# Homework 5: Recurrent Neural Networks

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## Exercise 1: Backpropagation through Time

Consider the RNN (Recurrent Neural Network) as:

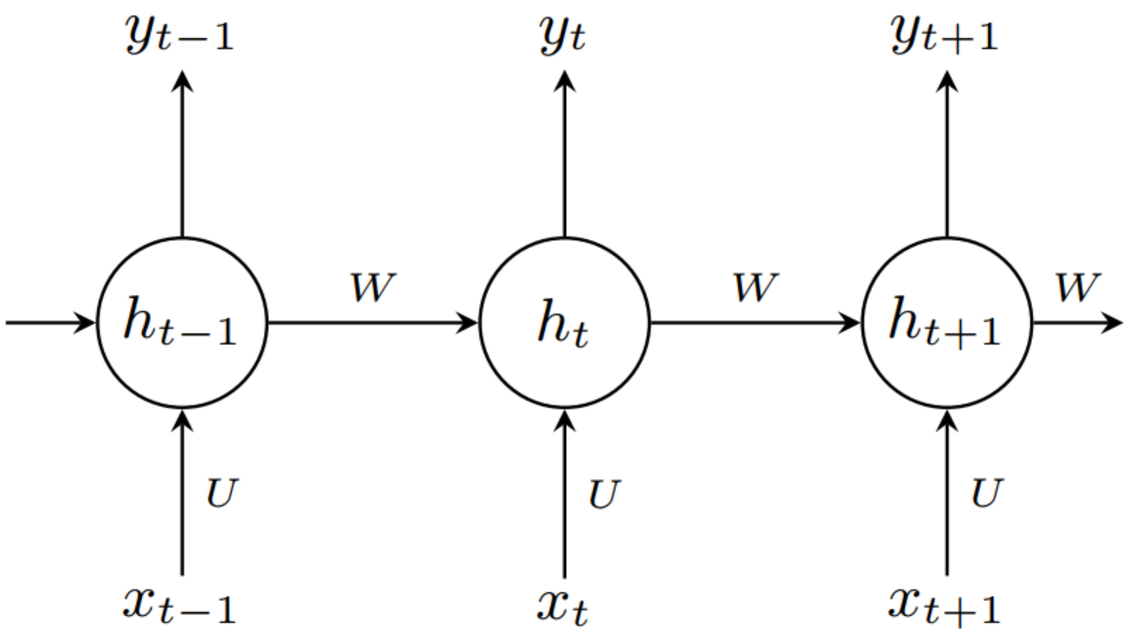


Figure 1: A recurrent neural network.

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 $W$.

## ex.1 (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 $\frac{\partial y}{\partial x} = \mathrm{diag}(\sigma')\ \mathrm{W} \in \mathbb{R}^{\mathrm{n}\times\mathrm{d}}$

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根据已知条件，可以通过链式法则得到：

$$\begin{aligned} \frac{\partial y}{\partial x} &= \frac{\partial\ \sigma(Wx)}{\partial x} \\ &= \frac{\partial\ \sigma(Wx)}{\partial Wx}\frac{\partial Wx}{\partial x} \end{aligned} \tag{1}$$

对于 $Wx$ 有：

$$Wx = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} \\ w_{21} & w_{22} & \cdots & w_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ w_{31} & w_{32} & \cdots & w_{3m} \\ w_{n1} & w_{n2} & \cdots & w_{nm} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} w_{11}x_1 + w_{12}x_2 + \cdots + w_{1m}x_m \\ w_{21}x_1 + w_{22}x_2 + \cdots + w_{1m}x_m \\ \vdots \\ w_{n1}x_1 + w_{n2}x_2 + \cdots + w_{nm}x_m \end{bmatrix} \tag{2}$$

假设 $p_i = w_{i1}x_1 + w_{i2}x_2 + \cdots + w_{im}x_m$ 因此对于 $\frac{\partial Wx}{\partial x}$：

$$\begin{aligned} \frac{\partial Wx}{\partial x} &= \begin{bmatrix} \frac{\partial p_1}{\partial x_1} & \frac{\partial p_1}{\partial x_2} & \cdots & \frac{\partial p_1}{\partial x_m} \\ \frac{\partial p_2}{\partial x_1} & \frac{\partial p_2}{\partial x_2} & \cdots & \frac{\partial p_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial p_n}{\partial x_1} & \frac{\partial p_n}{\partial x_2} & \cdots & \frac{\partial p_n}{\partial x_m} \end{bmatrix} \\ &= \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} \\ w_{21} & w_{22} & \cdots & w_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ w_{31} & w_{32} & \cdots & w_{3m} \\ w_{n1} & w_{n2} & \cdots & w_{nm} \end{bmatrix} = W \end{aligned} \tag{3}$$

