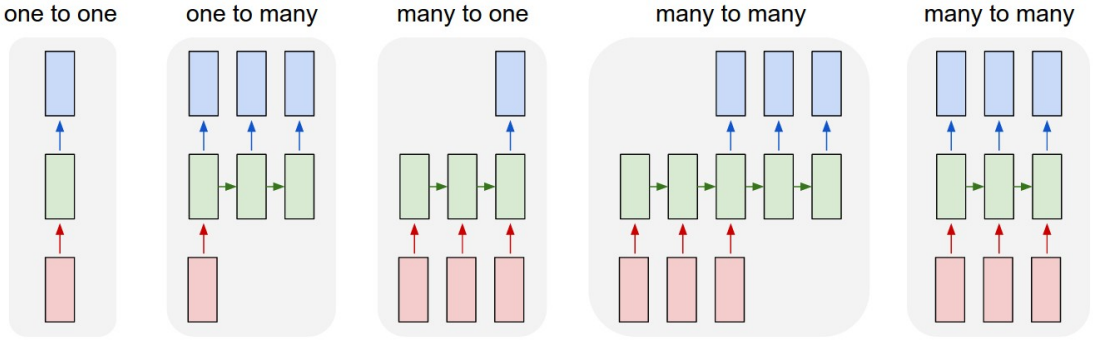
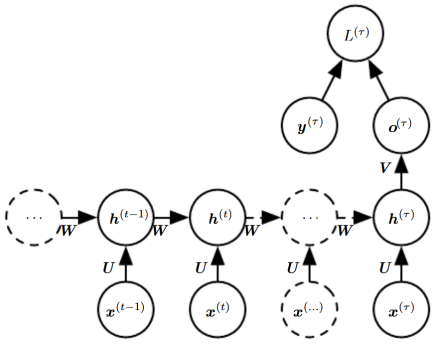
14 Recurrent neural networks

Recurrent neural networks (RNNs) are designed for features that are recurrent (e.g., time series). A good description of the various applications of RNNs is in Karpathy's blog. This figure from that blog illustrates various purposes of RNNs.



14.1 Many-to-one RNN models

The "**many-to-one**" type is probably the most common type of RNN models. For example, we may want to use the weather information in the past 10 days to predict the temperature tomorrow. It can also be illustrated below (DL Figure 10.5).



For this model, each observation consists of a set of input vectors, $\{x^{(1)}, \ldots, x^{(k)}\}$, and an output y, which can be a scalar or a vector. The value k may vary from one observation to another. The model is effectively a feedforward neural network with k hidden layers: $h^{(t)}$ $(t = 1, \cdots, k)$; we set $h^{(0)} = 0$. All these layers have the same number of nodes (often called **units** in RNN). Each hidden layer $h^{(t)}$ has inputs not only from the previous layer $h^{(t-1)}$, but also from the input vector $x^{(t)}$. The output layer has inputs from $h^{(k)}$. A key feature of the RNN is that all these hidden layers **share the same weights** W and U and **bias** b:

$$h^{(t)} = \tanh(Wh^{(t-1)} + Ux^{(t)} + b) \quad (t = 1, \cdots, k).$$

That is, the RNN layer is applied repeatedly to each input vector; in other words, it is updated repeatedly given every new input vector. After we have gone through all the input vectors, the output layer has weights V and c:

$$\hat{y} = f(Vh^{(k)} + c),$$

where $f()$ is an activation function (e.g., softmax if outcome is multinomial). If the input vector $x^{(t)}$ is p-dimensional and each RNN layer $h^{(t)}$ has q units, then W is $q \times q$, U is $q \times p$, and b is $q \times 1$. So the total number of parameters for this "many-to-one" RNN layer is $q(p + q + 1)$.

In summary, when this RNN model is applied to an observation with k input vectors, it works in the following way:

- Initialize vector $h^{(0)} = 0$;
- At step t $(t = 1, \ldots, k)$, $h^{(t)} = \tanh(Wh^{(t-1)} + Ux^{(t)} + b)$;
- $\hat{y} = f(Vh^{(k)} + c)$.

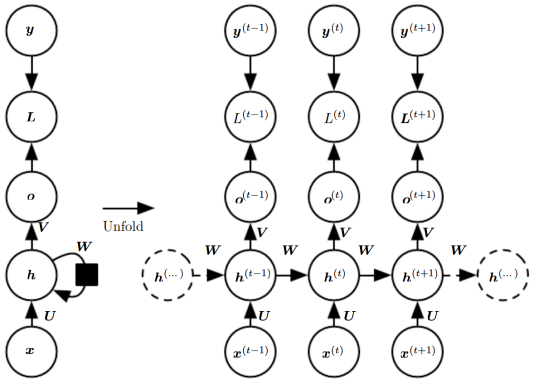
Let $L(y, \hat{y})$ be the cost function, where $\hat{y}$ is a function of $(x^{(1)}, \ldots, x^{(k)})$. Because of the parameter sharing, the gradient of $L(y, \hat{y})$ with respect to W is the sum of the gradients with respect to all the individual W's. Similarly for the gradients with respect to U and b.

