropping some memories, and then it adds some new memories via the addition operation (which adds the memories that were selected by an *input gate*). The result $\mathbf{c}_{(t)}$ is sent straight out, without any further transformation. So, at each time step, some memories are dropped and some memories are added. Moreover, after the addition operation, the long-term state is copied and passed through the tanh function, and then the result is filtered by the *output gate*. This produces the short-term state $\mathbf{h}_{(t)}$ (which is equal to the cell's output for this time step, $\mathbf{y}_{(t)}$). Now let's look at where new memories come from and how the gates work.

First, the current input vector $\mathbf{x}_{(t)}$ and the previous short-term state $\mathbf{h}_{(t-1)}$ are fed to four different fully connected layers. They all serve a different purpose:

- The main layer is the one that outputs $\mathbf{g}_{(t)}$. It has the usual role of analyzing the current inputs $\mathbf{x}_{(t)}$ and the previous (short-term) state $\mathbf{h}_{(t-1)}$. In a basic cell, there is nothing other than this layer, and its output goes straight out to $\mathbf{y}_{(t)}$ and $\mathbf{h}_{(t)}$. In contrast, in an LSTM cell this layer's output does not go straight out, but instead its most important parts are stored in the long-term state (and the rest is dropped).
- The three other layers are *gate controllers*. Since they use the logistic activation function, their outputs range from 0 to 1. As you can see, their outputs are fed to element-wise multiplication operations, so if they output 0s they close the gate, and if they output 1s they open it. Specifically:
  - The *forget gate* (controlled by $\mathbf{f}_{(t)}$) controls which parts of the long-term state should be erased.
  - The *input gate* (controlled by $\mathbf{i}_{(t)}$) controls which parts of $\mathbf{g}_{(t)}$ should be added to the long-term state.
  - Finally, the *output gate* (controlled by $\mathbf{o}_{(t)}$) controls which parts of the long-term state should be read and output at this time step, both to $\mathbf{h}_{(t)}$ and to $\mathbf{y}_{(t)}$.

Equation 15-3. LSTM computations

$$
\begin{aligned}
\mathbf{i}_{(t)} &= \sigma\left(\mathbf{W}_{xi}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hi}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_i\right) \\
\mathbf{f}_{(t)} &= \sigma\left(\mathbf{W}_{xf}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hf}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_f\right) \\
\mathbf{o}_{(t)} &= \sigma\left(\mathbf{W}_{xo}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{ho}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_o\right) \\
\mathbf{g}_{(t)} &= \tanh\left(\mathbf{W}_{xg}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hg}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_g\right) \\
\mathbf{c}_{(t)} &= \mathbf{f}_{(t)} \otimes \mathbf{c}_{(t-1)} + \mathbf{i}_{(t)} \otimes \mathbf{g}_{(t)} \\
\mathbf{y}_{(t)} &= \mathbf{h}_{(t)} = \mathbf{o}_{(t)} \otimes \tanh\left(\mathbf{c}_{(t)}\right)
\end{aligned}
$$

In this equation:

- $\mathbf{W}_{xi}$, $\mathbf{W}_{xf}$, $\mathbf{W}_{xo}$, $\mathbf{W}_{xg}$ are the weight matrices of each of the four layers for their connection to the input vector $\mathbf{x}_{(t)}$.
- $\mathbf{W}_{hi}$, $\mathbf{W}_{hf}$, $\mathbf{W}_{ho}$, and $\mathbf{W}_{hg}$ are the weight matrices of each of the four layers for their connection to the previous short-term state $\mathbf{h}_{(t-1)}$.
- $\mathbf{b}_i$, $\mathbf{b}_f$, $\mathbf{b}_o$, and $\mathbf{b}_g$ are the bias terms for each of the four layers. Note that TensorFlow initializes $\mathbf{b}_f$ to a vector full of 1s instead of 0s. This prevents forgetting everything at the beginning of training.

Gated Recurrent Unit (GRU)

The GRU cell is a simplified version of the LSTM cell, and it seems to perform just as well