对于 $\frac{\partial\ \sigma(Wx)}{\partial Wx}$，令 $y_i = \sigma(p_i), \qquad i = 1, 2, \cdots, n$ 则有：

$$
\begin{aligned}
\frac{\partial\, \sigma(Wx)}{\partial Wx} &= \frac{\partial y}{\partial p} \\
&= \begin{bmatrix} \frac{\partial y_1}{p_1} & \frac{\partial y_2}{p_1} & \cdots & \frac{\partial y_n}{p_1} \\ \frac{\partial y_2}{p_1} & \frac{\partial y_2}{p_2} & \cdots & \frac{\partial y_2}{p_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_n}{p_1} & \frac{\partial y_n}{p_2} & \cdots & \frac{\partial y_n}{p_n} \end{bmatrix} \\
&= \begin{bmatrix} \sigma'(p_1) & 0 & \cdots & 0 & \\ 0 & \sigma'(p_2) & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \\ 0 & 0 & 0 & \cdots & \sigma'(p_n) \end{bmatrix} \\
&= \operatorname{diag}(\sigma')
\end{aligned} \tag{4}
$$

根据式$(1),(3),(4)$可得

$$
\frac{\partial y}{\partial x} = \operatorname{diag}(\sigma')\mathrm{W} \in \mathbb{R}^{\mathrm{n}\times\mathrm{d}}
$$

## ex.1 (b)

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

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根据 $L = \sum_{t=0}^{T} L_t$ 的定义，可以得到

$$
\begin{aligned}
\frac{\partial L}{\partial W} &= \frac{\partial}{\partial W} \sum_{t=0}^{T} L_t \\
&= \sum_{t=0}^{T} \frac{\partial L_t}{\partial W}
\end{aligned} \tag{5}
$$

由于 $L_t$ 是和 $h_t$ 有关的一个标量损失，并且 $h_t$ 有如下表示：

$$
\begin{cases}
h_t & = \sigma(Wh_{t-1} + Ux_t) \\
h_{t-1} & = \sigma(Wh_{t-2} + Ux_{t-1}) \\
 & \vdots \\
h_1 & = \sigma(Wh_0, +Ux_1) \\
h_0 & = \sigma(Wh_f + Ux_0),\ h_f \text{ 和 } W \text{ 无关}
\end{cases} \tag{6}
$$

因此可以得到：

$$
\begin{aligned}
\frac{\partial L_t}{\partial W} &= \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial W}\right) + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_{t-1}}\frac{\partial h_{t-1}}{\partial W}\right) + \cdots + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_{t-1}}\cdots\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial W}\right) + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_{t-1}}\cdots\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial W}\right) \\
&= \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_t}\frac{\partial h_t}{\partial W}\right) + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_{t-1}}\frac{\partial h_{t-1}}{\partial W}\right) + \cdots + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_1}\frac{\partial h_1}{\partial W}\right) + \left(\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_0}\frac{\partial h_0}{\partial W}\right) \\
&= \sum_{k=0}^{t} \frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial h_k}{\partial W}
\end{aligned} \tag{7}
$$

根据式 $(5),(7)$ 可以得到：

$$
\frac{\partial L}{\partial W} = \sum_{t=0}^{T}\sum_{k=0}^{t} \frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial h_k}{\partial W} \tag{8}
$$

