5. Sequence modeling with recurrent neural networks

5.2b. Training an RNN. The backpropagation through time

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- The derivation of the gradient with respect to parameters $\mathbf{W}_{oh}$ is done from the output of the recurrent neural network.
- It can be expressed as

$$\mathbf{f}(\mathbf{x}_t) = \text{softmax}\left(\mathbf{z}_t^{(o)}\right) = \text{softmax}\left(\mathbf{W}_{oh}^{\top}\mathbf{h}_t + \mathbf{b}_o\right) \tag{1}$$

- This matrix is not revisited in the recursion.

- The derivative of the cost function at instant t with respect to parameter $w_{oh,i,j}$ is

$$\begin{aligned}\frac{dJ_{ML}}{dw_{oh,i,j}} &= \sum_{t=1}^{T} \frac{dJ_{ML}}{do_{j,t}} \frac{do_{j,t}}{dz^{(o)}_{j,t}} \frac{dz_{j,t}}{dw_{oh,i,j}} \\ &= \sum_{t=1}^{T} \frac{dJ_{ML}}{do_{j,t}} o'_{j,t} h_{i,t} \\ &= \sum_{t=1}^{T} \delta_{j,t} h_{i,t}\end{aligned} \tag{2}$$

Derivation of the gradients

Gradient with respect to the output weights

- In vector notation, the gradient with respect matrix $\mathbf{W}_{oh}$ is then

$$\nabla_{\mathbf{W}_{oh}} J_{ML}\left(\mathbf{o}_t\right) = \sum_{t=1}^{T} \mathbf{h}_t \boldsymbol{\delta}_t^\top \tag{3}$$

where $\boldsymbol{\delta}_t$ has components $\delta_{j,t}$. When the output of the RNN is a softmax, $\delta_{j,t} = \text{softmax}(z_{j,t}) - y_{j,t}$, therefore

$$\boldsymbol{\delta}_t = \text{softmax}(\mathbf{z}_t^{(o)}) - \mathbf{y}_t \tag{4}$$

- The derivation can be repeated for biases $\mathbf{b}_o$

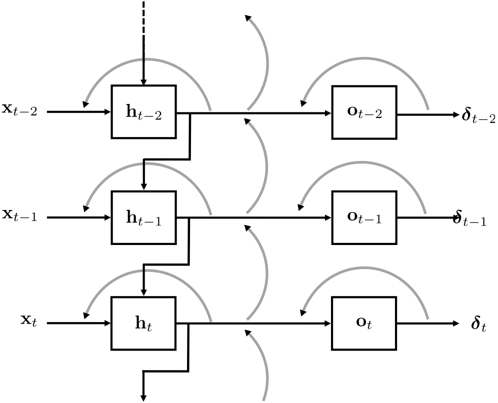
$$\begin{aligned}\frac{dJ_{ML}}{db_{o,j}} &= \sum_{t=1}^{T} \frac{dJ_{ML}}{do_{j,t}} \frac{do_{j,t}}{dz_{j,t}^{(o)}} \frac{dz_{j,t}}{db_{o,j}} \\ &= \sum_{t=1}^{T} \frac{dJ_{ML}}{do_{j,t}} o'_{j,t} \\ &= \sum_{t=1}^{T} \delta_{j,t}\end{aligned} \tag{5}$$

- with the result

$$\nabla_{\mathbf{b}_o} J_{ML}\left(\mathbf{o}_t\right) = \sum_{t=1}^{T} \boldsymbol{\delta}_t \tag{6}$$

Derivation of the gradients

Gradient with respect to the output weights



- The error term $\boldsymbol{\delta}_t$ must be backpropagated through $\mathbf{W}_{oh}$ in order to reach $\mathbf{W}_{hx}$ at input $\mathbf{x}_t$.
- It has to be repeatedly backpropagated through $\mathbf{W}_{hh}$ in order to reach the input matrix at each one of the inputs $\mathbf{x}_{t-t'}$.

To compute directly the gradient with respect to the weights, the chain rule must be used as follows.

1. Compute the gradient ($\nabla_{\mathbf{h}_t} J_{ML}$) of the cost function respect to $\mathbf{h}_t$.
2. Compute the derivatives of the components of $\mathbf{h}_t$ with respect to each component of $\mathbf{z}_t^{(x)}$, which gives the derivative of the tanh activation.
3. Compute the gradient of $\mathbf{z}_t^{(x)}$ with respect to $\mathbf{W}_{hx}$, which gives vector $\mathbf{x}_t$.

- The product of these elements has to be written in the right order so the gradient has the same dimensions as matrix $\mathbf{W}_{hx}$.
- The result is

$$
\begin{aligned}
\nabla_{\mathbf{W}_{hx}} J_{ML} &= \sum_{t=1}^{T} \nabla_{\mathbf{W}_{hx}} \mathbf{z}_t^{(x)} \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^{\top} \frac{\delta \mathbf{h}_t}{\delta \mathbf{z}_t^{(x)}} \\
&= \sum_{t=1}^{T} \mathbf{x}_t \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^{\top} \operatorname{diag}\left(\tanh'\left(\mathbf{z}_t^{(x)}\right)\right)
\end{aligned}
\tag{7}
$$

where the derivative of the hyperbolic tangent activation is expressed as a Jacobian represented by a diagonal matrix.