Below is an example Keras code for such a "many-to-one" RNN model. In this example, $p = 10$ and $q = 32$; the number of parameters for the RNN layer is $32 \times (10 + 32 + 1) = 1376$. The output is a scalar (i.e., 1 unit), and it requires $32 + 1 = 33$ parameters.

```
library(keras)
model <- keras_model_sequential() %>%
  layer_simple_rnn(units = 32, input_shape = list(NULL, 10)) %>%
  layer_dense(units = 1)

summary(model)
```

14.2 Many-to-many RNN models

The "**many-to-many**" type can also be illustrated below (DL Figure 10.3). The model is often shown with a loop as the one on the left; its unfolded version is on the right.



For this model, each observation consists of a set of k input vectors and k outputs, $\{x^{(1)}, \ldots, x^{(k)}, y^{(1)}, \ldots, y^{(k)}\}$, where k may vary from one observation to another. For example, in word processing, an observation can be a sentence, with $x^{(t)}$ being a "phrase" of 5 contiguous words and $y^{(t)}$ being the next word. Then a sentence with 15 words would have $k = 10$ pairs of $(x^{(t)}, y^{(t)})$.

When this RNN model is applied to an observation of size k, it works in the following way:

- Initialize vector $h^{(0)} = 0$.
- At step t $(t = 1, \ldots, k)$, there are
  - A hidden vector $h^{(t)} = \tanh(Wh^{(t-1)} + Ux^{(t)} + b)$;
  - An output $\hat{y}^{(t)} = f(Vh^{(t)} + c)$, where $f()$ is an activation function.

Similar to the "many-to-one" model, this model has the **shared weights** W and U and **bias** b. Each hidden layer $h^{(t)}$ has inputs from the previous layer $h^{(t-1)}$ and the input vector $x^{(t)}$. Each output $\hat{y}^{(t)}$ has inputs from $h^{(t)}$. The paths to $\hat{y}^{(t)}$ $(t = 1, \ldots, k)$ also **share the same weights** V and **bias** c. This model has the same number of parameters as the "many-to-one" version, $q(p + q + 1)$.

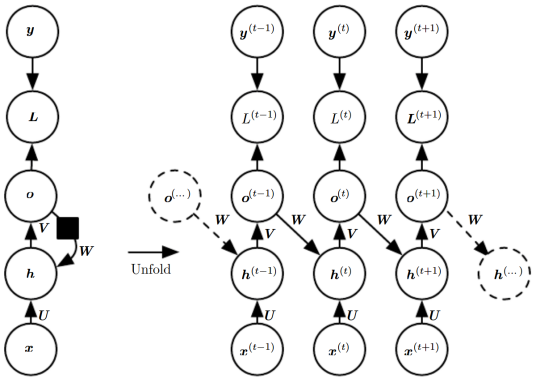
The cost for an observation of size k is $\sum_{t=1}^{k} L(y^{(t)}, \hat{y}^{(t)})$, where $\hat{y}^{(t)}$ is a function of $(x^{(1)}, \ldots, x^{(t)})$. Similar to the "many-to-one" model, because of parameter sharing, the gradient of $L(y, \hat{y})$ with respect to W is the sum of the gradients with respect to all the individual W's. Similarly for the gradients with respect to all other paramters.

Below is an example Keras code for such a "many-to-many" RNN layer. The specification `return_sequences=T` tells the model to output $h^{(t)}$ at every t; `time_distributed()` tells the model to evaluate the outcome at every t.

```
library(keras)
model <- keras_model_sequential() %>%
  layer_simple_rnn(units = 32, return_sequences=T, input_shape = list(NULL, 10)) %>%
```

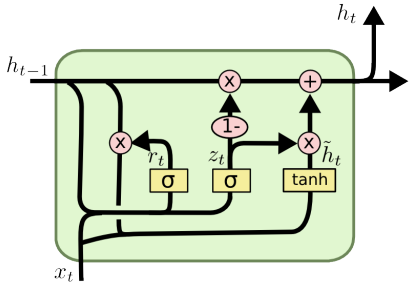
```
  time_distributed(layer_dense(units = 1))

summary(model)
```

An variation of this "many-to-many" model is below (DL Figure 10.4), which differs from the model above in that $h^{(t)} = \tanh(Wo^{(t-1)} + Ux^{(t)} + b)$, where $o^{(t)} = \hat{y}^{(t)} = Vh^{(t)} + c$. Here the dimensions of W are $q \times a$, where a is the dimension of $o^{(t)}$.