> 发现结果和题目有矛盾，$k$ 应该从0而不是1开始

# Exercise 2: Vanishing/Exploding Gradients in RNNs

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

## ex.2 (a)

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

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由式 $(7)$ 可得，当 $T=3$时，有:

$$
\begin{aligned}
\frac{\partial L}{\partial W} &= \sum_{t=0}^{T=3}\sum_{k=0}^{t}\frac{\partial L_t}{\partial h_t}\frac{\partial h_t}{\partial h_k}\frac{\partial h_k}{\partial W} \\
&= (\frac{\partial L_0}{\partial h_0}\frac{\partial h_0}{\partial h_0}\frac{\partial h_0}{\partial W}) + (\frac{\partial L_1}{\partial h_1}\frac{\partial h_1}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_1}{\partial h_1}\frac{\partial h_1}{\partial h_1}\frac{\partial h_1}{\partial W}) \\
&\quad + (\frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial h_2}\frac{\partial h_2}{\partial W}) \\
&\quad + (\frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_3}\frac{\partial h_3}{\partial W}) \\
&= (\frac{\partial L_0}{\partial h_0}\frac{\partial h_0}{\partial W}) + (\frac{\partial L_1}{\partial h_1}\frac{\partial h_1}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_1}{\partial h_1}\frac{\partial h_1}{\partial W}) \\
&\quad + (\frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L_2}{\partial h_2}\frac{\partial h_2}{\partial W}) \\
&\quad + (\frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_0}\frac{\partial h_0}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial W} + \frac{\partial L_3}{\partial h_3}\frac{\partial h_3}{\partial W})
\end{aligned}
\tag{9}
$$

根据式 $(6)$ 可以得到:

$$
\frac{\partial h_t}{\partial h_{t-1}} = \mathrm{diag}(\sigma')\mathrm{W} \in \mathbb{R}^{\mathrm{n\times d}} \tag{10}
$$

将上式合并，可以得到:

$$
\begin{aligned}
\frac{\partial L}{\partial W} = (\frac{\partial L_0}{\partial h_0}\frac{\partial h_0}{\partial W}) &+ [\frac{\partial L_1}{\partial h_1}(\mathrm{diag}(\sigma')\mathrm{W})\frac{\partial \mathrm{h}_0}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_1}{\partial \mathrm{h}_1}\frac{\partial \mathrm{h}_1}{\partial \mathrm{W}}] \\
&+ [\frac{\partial \mathrm{L}_2}{\partial \mathrm{h}_2}(\mathrm{diag}(\sigma')\mathrm{W})^2\frac{\partial \mathrm{h}_0}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_2}{\partial \mathrm{h}_2}(\mathrm{diag}(\sigma')\mathrm{W})\frac{\partial \mathrm{h}_1}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_2}{\partial \mathrm{h}_2}\frac{\partial \mathrm{h}_2}{\partial \mathrm{W}}] \\
&+ [\frac{\partial \mathrm{L}_3}{\partial \mathrm{h}_3}(\mathrm{diag}(\sigma')\mathrm{W})^3\frac{\partial \mathrm{h}_0}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_3}{\partial \mathrm{h}_3}(\mathrm{diag}(\sigma')\mathrm{W})^2\frac{\partial \mathrm{h}_1}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_3}{\partial \mathrm{h}_3}(\mathrm{diag}(\sigma')\mathrm{W})\frac{\partial \mathrm{h}_2}{\partial \mathrm{W}} + \frac{\partial \mathrm{L}_3}{\partial \mathrm{h}_3}\frac{\partial \mathrm{h}_3}{\partial \mathrm{W}}]
\end{aligned}
\tag{11}
$$

在式 $(11)$ 看到，当 $T=3$ 时，需要乘 $(\mathrm{diag}(\sigma')\mathrm{W})$ 3次

## ex.2 (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 $\Lambda$ 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: $M^n = Q\Lambda^n Q^{-1}$.

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对于 $n=1$ 时，根据题目可得:

$$M^1 = Q\Lambda^1 Q^{-1} \tag{12}$$

对于 $n = t - 1$ 时，假设：

$$M^{t-1} = Q\Lambda^{t-1} Q^{-1} \tag{13}$$

那么在 $n = t$ 时，可以得到：

$$\begin{aligned} M^t &= M^{t-1}M \\ &= (Q\Lambda^{t-1}Q^{-1})(Q\Lambda Q^{-1}) \\ &= Q\Lambda^{t-1}\Lambda Q^{-1} \\ &= Q\Lambda^t Q^{-1} \end{aligned} \tag{14}$$

因此可以得到 $\prod_{i=1}^n M = Q\Lambda^t Q^{-1}$

## ex.2 (c)

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

$$W = Q\Lambda Q^{-1} = \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.5 \end{bmatrix} \begin{bmatrix} 0.9 & 0 \\ 0 & 0.4 \end{bmatrix} \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix}$$

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?

