# CS7015 (Deep Learning) : Lecture 14

## Sequence Learning Problems, Recurrent Neural Networks, Backpropagation Through Time (BPTT), Vanishing and Exploding Gradients, Truncated BPTT

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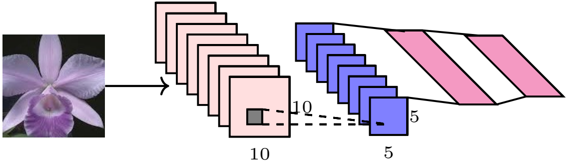
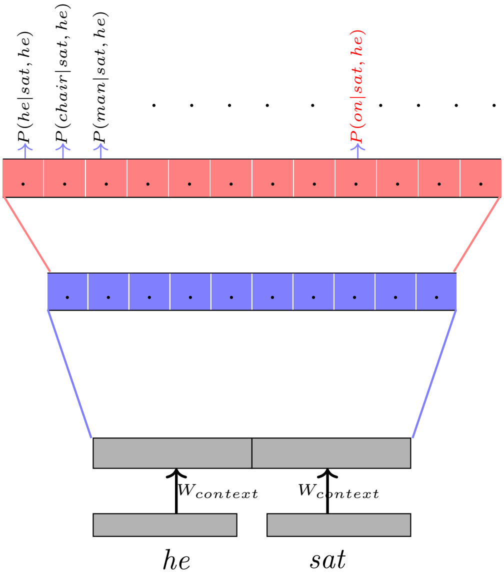
# Module 14.1: Sequence Learning Problems




- In feedforward and convolutional neural networks the size of the input was always fixed
- For example, we fed fixed size ($32 \times 32$) images to convolutional neural networks for image classification

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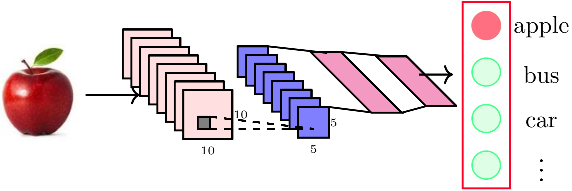
- Similarly in word2vec, we fed a fixed window ($k$) of words to the network

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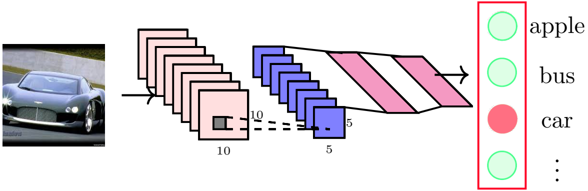
- For example, we fed fixed size ($32 \times 32$) images to convolutional neural networks for image classification
- Similarly in word2vec, we fed a fixed window ($k$) of words to the network
- Further, each input to the network was independent of the previous or future inputs

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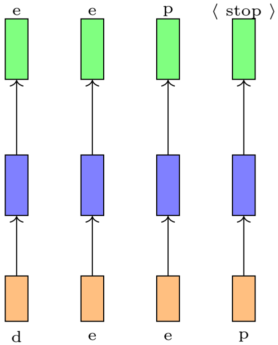
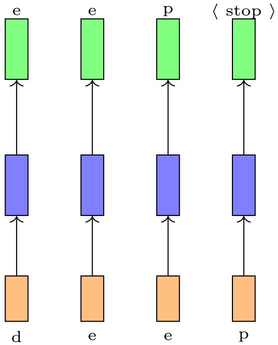
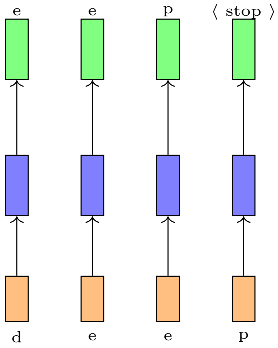
- For example, we fed fixed size ($32 \times 32$) images to convolutional neural networks for image classification
- Similarly in word2vec, we fed a fixed window ($k$) of words to the network
- Further, each input to the network was independent of the previous or future inputs
- For example, the computatations, outputs and decisions for two successive images are completely independent of each other