14.3 GRUs and LSTMs

Some RNNs have sophisticated operations inside a unit. One example is the **gated recurrent unit** (GRU) (Cho et al., 2014). The figure below is a "fully gated" version (from Olah's blog).



Below is the matrix representation of the operations across all units:

$$\begin{cases} z_t &= \sigma(W_z x_t + R_z h_{t-1} + b_z), \\ r_t &= \sigma(W_r x_t + R_r h_{t-1} + b_r), \\ \tilde{h}_t &= \tanh(W_a x_t + R_a(r_t \circ h_{t-1}) + b_a), \\ h_t &= (1 - z_t) \circ h_{t-1} + z_t \circ \tilde{h}_t. \end{cases} \quad \text{(update gate)}$$

Here the operator $\circ$ is the Hadamard product (i.e., element-wise product between two vectors). For a single unit, r_t, z_t, h_t are scalars, and $\circ$ becomes a regular product. In the GRU, $\tilde{h}_t$ is a new candidate h value. If z_t could take value 0 or 1, it would determine whether h_t is updated to be $\tilde{h}_t$ (when $z_t = 1$) or keeps the value of h_{t-1} (when $z_t = 0$). But since $0 < z_t < 1$, z_t serves as a weight for $\tilde{h}_t$, and $1 - z_t$ is the weight for h_{t-1}.

If the input $x^{(t)}$ is p-dimensional and a hidden layer has q GRUs, all W matrices are $q \times p$, all R matrices are $q \times q$, and all b vectors are $q \times 1$. So the total number of parameters for the GRU layer is $3q(p + q + 1)$.

Below is an example Keras code for a layer of GRUs. In this example, the number of parameters for the GRU layer is $3 \times 32 \times (10 + 32 + 1) = 4128$. The 1-dimensional output requires $32 + 1 = 33$ parameters.

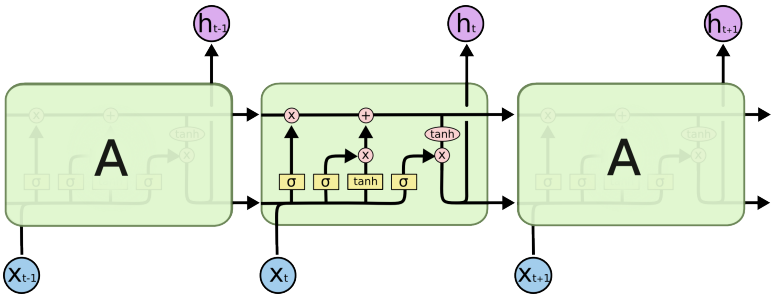
```
library(keras)
model <- keras_model_sequential() %>%
  layer_gru(units = 32, input_shape = list(NULL, 10)) %>%
```

```
  layer_dense(units = 1)

summary(model)
```

One can stack a GRU layer after another by specifying `return_sequences=T` in the first GRU layer so that it feeds as the input to the next GRU layer. The second GRU layer treats the $h^{(t)}$ from the first GRU layer as its $x^{(t)}$. In the example below, the second GRU layer has 64 units, requiring $3 \times 64 \times (32 + 64 + 1) = 18,624$ parameters.

```
library(keras)
model <- keras_model_sequential() %>%
  layer_gru(units = 32, return_sequences=T, input_shape = list(NULL, 10)) %>%
  layer_gru(units = 64, activation = "relu") %>%
  layer_dense(units = 1)

summary(model)
```

GRUs are a simplified version of **long short-term memory** (LSTM) networks (Hochreiter and Schmidhuber, 1997). An LSTM unit looks like the figure below. It has a separate "memory" thread in addition to the "hidden" thread. A nice description of the LSTM is given by Christopher Olah.