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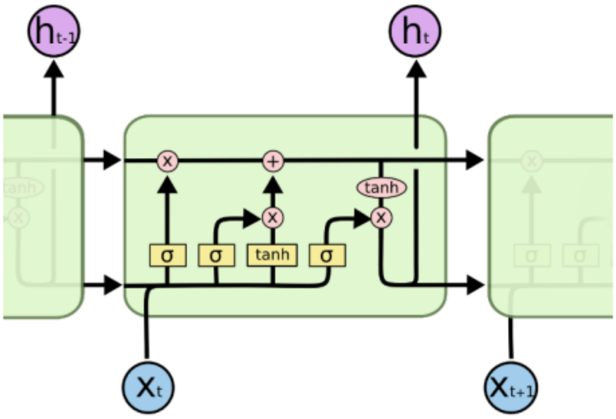
根据式 $(14)$ 可以得到：

$$\begin{aligned} W^{30} &= Q\Lambda^{30}Q^{-1} \\ &= \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix} \begin{bmatrix} 0.9^{30} & 0 \\ 0 & 0.4^{30} \end{bmatrix} \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix} \\ &= \begin{bmatrix} 0.015260 & 0.020348 \\ 0.020348 & 0.027130 \end{bmatrix} \end{aligned} \tag{15}$$

1. 从式 $(15)$ 可以看出，$\Lambda$ 得30次方会导致结果相对变小很多
2. 当 $W$ 的所有特征值的绝对值都小于1时，$\Lambda$ 对角线上的元素的绝对值也都会小于1，此时对于 $n$ 来说，其递增会导致 $\Lambda$ 指数递减，最终导致 $W^n$ 的值变得很小
3. 当 $W$ 的所有特征值的绝对值都打于1时，$\Lambda$ 对角线上的元素的绝对值也都会大于1，此时对于 $n$ 来说，其递增会导致 $\Lambda$ 指数递增，最终导致 $W^n$ 的值变得很大
4. 当 $W$ 的所有特征值的绝对值都等于1时，$\Lambda$ 对角线上的元素的绝对值也都会等于1，此时对于 $n$ 来说，其无论怎么变化，$\Lambda$ 不变，最终 $W^n$ 的值不变

# 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 http://colah.github.io/posts/2015-08-Understanding-LSTMs/ . Consider the LSTM in Figure 2.




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

Figure 2: A Long Short Term Memory network.

## ex.3 (a)

What do the gates $f_t, i_t$ and $o_t$ do?

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- 遗忘门 $f_t$：选择上一时刻状态 $C_{t-1}$ 的部分信息融入当前状态 $C_t$，选择性的将 $C_{t-1}$ 中与当前词 $x_t$ 无关的内容遗忘并保留有用的信息
- 输入门 $i_t$：判断当前词 $x_t$ 的信息，选择性的进行保留进细胞当前状态 $C_t$ 或者丢弃
- 输出门 $o_t$：判断当前细胞状态 $C_t$ 的有用信息，并选择性的输出到隐层 $h_t$ 中

## ex.3 (b)

Which of the quantities next to the figure are always positive?

Let's now try to understand how this architecture approaches the vanishing gradients problem. To calculate the gradient $\frac{\partial L}{\partial \theta}$ , where $\theta$ 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 $C_{t-1}, \cdots, C_0$, so we get a formula of the form:

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

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

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对于 $f_t, i_t$ 和 $o_t$ 来说，采用了 Sigmoid 函数，而该函数值域为 $(0,1)$，因此符号总是为正的

对于 $\tilde{C}_t$ 由于 Tanh 函数的值域为 $(-1,1)$，因此 $\tilde{C}_t$，$h_t$ 和 $C_t$ 都可能符号为负

## ex.3 (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?

---

$$\frac{\partial C_t}{\partial C_k} = \prod_{i=k+1}^{t} \frac{\partial C_t}{\partial C_{t-1}} = \prod_{i=k+1}^{t} 1 = 1 \tag{16}$$

显然，梯度为1