Homework 3: Recurrent Neural Networks

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1 Exercise 1: Backpropagation through Time

Consider the RNN (Recurrent Neural Network) in Figure 1:

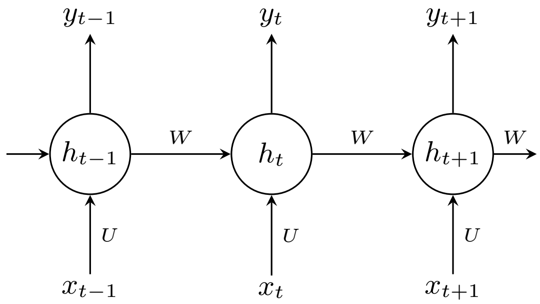


Figure 1: A recurrent neural network.

Each state h_t is given by:

$$h_t = \sigma(Wh_{t-1} + Ux_t), \text{where } \sigma(z) = \frac{1}{1+\exp(-z)}.$$

Let L be a loss function defined as the sum over the losses L_t at every time step until time T: $L = \sum_{t=0}^{T} L_t$, where L_t is a scalar loss depending on h_t.

In the following, we want to derive the gradient of this loss function with respect to the parameter W.

(a) Suppose we have $y = \sigma(Wx)$ where $y \in \mathbb{R}^n, x \in \mathbb{R}^d$ and $W \in \mathbb{R}^{n\times d}$. Derive the Jacobian $\frac{\partial y}{\partial x} = \text{diag}(\sigma')W \in \mathbb{R}^{n\times d}$.

Answer. $\frac{\partial y}{\partial x} = \frac{\partial \sigma(Wx)}{\partial x} = \frac{\partial \sigma(Wx)}{\partial (Wx)} \times \frac{\partial (Wx)}{\partial x} = \text{diag}(\sigma')W$.

(b) Derive the quantity $\frac{\partial L}{\partial W} = \sum_{t=0}^{T} \sum_{k=1}^{t} \frac{\partial L_t}{\partial h_t} \frac{\partial h_t}{\partial h_k} \frac{\partial h_k}{\partial W}$.

Answer. $\frac{\partial L}{\partial W} = \frac{\partial (\sum_{t=0}^{T} L_t)}{\partial W} = \sum_{t=0}^{T} (\frac{\partial L_t}{h_t} \times \frac{\partial h_t}{\partial W}) = \sum_{t=0}^{T} \sum_{k=0}^{t-1} (\frac{\partial L_t}{\partial h_t} \times \frac{\partial h_t}{\partial h_{t-k}} \times \frac{\partial h_{t-k}}{\partial W}) = \sum_{t=0}^{T} \sum_{k=1}^{t} (\frac{\partial L_t}{\partial h_t} \times \frac{\partial h_t}{\partial h_k} \times \frac{\partial h_k}{\partial W})$.

2 Exercise 2: Vanishing/Exploding Gradients in RNNs

In this exercise, we want to understand why RNNs (Recurrent Neural Networks) are especially prone to the Vanishing/Exploding Gradients problem and what role the eigenvalues of the weight matrix play. Consider part (b) of exercise 1 again.

(a) Write down $\frac{\partial L}{\partial W}$ as expanded sum for $T = 3$. You should see that if we want to back-propagate through n timesteps, we have to multiply the matrix $\text{diag}(\sigma')W$ n times with itself.

Answer. When $T = 3$, $\frac{\partial L}{\partial W} = \sum_{t=0}^{3}\sum_{k=1}^{t}(\frac{\partial L_t}{\partial h_t} \times \frac{\partial h_t}{\partial h_k} \times \frac{\partial h_k}{\partial W})$. Considering $h_t = \sigma(Wh_{t-1} + U_{x_t})$, $\frac{\partial h_t}{\partial h_{t-1}} = \text{diag}(\sigma')W$. Hence that $\frac{\partial h_n}{\partial h_0} = [\text{diag}(\sigma')W]^n$ for back-propagating through n timesteps. Specifically, if back-propagate through 3 timesteps, $\frac{\partial h_n}{\partial h_0} = [\text{diag}(\sigma')W]^3$.

(b) Remember that any diagonalizable (square) matrix M can be represented by its eigendecomposition $M = Q\Lambda Q^{-1}$ where Q is a matrix whose i-th column corresponds to the i-th eigenvector of M and Λ is a diagonal matrix with the corresponding eigenvalues placed on the diagonals. Recall that every eigenvector v_i satisfies this linear equation $Mv_i = \lambda_i v_i$, where $\lambda_i = \Lambda_{ii}$ is an eigenvalue of M. Proof by induction that for such a matrix the product $\prod_{i=1}^{n} M$ can be represented as: $M^n = Q\Lambda^n Q^{-1}$.

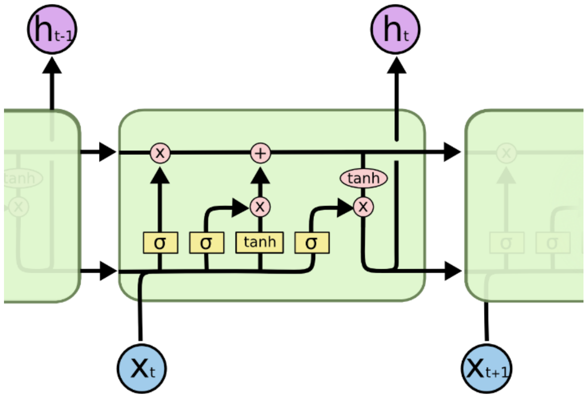
Answer. $M^n = (Q\Lambda Q^{-1})^n = \prod_{i=1}^{n}(Q\Lambda Q^{-1}) = Q\Lambda^n Q^{-1}$.

