Deep learning

12.2. LSTM and GRU

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The Long-Short Term Memory unit (LSTM) by Hochreiter and Schmidhuber (1997), is a recurrent network that originally had a gating of the form

$$c_t = c_{t-1} + i_t \odot g_t$$

where $c_t$ is a recurrent state, $i_t$ is a gating function and $g_t$ is a full update. This assures that the derivatives of the loss w.r.t. $c_t$ does not vanish.
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This original architecture was improved with a forget gate (Gers et al., 2000), resulting in the standard LSTM used today.

In what follows we consider notation and variant from Jozefowicz et al. (2015).
The recurrent state is composed of a “cell state” $c_t$ and an “output state” $h_t$. Gate $f_t$ modulates if the cell state should be forgotten, $i_t$ if the new update should be taken into account, and $o_t$ if the output state should be reset.
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$$f_t = \text{sigm} \left( W_{(x f)} x_t + W_{(h f)} h_{t-1} + b(f) \right)$$  \hspace{1cm} \text{(forget gate)}

$$i_t = \text{sigm} \left( W_{(x i)} x_t + W_{(h i)} h_{t-1} + b(i) \right)$$  \hspace{1cm} \text{(input gate)}

$$g_t = \tanh \left( W_{(x c)} x_t + W_{(h c)} h_{t-1} + b(c) \right)$$  \hspace{1cm} \text{(full cell state update)}

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$  \hspace{1cm} \text{(cell state)}

$$o_t = \text{sigm} \left( W_{(x o)} x_t + W_{(h o)} h_{t-1} + b(o) \right)$$  \hspace{1cm} \text{(output gate)}

$$h_t = o_t \odot \tanh(c_t)$$  \hspace{1cm} \text{(output state)}
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\[
\begin{align*}
    f_t &= \text{sigm} \left( W_{(x \, f)} x_t + W_{(h \, f)} h_{t-1} + b(f) \right) & \text{(forget gate)} \\
    i_t &= \text{sigm} \left( W_{(x \, i)} x_t + W_{(h \, i)} h_{t-1} + b(i) \right) & \text{(input gate)} \\
    g_t &= \text{tanh} \left( W_{(x \, c)} x_t + W_{(h \, c)} h_{t-1} + b(c) \right) & \text{(full cell state update)} \\
    c_t &= f_t \odot c_{t-1} + i_t \odot g_t & \text{(cell state)} \\
    o_t &= \text{sigm} \left( W_{(x \, o)} x_t + W_{(h \, o)} h_{t-1} + b(o) \right) & \text{(output gate)} \\
    h_t &= o_t \odot \tanh(c_t) & \text{(output state)}
\end{align*}
\]

As pointed out by Gers et al. (2000), the forget bias \( b(f) \) should be initialized with large values so that initially \( f_t \approx 1 \) and the gating has no effect.
The recurrent state is composed of a “cell state” $c_t$ and an “output state” $h_t$. Gate $f_t$ modulates if the cell state should be forgotten, $i_t$ if the new update should be taken into account, and $o_t$ if the output state should be reset.

$$f_t = \text{sigm} \left( W(x_f)x_t + W(h_f)h_{t-1} + b(f) \right) \quad \text{(forget gate)}$$

$$i_t = \text{sigm} \left( W(x_i)x_t + W(h_i)h_{t-1} + b(i) \right) \quad \text{(input gate)}$$

$$g_t = \tanh \left( W(x_c)x_t + W(h_c)h_{t-1} + b(c) \right) \quad \text{(full cell state update)}$$

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t \quad \text{(cell state)}$$

$$o_t = \text{sigm} \left( W(x_o)x_t + W(h_o)h_{t-1} + b(o) \right) \quad \text{(output gate)}$$

$$h_t = o_t \odot \tanh(c_t) \quad \text{(output state)}$$

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This model was extended by Gers et al. (2003) with “peephole connections” that allow gates to depend on $c_{t-1}$. 
Prediction is done from the $h_t$ state, hence called the output state.
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PyTorch’s `torch.nn.LSTM` implements this model.

Its processes several sequences, and returns two tensors, with $D$ the number of layers and $T$ the sequence length:

- the outputs for all the layers at the last time step: $h^1_T$ and $h^D_T$, and
- the outputs of the last layer at each time step: $h^D_1, \ldots, h^D_T$.

The initial recurrent states $h^1_0, \ldots, h^D_0$ and $c^1_0, \ldots, c^D_0$ can also be specified.
PyTorch’s RNNs can process batches of sequences of same length, that can be encoded in a regular tensor, or batches of sequences of various lengths using the type `nn.utils.rnn.PackedSequence`.