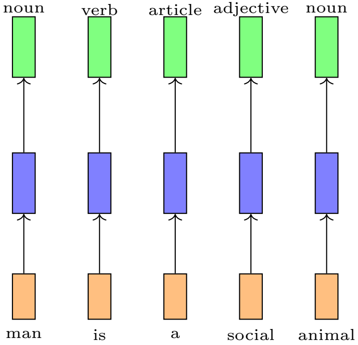

- In many applications the input is not of a fixed size
- Further successive inputs may not be independent of each other
- For example, consider the task of auto completion
- Given the first character ‘d’ you want to predict the next character ‘e’ and so on



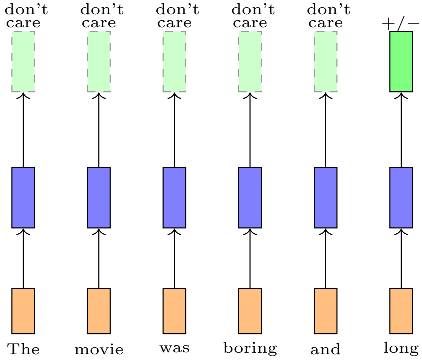

- Notice a few things
- First, successive inputs are no longer independent (while predicting 'e' you would want to know what the previous input was in addition to the current input)
- Second, the length of the inputs and the number of predictions you need to make is not fixed (for example, "learn", "deep", "machine" have different number of characters)
- Third, each network (orange-blue-green structure) is performing the same task (**input** : character **output** : character)



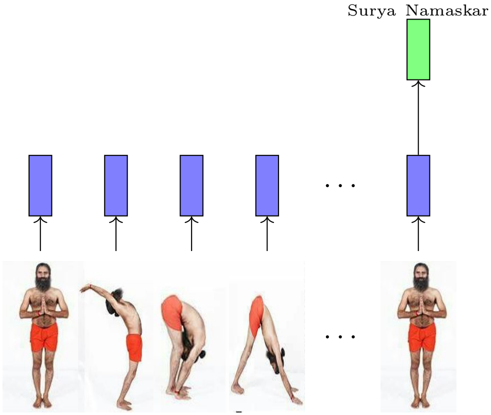

- These are known as sequence learning problems
- We need to look at a sequence of (dependent) inputs and produce an output (or outputs)
- Each input corresponds to one time step
- Let us look at some more examples of such problems




- Consider the task of predicting the part of speech tag (noun, adverb, adjective verb) of each word in a sentence
- Once we see an adjective (social) we are almost sure that the next word should be a noun (man)
- Thus the current output (noun) depends on the current input as well as the previous input
- Further the size of the input is not fixed (sentences could have arbitrary number of words)
- Notice that here we are interested in producing an output at each time step
- Each network is performing the same task (**input** : word, **output** : tag)




- Sometimes we may not be interested in producing an output at every stage
- Instead we would look at the full sequence and then produce an output
- For example, consider the task of predicting the polarity of a movie review
- The prediction clearly does not depend only on the last word but also on some words which appear before
- Here again we could think that the network is performing the same task at each step (input : word, output : +/−) but it's just that we don't care about intermediate outputs



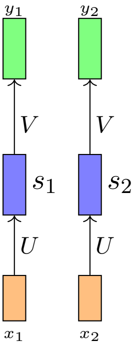

- Sequences could be composed of anything (not just words)
- For example, a video could be treated as a sequence of images
- We may want to look at the entire sequence and detect the activity being performed

# Module 14.2: Recurrent Neural Networks

How do we model such tasks involving sequences ?

### Wishlist

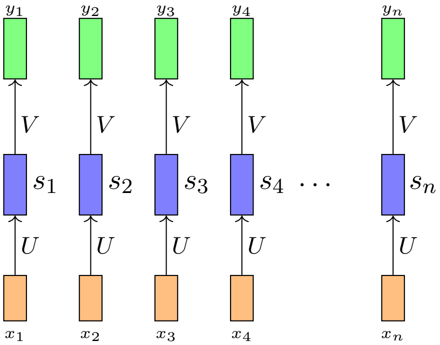
- Account for dependence between inputs
- Account for variable number of inputs
- Make sure that the function executed at each time step is the same
- We will focus on each of these to arrive at a model for dealing with sequences