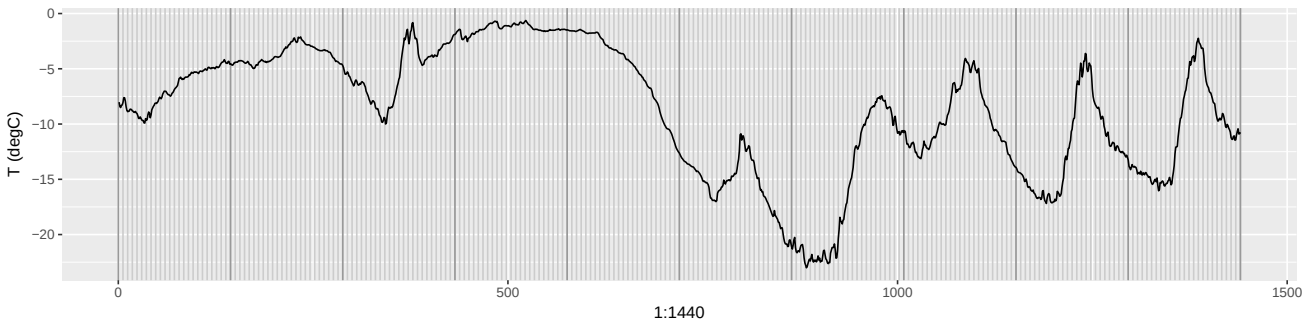
An LSTM layer with q units has $4q(p + q + 1)$ parameters. In the example below, $4 \times 32 \times (10 + 32 + 1) = 5504$.

```
library(keras)
model <- keras_model_sequential() %>%
  layer_lstm(units = 32, input_shape = list(NULL, 10)) %>%
  layer_dense(units = 1)

summary(model)
```

14.4 Example: Time series forecasting (many-to-one)

https://tensorflow.rstudio.com/blog/time-series-forecasting-with-recurrent-neural-networks.html

In this weather time series dataset, temperature and 13 other relevant variables (e.g., air pressure) were recorded every 10 minutes for 8 years from 2009 to 2016 in Jena, Germany. Below are the temperatures in the first 10 days of 2009. There are $6 \times 24 \times 10 = 1440$ values.



The authors want to predict the temperature 24 hours from now given the data in the last 10 days (temperature + 13 other variables). Instead of using the full 10 days data as the input, they sampled hourly (i.e., took every 6th observation; $k = 240$). In a FFNN, there would be a total of $240 \times 14 = 3360$ input neurons. For the RNN model below, the GRU layer has 240 unfolded layers, each with a 14-vector as the input, and a scalar output after the last unfolded layer.

```
library(keras)
model <- keras_model_sequential() %>%
  layer_gru(units = 32, input_shape = list(NULL, 14)) %>%
  layer_dense(units = 1)
summary(model)
```

14.5 Milestones of ANNs:

- Backpropagation (Rumelhart et al. 1986)
- MNIST dataset (1998): 70,000 28×28 images of handwritten digits, 10 classes
- **LeNet**: CNN was developed and applied to MNIST (LeCun et al. 1998)
- LSTM, a type of RNN (Hochreiter and Schmidhuber, 1997)
- NN in natural language processing (Bengio et al., 2003)
- Netflix Prize (2006–2009)
- CIFAR-10/CIFAR-100 datasets (2009): 60,000 32×32 images, in 10 and 100 classes.
- ImageNet dataset (Fei-Fei Li): Initially 3.2 million images in 5,247 "synonym sets" or "synsets". Now over 14 million images. 1000 synsets have SIFT (scale-invariant feature transform) features.
- ILSVRC (ImageNet Large Scale Visual Recognition Challenge) (2010–2017): **The catalyst for the AI boom**.
  - **AlexNet** (Krizhevsky, Sutskever, Hinton, 2012) **brought DL into the mainstream**. It won the 2012 ILSVRC (top-5 error rate 15.4%, same below; 11x11 filters). They used ReLU rather than the conventional tanh function, and introduced dropout layers to overcome *overfitting.
  - **VGG Net** (Simonyan and Zisserman, 2014) won the "classification+localization" category of the 2014 ILSVRC (error rate 7.3%; 3x3 filters). Showed that simple deep structures work for hierarchical feature extraction.
  - **GoogLeNet/inception** (Szegedy et al., 2014) won 2014 ILSVRC (error rate 6.7%). Introduced the inception module, with CNN layers not stacked up sequentially. Later improvement: BN-inception-2 (error rate 4.8% with batch normalization) (Ioffe, Szegedy, 2015), inception-3 (error rate 3.6%) (Szegedy et al., 2015).
  - Microsoft **ResNet** (He et al. 2015) won 2015 ILSVRC (error rate 3.6%). Introduced residual block to reduce overfitting.
- Generative adversarial nets (GANs) (Goodfellow et al. 2014)
- AlphaGo (2016), AlphaGo Zero (2017), AlphaZero (2018)
- 2018 Turing Award to three pioneers in deep learning: Geoffrey Hinton, Yoshua Bengio, Yann LeCun.

Below is a figure from a 2017 article on the impact of the ImageNet dataset and the ILSVRC: The data that transformed AI research — and possibly the world. It shows the great performance improvements made every year between 2012 and 2015.