Such an object can be created with `nn.utils.rnn.pack_padded_sequence`, which expects as argument a first tensor of $x_{n,t}$s $N \times T \times \ldots$ padded with zeros, and a second tensor of $T_n$s.
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```python
>>> from torch.nn.utils.rnn import pack_padded_sequence
>>> pack_padded_sequence(torch.tensor([[1.], [2.]], ... [[3.], [4.]], ... [[5.], [0.]]), ... [3, 2])
PackedSequence(data=tensor([[1.], ... [5.]]), batch_sizes=tensor([2, 2, 1]))
```
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  [3.],
  [4.],
  [5.]]), batch_sizes=tensor([2, 2, 1]))
```

⚠️ The sequences must be sorted by decreasing lengths.
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Such an object can be created with `nn.utils.rnn.pack_padded_sequence`, which expects as argument a first tensor of $x_n$, $t_s$ $N \times T \times \ldots$ padded with zeros, and a second tensor of $T$ $n$.

```python
>>> import torch.nn.utils.rnn as rnn
>>> print(rnn.pack_padded_sequence(torch.tensor([[1.], [2.]],
...                                          [[3.], [4.]],
...                                          [[5.], [0.]]),
...                                          [3, 2])
<torch.nn.utils.rnn.PackedSequence object at 0x7fa1a5d20590>
```

⚠️ The sequences must be sorted by decreasing lengths.

`nn.utils.rnn.pad_packed_sequence` converts back to a padded tensor.
We implement a small model to test it on the toy task of lecture 12.1. “Recurrent Neural Networks”.

```python
class LSTMNet(nn.Module):
    def __init__(self, dim_input, dim_recurrent, num_layers, dim_output):
        super().__init__()
        self.lstm = nn.LSTM(input_size = dim_input,
                             hidden_size = dim_recurrent,
                             num_layers = num_layers)
        self.fc_o2y = nn.Linear(dim_recurrent, dim_output)

    def forward(self, input):
        # Get the last layer's last time step activation
        output, _ = self.lstm(input.permute(1, 0, 2))
        output = output[-1]
        return self.fc_o2y(F.relu(output))
```

| permute makes the tensor $T \times N \times \ldots$ as expected by LSTM.forward, and for simplicity, we consider all sequences to be of same length when picking the last step. |
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The diagram shows a graph with the x-axis labeled "Sequence length" and the y-axis labeled "Error". The graph compares the performance of different models, including elman, gating, and lstm, across varying sequence lengths. The elman model shows a significant increase in error as the sequence length increases, while the gating and lstm models maintain relatively low error levels throughout the sequence lengths depicted.
The LSTM were simplified into the Gated Recurrent Unit (GRU) by Cho et al. (2014), with a gating for the recurrent state, and a reset gate.

\[
\begin{align*}
    r_t &= \text{sigmoid} \left( W_{(x \ r)} x_t + W_{(h \ r)} h_{t-1} + b_{(r)} \right) & \text{(reset gate)} \\
    z_t &= \text{sigmoid} \left( W_{(x \ z)} x_t + W_{(h \ z)} h_{t-1} + b_{(z)} \right) & \text{(forget gate)} \\
    \tilde{h}_t &= \tanh \left( W_{(x \ h)} x_t + W_{(h \ h)} (r_t \odot h_{t-1}) + b_{(h)} \right) & \text{(full update)} \\
    h_t &= z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t & \text{(hidden update)}
\end{align*}
\]
class GRUNet(nn.Module):
    def __init__(self, dim_input, dim_recurrent, num_layers, dim_output):
        super().__init__()
        self.gru = nn.GRU(input_size = dim_input,
                          hidden_size = dim_recurrent,
                          num_layers = num_layers)
        self.fc_y = nn.Linear(dim_recurrent, dim_output)

    def forward(self, input):
        # Get the last layer's last time step activation
        output, _ = self.gru(input.permute(1, 0, 2))
        output = output[-1]
        return self.fc_y(F.relu(output))

permute makes the tensor $T \times N \times \ldots$ as expected by `GRU.forward`,
and for simplicity, we consider all sequences to be of same length when
picking the last step.
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The specific form of these units prevents the gradient from vanishing, but it may still be excessively large on certain mini-batch.

The standard strategy to solve this issue is gradient norm clipping (Pascanu et al., 2013), which consists of re-scaling the norm of the gradient to a fixed threshold $\delta$ when it is above:

$$\tilde{\nabla} f = \frac{\nabla f}{\|\nabla f\|} \min (\|\nabla f\|, \delta).$$
The function `torch.nn.utils.clip_grad_norm` applies this operation to the gradient of a model, as defined by an iterator through its parameters:

```python
>>> x = torch.empty(10)
>>> x.grad = x.new(x.size()).normal_()
>>> y = torch.empty(5)
>>> y.grad = y.new(y.size()).normal_()
>>> torch.cat((x.grad, y.grad)).norm()
tensor(4.0303)
>>> torch.nn.utils.clip_grad_norm_((x, y), 5.0)
tensor(4.0303)
>>> torch.cat((x.grad, y.grad)).norm()
tensor(4.0303)
>>> torch.nn.utils.clip_grad_norm_((x, y), 1.25)
tensor(4.0303)
>>> torch.cat((x.grad, y.grad)).norm()
tensor(1.2500)
```
Jozefowicz et al. (2015) conducted an extensive exploration of different recurrent architectures through meta-optimization, and even though some units simpler than LSTM or GRU perform well, they wrote:

“We have evaluated a variety of recurrent neural network architectures in order to find an architecture that reliably out-performs the LSTM. Though there were architectures that outperformed the LSTM on some problems, we were unable to find an architecture that consistently beat the LSTM and the GRU in all experimental conditions.”

(Jozefowicz et al., 2015)
The end
References