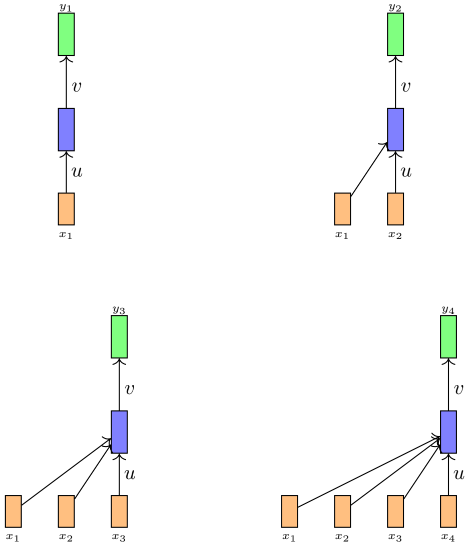

- What is the function being executed at each time step ?

$$
\begin{aligned}
s_i &= \sigma(Ux_i + b) \\
y_i &= \mathcal{O}(Vs_i + c) \\
i &= \text{timestep}
\end{aligned}
$$

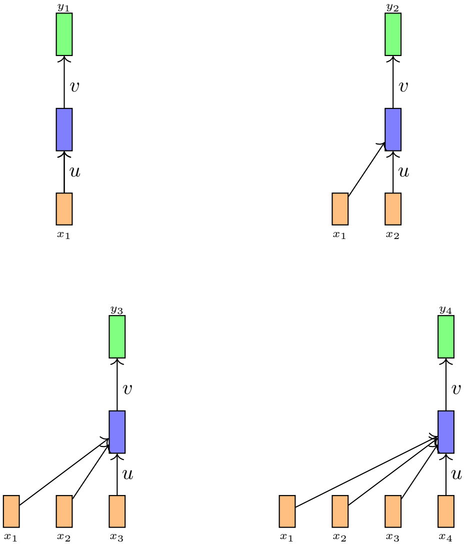
- Since we want the same function to be executed at each timestep we should share the same network (i.e., same parameters at each timestep)




- This parameter sharing also ensures that the network becomes agnostic to the length (size) of the input
- Since we are simply going to compute the same function (with same parameters) at each timestep, the number of timesteps doesn't matter
- We just create multiple copies of the network and execute them at each timestep



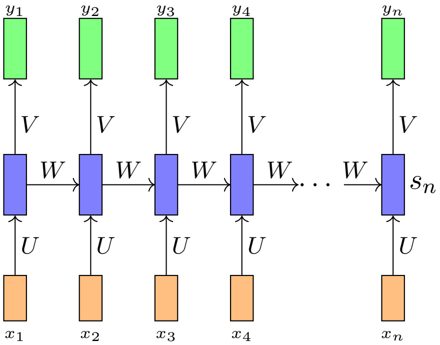

- How do we account for dependence between inputs ?
- Let us first see an infeasible way of doing this
- At each timestep we will feed all the previous inputs to the network
- Is this okay ?
- No, it violates the other two items on our wishlist
- How ? Let us see




- First, the function being computed at each time-step now is different

$$
\begin{aligned}
y_1 &= f_1(x_1) \\
y_2 &= f_2(x_1, x_2) \\
y_3 &= f_3(x_1, x_2, x_3)
\end{aligned}
$$

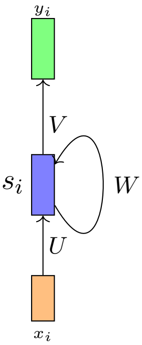
- The network is now sensitive to the length of the sequence
- For example a sequence of length 10 will require $f_1, \ldots, f_{10}$ whereas a sequence of length 100 will require $f_1, \ldots, f_{100}$



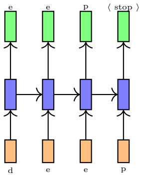

- The solution is to add a recurrent connection in the network,

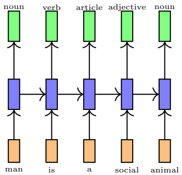
$$s_i = \sigma(Ux_i + Ws_{i-1} + b)$$
$$y_i = \mathcal{O}(Vs_i + c)$$
$$or$$
$$y_i = f(x_i, s_{i-1}, W, U, V, b, c)$$

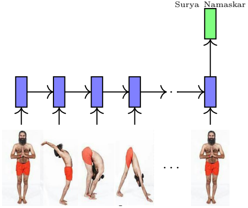
- $s_i$ is the state of the network at timestep $i$
- The parameters are $W, U, V, c, b$ which are shared across timesteps
- The same network (and parameters) can be used to compute $y_1, y_2, \dots, y_{10}$ or $y_{100}$