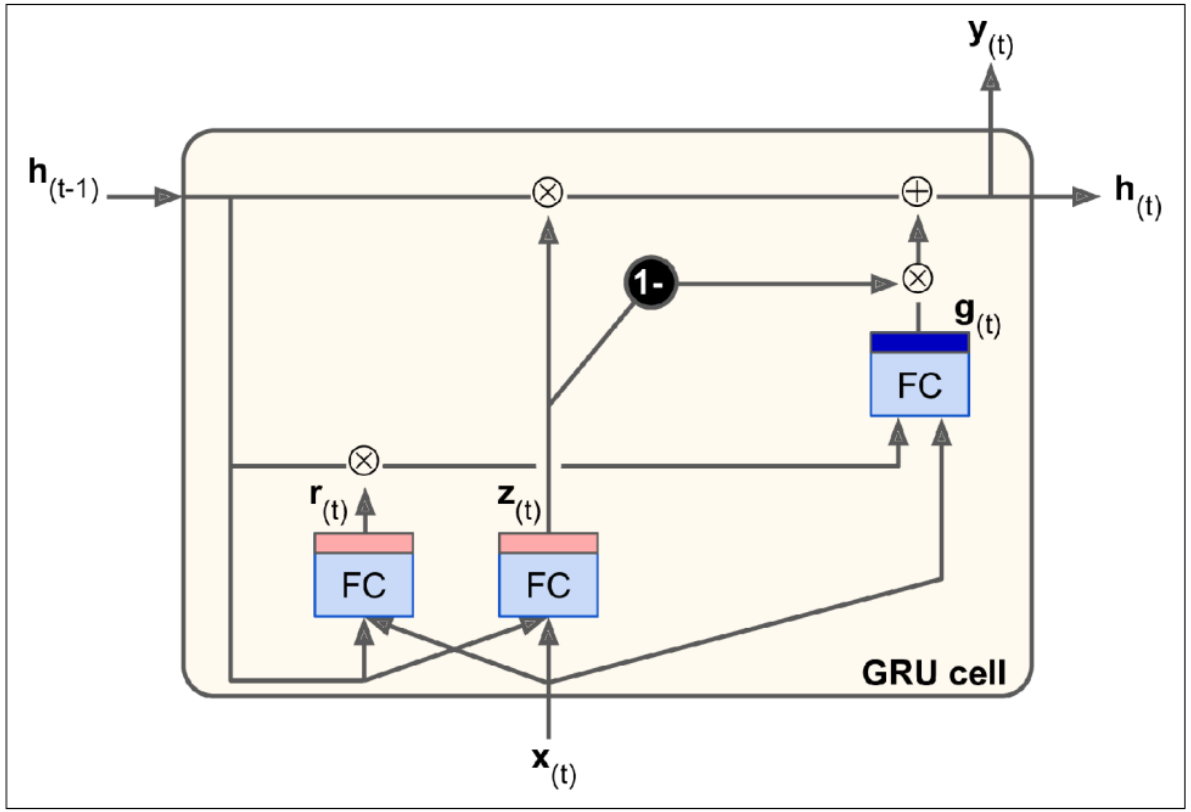


Figure 15-10. GRU cell

- Both state vectors are merged into a single vector $\mathbf{h}_{(t)}$.
- A single gate controller $\mathbf{z}_{(t)}$ controls both the forget gate and the input gate. If the gate controller outputs a 1, the forget gate is open (= 1) and the input gate is closed (1 – 1 = 0). If it outputs a 0, the opposite happens. In other words, whenever a memory must be stored, the location where it will be stored is erased first. This is actually a frequent variant to the LSTM cell in and of itself.
- There is no output gate; the full state vector is output at every time step. However, there is a new gate controller $\mathbf{r}_{(t)}$ that controls which part of the previous state will be shown to the main layer ($\mathbf{g}_{(t)}$).

Equation 15-4. GRU computations

$$\mathbf{z}_{(t)} = \sigma\left(\mathbf{W}_{xz}{}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hz}{}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_z\right)$$

$$\mathbf{r}_{(t)} = \sigma\left(\mathbf{W}_{xr}{}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hr}{}^{\top}\mathbf{h}_{(t-1)} + \mathbf{b}_r\right)$$

$$\mathbf{g}_{(t)} = \tanh\left(\mathbf{W}_{xg}{}^{\top}\mathbf{x}_{(t)} + \mathbf{W}_{hg}{}^{\top}\left(\mathbf{r}_{(t)} \otimes \mathbf{h}_{(t-1)}\right) + \mathbf{b}_g\right)$$

$$\mathbf{h}_{(t)} = \mathbf{z}_{(t)} \otimes \mathbf{h}_{(t-1)} + \left(1 - \mathbf{z}_{(t)}\right) \otimes \mathbf{g}_{(t)}$$

Keras provides a `keras.layers.GRU` layer (based on the `keras.layers.GRUCell` memory cell); using it is just a matter of replacing `SimpleRNN` or `LSTM` with `GRU`.

LSTM and GRU cells are one of the main reasons behind the success of RNNs. Yet while they can tackle much longer sequences than simple RNNs, they still have a fairly limited short-term memory, and they have a hard time learning long-term patterns in sequences of 100 time steps or more, such as audio samples, long time series, or long sentences. One way to solve this is to shorten the input sequences, for example using 1D convolutional layers.