(c) Consider the weight matrix $\begin{bmatrix} 0.58 & 0.24 \\ 0.24 & 0.72 \end{bmatrix}$. Its eigendecomposition is:

$$W = Q\Lambda Q^{-1} = \begin{bmatrix} 0.8 & -0.6 \\ 0.6 & 0.8 \end{bmatrix} \begin{bmatrix} 0.4 & 0 \\ 0 & 0.9 \end{bmatrix} \begin{bmatrix} 0.8 & 0.6 \\ -0.6 & 0.8 \end{bmatrix}$$

Calculate W^{30}. What do you observe? What happens in general if the absolute value of all eigenvalues of W is smaller than 1? What happens if the absolute value of any eigenvalue of W is larger than 1? What if all eigenvalues are 1?

Answer. $W^{30} = \begin{bmatrix} 0.015261 & -0.020348 \\ -0.020348 & 0.027130 \end{bmatrix}$. When absolutes of all W's eigenvalues are all smaller than 1, values in W^{30} are pretty small, meaning the gradients are vanishing. While absolutes of all W's eigenvalues are all larger than 1, values in W^{30} are relatively large. When absolutes of all W's eigenvalues all equal to 1, the diagonals of W^{30} are 1.



$$
\begin{aligned}
f_t &= \sigma(W_f h_{t-1} + U_f x_t) \\
i_t &= \sigma(W_i h_{t-1} + U_i x_t) \\
o_t &= \sigma(W_o h_{t-1} + U_o x_t) \\
\tilde{C}_t &= \tanh(W_c h_{t-1} + U_c x_t) \\
C_t &= f_t \odot C_{t-1} + i_t \odot \tilde{C}_t \\
h_t &= o_t \odot \tanh(C_t)
\end{aligned}
$$

Figure 2: A Long Short Term Memory network.

3 Exercise 3: LSTMs

Recall the elements of a module in an LSTM and the corresponding computations, where $\odot$ stands for pointwise multiplication. For a good explanation on LSTMs you can refer to `https://colah.github.io/posts/2015-08-Understanding-LSTMs/`. Consider the LSTM in Figure 2.

(a) What do the gates f_t, i_t and o_t do?

Answer. f_t is forget gate, deciding the reserving information. i_t is input gate, deciding the updating information. o_t is output gate, deciding the outputting information.

(b) Which of the quantities next to the figure are always positive?

Answer. Gate f_t, i_t, and o_t. This architecture tackles the gradient vanishing problem by the follows. To calculate $\frac{\partial L}{\partial \theta}$, where θ is (W_f, W_o, W_i, W_c), we need to consider C_t as h_t in RNN. Since C_t depends on its previous state C_{t-1}, we have $\frac{\partial L}{\partial W} = \sum_{t=0}^{T} (\frac{\partial L_t}{h_t} \times \frac{\partial h_t}{\partial W}) = \sum_{t=0}^{T} \sum_{k=1}^{t} (\frac{\partial L_t}{\partial C_t} \times \frac{\partial C_t}{\partial C_k} \times \frac{\partial C_k}{\partial W})$.

Note that the real formula is more complicated, where we also need to take f_t, i_t, and $\tilde{C}_t$ into consideration. But the effect of these factors is negligible.

Let's now try to understand how this architecture approaches the vanishing gradients problem. To calculate the gradient $\frac{\partial L}{\partial \theta}$, where θ stands for the parameters (W_f, W_o, W_i, W_c), we now have to consider the cell state C_t instead of h_t. Like h_t in normal RNNs, C_t will also depend on the previous cell states $C_{t-1}, \dots, C_0$, so we get a formula of the form:

$$\frac{\partial L}{\partial W} = \sum_{t=0}^{T} \sum_{k=1}^{t} \frac{\partial L}{\partial C_t} \frac{\partial C_t}{\partial C_k} \frac{\partial C_k}{\partial W},$$

where note that the real formula is a bit more complicated since C_t also depends on f_t, i_t and $\widetilde{C}_t$, which in turn all depend on W, but this can be neglected.

(c) We know that $\frac{\partial C_t}{\partial C_k} = \prod_{i=k+1}^{t} \frac{\partial C_t}{\partial C_{t-1}}$. Let $f_t = 1$ and $i_t = 0$ such that $C_t = C_{t-1}$ for all t. What is the gradient $\frac{\partial C_t}{\partial C_k}$ in this case?

Answer. When $f_t = 1$ and $i_t = 0$, $\frac{\partial C_t}{\partial C_k} = \prod_{i=k+1}^{t} \frac{\partial (f_i \odot C_{i-1} + i_i \odot \tilde{C}_i)}{\partial C_{i-1}} = \prod_{i=k+1}^{t} \frac{\partial C_{i-1}}{\partial C_{i-1}} = 1.$

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