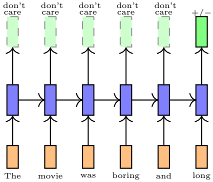



- This can be represented more compactly



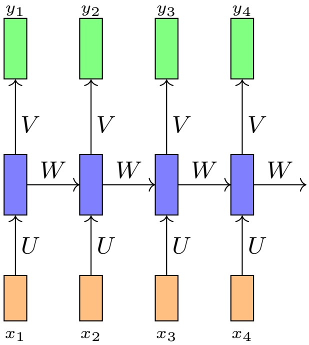




- Let us revisit the sequence learning problems that we saw earlier
- We now have recurrent connections between time steps which account for dependence between inputs

# Module 14.3: Backpropagation through time




- Before proceeding let us look at the dimensions of the parameters carefully

$$x_i \in \mathbb{R}^n \quad \text{(n-dimensional input)}$$

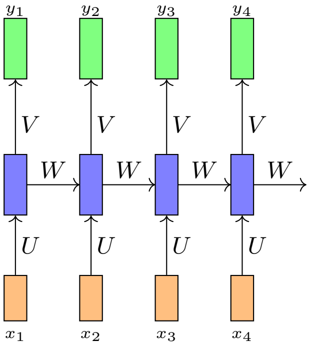
$$s_i \in \mathbb{R}^d \quad \text{(d-dimensional state)}$$

$$y_i \in \mathbb{R}^k \quad \text{(say k classes)}$$

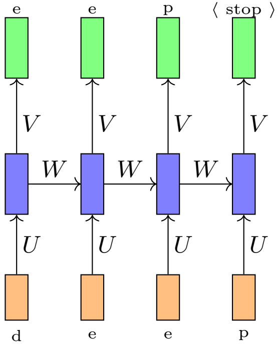
$$U \in \mathbb{R}^{n \times d}$$

$$V \in \mathbb{R}^{d \times k}$$

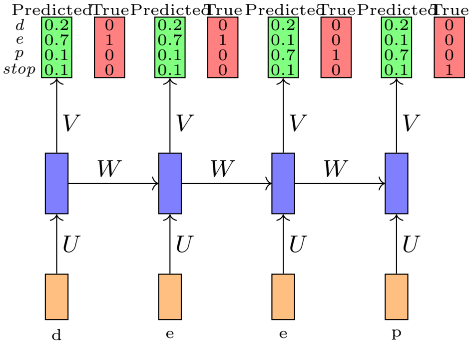
$$W \in \mathbb{R}^{d \times d}$$



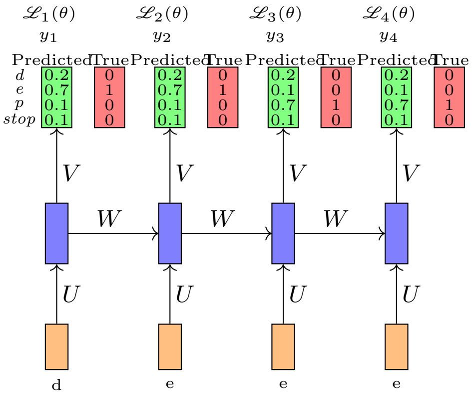

- How do we train this network ? (**Ans**: using backpropagation)
- Let us understand this with a concrete example




- Suppose we consider our task of auto-completion (predicting the next character)
- For simplicity we assume that there are only 4 characters in our vocabulary (d,e,p, <stop>)
- At each timestep we want to predict one of these 4 characters
- What is a suitable output function for this task ? **(softmax)**
- What is a suitable loss function for this task ? **(cross entropy)**




- Suppose we initialize $U, V, W$ randomly and the network predicts the probabilities as shown
- And the true probabilities are as shown
- We need to answer two questions
- What is the total loss made by the model ?
- How do we backpropagate this loss and update the parameters ($\theta = \{U, V, W, b, c\}$) of the network ?