- A similar result can be found for the biases

$$\nabla_{\mathbf{b}_h} J_{ML} = \sum_{t=1}^{T} \operatorname{diag}\left(\tanh'\left(\mathbf{z}_t^{(x)}\right)\right)\left(\nabla_{\mathbf{h}_t} J_{ML}\right) \tag{8}$$

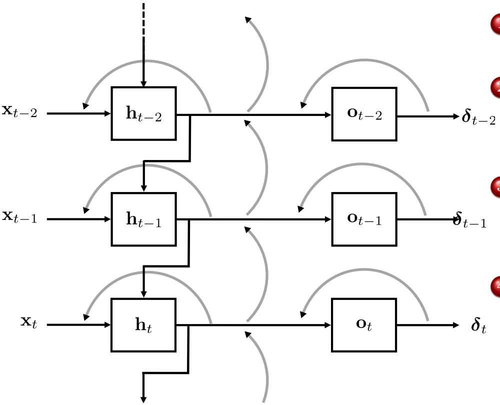
$$\nabla_{\mathbf{b}_h} J_{ML} = \sum_{t=1}^{T} \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^{\top} \operatorname{diag}\left(\tanh'\left(\mathbf{z}_t^{(x)}\right)\right) \tag{9}$$

- The above equations have the same form as any previously computed gradient: it is the product of
  1. the input sample $\mathbf{x}_t$ as a column vector
  2. a vector representing the backpropagated error
- The error is embedded in the (recursive) gradient with respect to the hidden state. This is, the error backpropagated to the input can be written as

$$\boldsymbol{\delta}_t^{(bp)} = \text{diag}\left(tanh'\left(\mathbf{z}_t^{(x)}\right)\right)\left(\nabla_{\mathbf{h}_t} J_{ML}\right)$$

.

For this set of weights, the backpropagation of the error at instant t



1. Starts from the output $\mathbf{o}_t$.
2. It is transformed with output weights $\mathbf{W}_{oh}$
3. This error is used to update $\mathbf{W}_{hh}$. The input is is $\mathbf{h}_{t-1}$.
4. The backpropagation then goes to the previous time instant, which requires another transformation of the error $\mathbf{W}_{hh}$.

- To see this, we can compute the gradient with respect to the hidden weights.

$$
\begin{aligned}
\nabla_{\mathbf{W}_{hh}} J_{ML} &= \sum_{t=1}^{T} \nabla_{\mathbf{W}_{hh}} \mathbf{z}_t^x \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^\top \frac{\delta \mathbf{h}_t}{\delta \mathbf{z}_t^{(x)}} \\
&= \sum_{t=1}^{T} \mathbf{h}_{t-1} \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^\top \operatorname{diag}\left(tanh'\left(\mathbf{z}_t^{(x)}\right)\right)
\end{aligned}
\tag{10}
$$

- The gradient of $\mathbf{z}_t$ is computed now with respect to $\mathbf{W}_{hh}$.
- The result is the input to these weights $\mathbf{h}_{t-1}$.
- This is known as backpropagation through time (BPTT).
- For $\mathbf{b}_h$, if we remove $\mathbf{h}_{t-1}$ from (10), we obtain the same result as in Eq. (8).

- Compute the output errors $\boldsymbol{\delta}_t$, $1 \leq t \leq T$.
- Use these errors to update the output weights with Eqs. (3) and (6).

$$\begin{aligned} \mathbf{W}_{oh} &\leftarrow \mathbf{W}_{oh} - \mu \sum_{t=1}^{T} \mathbf{h}_t \boldsymbol{\delta}_t^\top \\ \mathbf{b}_{oh} &\leftarrow \mathbf{b}_{oh} - \mu \sum_{t=1}^{T} \boldsymbol{\delta}_t \end{aligned} \tag{11}$$

Summary of the backpropagation through time

Input weights and hidden state weights

- Compute the gradient with respect to the hidden states

$$\nabla_{\mathbf{h}_t} J_{ML} = \mathbf{W}_{oh}\boldsymbol{\delta}_t + \mathbf{W}_{hh}\mathrm{diag}\left(\tanh'\left(\mathbf{z}_{t+1}^{(x)}\right)\right)\left(\nabla_{\mathbf{h}_{t+1}} J_{ML}\right) \quad (12)$$

- Update with Eqs. (7), (8), and (10).

$$\begin{aligned}
\mathbf{W}_{hx} &\leftarrow \mathbf{W}_{hx} - \mu \sum_{t=1}^{T} \mathbf{x}_t \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^\top \mathrm{diag}\left(\tanh'\left(\mathbf{z}_t^{(x)}\right)\right) \\
\mathbf{b}_h &\leftarrow \mathbf{b}_h - \mu \sum_{t=1}^{T} \mathrm{diag}\left(tanh'\left(\mathbf{z}_t^{(x)}\right)\right)\left(\nabla_{\mathbf{h}_t} J_{ML}\right)
\end{aligned} \quad (13)$$

$$\mathbf{W}_{hh} \leftarrow \mathbf{W}_{hh} - \mu \sum_{t=1}^{T} \mathbf{h}_{t-1} \left(\nabla_{\mathbf{h}_t} J_{ML}\right)^\top \mathrm{diag}\left(\tanh'\left(\mathbf{z}_t^{(x)}\right)\right) \quad (14)$$