- The total loss is simply the sum of the loss over all time-steps

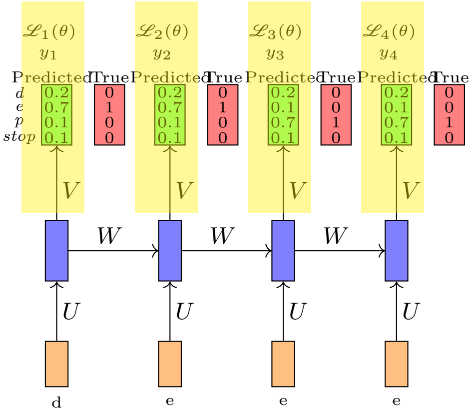
$$\mathscr{L}(\theta) = \sum_{t=1}^{T} \mathscr{L}_t(\theta)$$

$$\mathscr{L}_t(\theta) = -log(y_{tc})$$

$$y_{tc} = \text{predicted probability of true character at time-step } t$$

$$T = \text{number of timesteps}$$

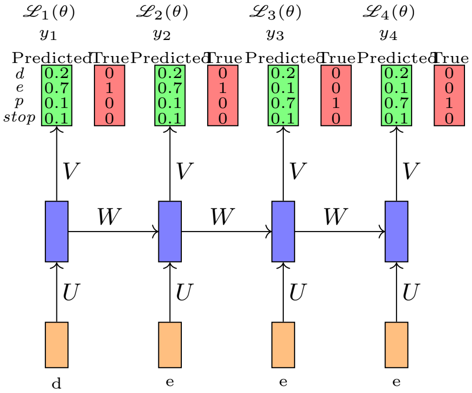
- For backpropagation we need to compute the gradients w.r.t. $W, U, V, b, c$
- Let us see how to do that




- Let us consider $\frac{\partial \mathscr{L}(\theta)}{\partial V}$ ($V$ is a matrix so ideally we should write $\nabla_v \mathscr{L}(\theta)$)

$$\frac{\partial \mathscr{L}(\theta)}{\partial V} = \sum_{t=1}^{T} \frac{\partial \mathscr{L}_t(\theta)}{\partial V}$$

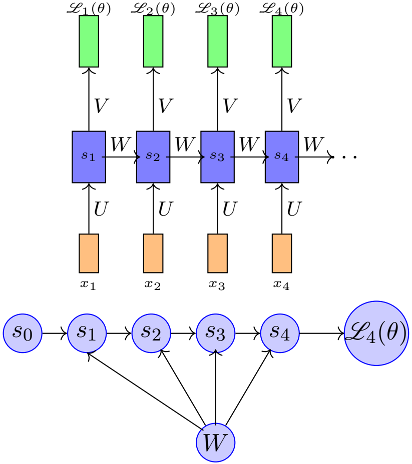
- Each term is the summation is simply the derivative of the loss w.r.t. the weights in the output layer
- We have already seen how to do this when we studied backpropagation




- Let us consider the derivative $\frac{\partial \mathscr{L}(\theta)}{\partial W}$

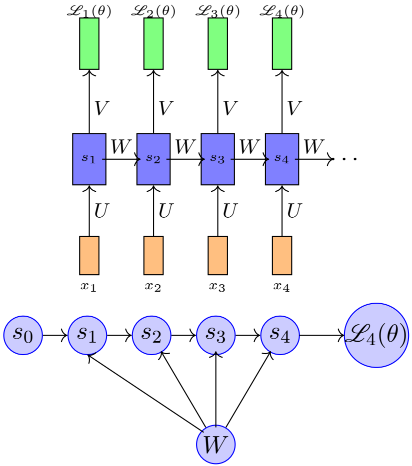
$$\frac{\partial \mathscr{L}(\theta)}{\partial W} = \sum_{t=1}^{T} \frac{\partial \mathscr{L}_t(\theta)}{\partial W}$$

- By the chain rule of derivatives we know that $\frac{\partial \mathscr{L}_t(\theta)}{\partial W}$ is obtained by summing gradients along all the paths from $\mathscr{L}_t(\theta)$ to $W$
- What are the paths connecting $\mathscr{L}_t(\theta)$ to $W$ ?
- Let us see this by considering $\mathscr{L}_4(\theta)$




- $\mathscr{L}_4(\theta)$ depends on $s_4$
- $s_4$ in turn depends on $s_3$ and $W$
- $s_3$ in turn depends on $s_2$ and $W$
- $s_2$ in turn depends on $s_1$ and $W$
- $s_1$ in turn depends on $s_0$ and $W$

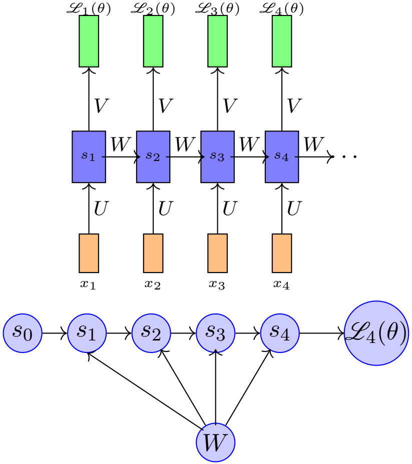
  where $s_0$ is a constant starting state.




- What we have here is an ordered network
- In an ordered network each state variable is computed one at a time in a specified order (first $s_1$, then $s_2$ and so on)
- Now we have

$$\frac{\partial \mathscr{L}_4(\theta)}{\partial W} = \frac{\partial \mathscr{L}_4(\theta)}{\partial s_4} \frac{\partial s_4}{\partial W}$$

- We have already seen how to compute $\frac{\partial \mathscr{L}_4(\theta)}{\partial s_4}$ when we studied backprop
- But how do we compute $\frac{\partial s_4}{\partial W}$




- Recall that

$$s_4 = \sigma(W s_3 + b)$$

- In such an ordered network, we can't compute $\frac{\partial s_4}{\partial W}$ by simply treating $s_3$ as a constant (because it also depends on $W$)
- In such networks the total derivative $\frac{\partial s_4}{\partial W}$ has two parts
- **Explicit** : $\frac{\partial^+ s_4}{\partial W}$, treating all other inputs as constant
- **Implicit** : Summing over all indirect paths from $s_4$ to $W$
- Let us see how to do this

$$\frac{\partial s_4}{\partial W} = \underbrace{\frac{\partial^+ s_4}{\partial W}}_{\text{explicit}} + \underbrace{\frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial W}}_{\text{implicit}}$$

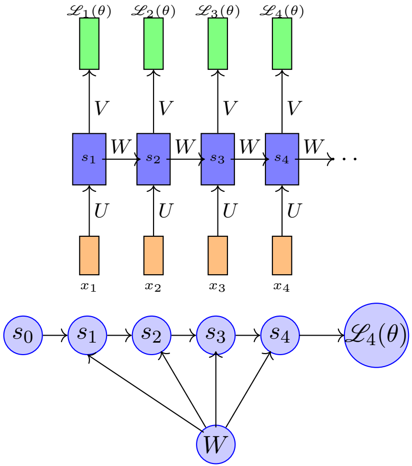
$$= \frac{\partial^+ s_4}{\partial W} + \frac{\partial s_4}{\partial s_3}\left[\underbrace{\frac{\partial^+ s_3}{\partial W}}_{\text{explicit}} + \underbrace{\frac{\partial s_3}{\partial s_2}\frac{\partial s_2}{\partial W}}_{\text{implicit}}\right]$$

$$= \frac{\partial^+ s_4}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial^+ s_3}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial s_2}\left[\frac{\partial^+ s_2}{\partial W} + \frac{\partial s_2}{\partial s_1}\frac{\partial s_1}{\partial W}\right]$$

$$= \frac{\partial^+ s_4}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial^+ s_3}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial s_2}\frac{\partial^+ s_2}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial s_2}\frac{\partial s_2}{\partial s_1}\left[\frac{\partial^+ s_1}{\partial W}\right]$$

For simplicity we will short-circuit some of the paths

$$\frac{\partial s_4}{\partial W} = \frac{\partial s_4}{\partial s_4}\frac{\partial^+ s_4}{\partial W} + \frac{\partial s_4}{\partial s_3}\frac{\partial^+ s_3}{\partial W} + \frac{\partial s_4}{\partial s_2}\frac{\partial^+ s_2}{\partial W} + \frac{\partial s_4}{\partial s_1}\frac{\partial^+ s_1}{\partial W} = \sum_{k=1}^{4}\frac{\partial s_4}{\partial s_k}\frac{\partial^+ s_k}{\partial W}$$




- Finally we have

$$\frac{\partial \mathscr{L}_4(\theta)}{\partial W} = \frac{\partial \mathscr{L}_4(\theta)}{\partial s_4} \frac{\partial s_4}{\partial W}$$

$$\frac{\partial s_4}{\partial W} = \sum_{k=1}^{4} \frac{\partial s_4}{\partial s_k} \frac{\partial^+ s_k}{\partial W}$$

$$\therefore \frac{\partial \mathscr{L}_t(\theta)}{\partial W} = \frac{\partial \mathscr{L}_t(\theta)}{\partial s_t} \sum_{k=1}^{t} \frac{\partial s_t}{\partial s_k} \frac{\partial^+ s_k}{\partial W}$$

- This algorithm is called backpropagation through time (BPTT) as we backpropagate over all previous time steps

# Module 14.4: The problem of Exploding and Vanishing Gradients

- We will now focus on $\frac{\partial s_t}{\partial s_k}$ and highlight an important problem in training RNN's using BPTT

$$\frac{\partial s_t}{\partial s_k} = \frac{\partial s_t}{\partial s_{t-1}} \frac{\partial s_{t-1}}{\partial s_{t-2}} \dots \frac{\partial s_{k+1}}{\partial s_k}$$
$$= \prod_{j=k}^{t-1} \frac{\partial s_{j+1}}{\partial s_j}$$

- Let us look at one such term in the product (i.e., $\frac{\partial s_{j+1}}{\partial s_j}$)

$$a_j = [a_{j1}, a_{j2}, a_{j3}, \dots a_{jd},]$$
$$s_j = [\sigma(a_{j1}), \sigma(a_{j2}), \dots \sigma(a_{jd})]$$

$$\frac{\partial s_j}{\partial a_j} = \begin{bmatrix} \frac{\partial s_{j1}}{\partial a_{j1}} & \frac{\partial s_{j2}}{\partial a_{j1}} & \frac{\partial s_{j3}}{\partial a_{j1}} & \cdots \\ \frac{\partial s_{j1}}{\partial a_{j2}} & \frac{\partial s_{j2}}{\partial a_{j2}} & \ddots & \\ \vdots & \vdots & \vdots & \frac{\partial s_{jd}}{\partial a_{jd}} \end{bmatrix}$$
$$= \begin{bmatrix} \sigma^{'}(a_{j1}) & 0 & 0 & 0 \\ 0 & \sigma^{'}(a_{j2}) & 0 & 0 \\ 0 & 0 & \ddots & \\ 0 & 0 & \dots & \sigma^{'}(a_{jd}) \end{bmatrix}$$
$$= diag(\sigma^{'}(a_j))$$

- We are interested in $\frac{\partial s_j}{\partial s_{j-1}}$

$$a_j = W s_j + b$$
$$s_j = \sigma(a_j)$$

$$\frac{\partial s_j}{\partial s_{j-1}} = \frac{\partial s_j}{\partial a_j} \frac{\partial a_j}{\partial s_{j-1}}$$
$$= diag(\sigma^{'}(a_j))W$$

- We are interested in the magnitude of $\frac{\partial s_j}{\partial s_{j-1}} \leftarrow$ if it is small (large) $\frac{\partial s_t}{\partial s_k}$ and hence $\frac{\partial \mathscr{L}_t}{\partial W}$ will vanish (explode)

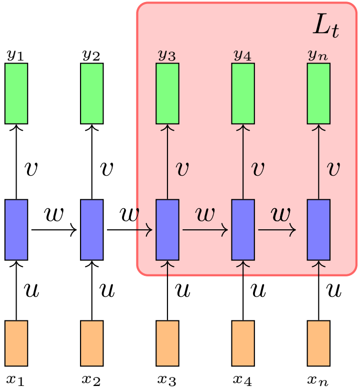
$$\left\| \frac{\partial s_j}{\partial s_{j-1}} \right\| = \left\| diag(\sigma^{'}(a_j))W \right\|$$
$$\leq \left\| diag(\sigma^{'}(a_j) \right\| \|W\|$$

$\because \sigma(a_j)$ is a bounded function (sigmoid, tanh) $\sigma^{'}(a_j)$ is bounded

$$\sigma^{'}(a_j) \leq \frac{1}{4} = \gamma \, [\text{if } \sigma \text{ is logistic }]$$
$$\leq 1 = \gamma \, [\text{if } \sigma \text{ is tanh }]$$
$$\left\| \frac{\partial s_j}{\partial s_{j-1}} \right\| \leq \gamma \|W\|$$
$$\leq \gamma\lambda$$

$$\left\| \frac{\partial s_t}{\partial s_k} \right\| = \left\| \prod_{j=k+1}^{t} \frac{\partial s_j}{\partial s_{j-1}} \right\|$$
$$\leq \prod_{j=k+1}^{t} \gamma\lambda$$
$$\leq (\gamma\lambda)^{t-k}$$

- If $\gamma\lambda < 1$ the gradient will vanish
- If $\gamma\lambda > 1$ the gradient could explode
- This is known as the problem of vanishing/ exploding gradients




- One simple way of avoiding this is to use truncated backpropogation where we restrict the product to $\tau(< t - k)$ terms

# Module 14.5: Some Gory Details

$$\underbrace{\frac{\partial \mathscr{L}_t(\theta)}{\partial W}}_{\in \mathbb{R}^{d\times d}} = \underbrace{\frac{\partial \mathscr{L}_t(\theta)}{\partial s_t}}_{\in \mathbb{R}^{1\times d}} \sum_{k=1}^{t} \underbrace{\frac{\partial s_t}{\partial s_k}}_{\in \mathbb{R}^{d\times d}} \underbrace{\frac{\partial^+ s_k}{\partial W}}_{\in \mathbb{R}^{d\times d\times d}}$$

- We know how to compute $\frac{\partial \mathscr{L}_t(\theta)}{\partial s_t}$ (derivative of $\mathscr{L}_t(\theta)$ (scalar) w.r.t. last hidden layer (vector)) using backpropagation
- We just saw a formula for $\frac{\partial s_t}{\partial s_k}$ which is the derivative of a vector w.r.t. a vector)
- $\frac{\partial^+ s_k}{\partial W}$ is a tensor $\in \mathbb{R}^{d\times d\times d}$, the derivative of a vector $\in \mathbb{R}^d$ w.r.t. a matrix $\in \mathbb{R}^{d\times d}$
- How do we compute $\frac{\partial^+ s_k}{\partial W}$ ? Let us see

- We just look at one element of this $\frac{\partial^+ s_k}{\partial W}$ tensor
- $\frac{\partial^+ s_{kp}}{\partial W_{qr}}$ is the $(p, q, r)$-th element of the 3d tensor

  $a_k = W s_{k-1} + b$

  $s_k = \sigma(a_k)$

$$a_k = W s_{k-1}$$

$$\begin{bmatrix} a_{k1} \\ a_{k2} \\ \vdots \\ a_{kp} \\ \vdots \\ a_{kd} \end{bmatrix} = \begin{bmatrix} W_{11} & W_{12} & \dots & W_{1d} \\ \vdots & \vdots & \vdots & \vdots \\ W_{p1} & W_{p2} & \dots & W_{pd} \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} s_{k-1,1} \\ s_{k-1,2} \\ \vdots \\ s_{k-1,p} \\ \vdots \\ s_{k-1,d} \end{bmatrix}$$

$$a_{kp} = \sum_{i=1}^{d} W_{pi} s_{k-1,i}$$

$$s_{kp} = \sigma(a_{kp})$$

$$\frac{\partial s_{kp}}{\partial W_{qr}} = \frac{\partial s_{kp}}{\partial a_{kp}} \frac{\partial a_{kp}}{\partial W_{qr}}$$

$$= \sigma'(a_{kp}) \frac{\partial a_{kp}}{\partial W_{qr}}$$

$$\frac{\partial a_{kp}}{\partial W_{qr}} = \frac{\partial \sum_{i=1}^{d} W_{pi} s_{k-1,i}}{\partial W_{qr}}$$

$$= s_{k-1,i} \quad \text{if} \quad p = q \quad \text{and} \quad i = r$$

$$= 0 \quad \text{otherwise}$$

$$\frac{\partial s_{kp}}{\partial W_{qr}} = \sigma'(a_{kp}) s_{k-1,r} \quad \text{if} \quad p = q \quad \text{and} \quad i = r$$

$$= 0 \quad \text{otherwise}$$