RNN vanishing/exploding gradient problem

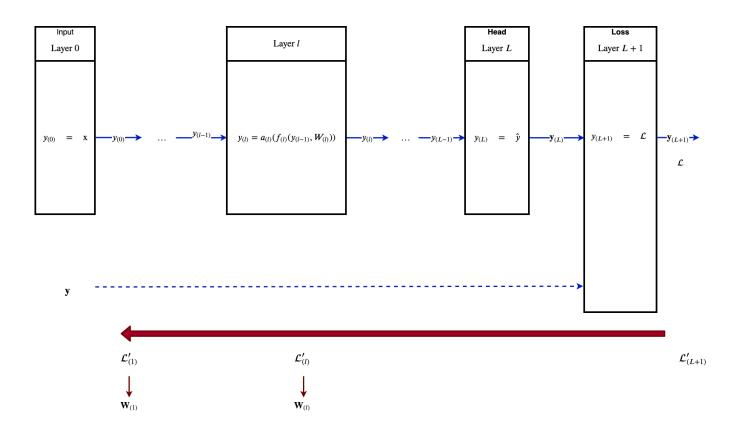
Training Deep Networks is hard: Review

As we learned in the module on Vanishing and Exploding Gradients

- Training a very deep (many layer) network is difficult
- Because as the gradient flows backwards (from Loss layer to Input layer)
- The Loss Gradients successively either diminish or expand

Let's quickly review the issue of vanishing and exploding gradients. Here is the picture of gradient flow during Back propagation:

Backward pass: Loss to Weights



The Loss Gradient of layer l

$$\mathcal{L}_{(l)}' = rac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l)}}$$

flows backwards from Loss Layer (L+1) inductively as:

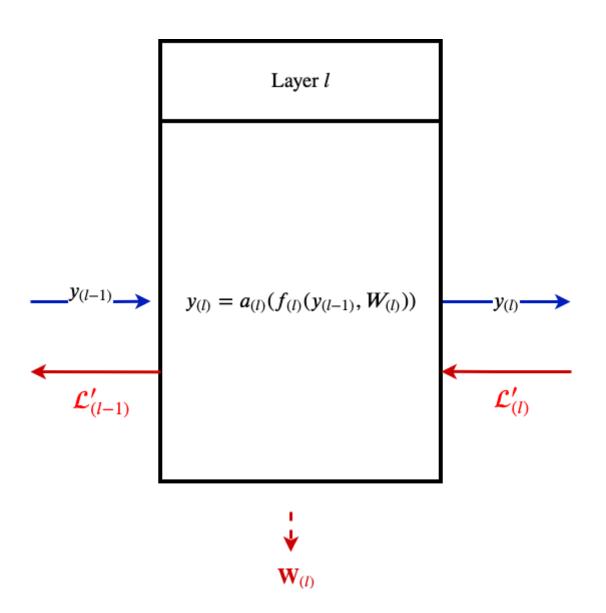
$$egin{array}{lll} \mathcal{L}'_{(l-1)} & = & rac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l-1)}} \ & = & rac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l)}} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \ & = & \mathcal{L}'_{(l)} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \end{array}$$

Moreover, from the Loss Gradient and a local gradient $rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{W}_{(l)}}$ at layer l

- We can compute the derivative of the loss with respect to the layer's weights
- Which is used in the update equation for Gradient Descent
- To modify the estimate of the layer's weights
- In the direction of decreasing Loss

$$rac{\partial \mathcal{L}}{\partial \mathbf{W}_{(l)}} \;\; = \;\; rac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l)}} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{W}_{(l)}} \;\; = \;\; \mathcal{L}'_{(l)} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{W}_{(l)}}$$

Forward and Backward pass: Detail



The issue arises in the second term $\frac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}}$ of the inductive update of the Loss Gradient

$$\mathcal{L}'_{(l-1)} \;\; = \;\; \mathcal{L}'_{(l)} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}}$$

Since

$$\mathbf{y}_{(l)} = a_{(l)}\left(f_{(l)}(\mathbf{y}_{(l-1)},\mathbf{W}_{(l)})
ight)$$

The derivative

$$rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \;\; = a'_{(l)} f'_{(l)}$$

where

$$egin{array}{lll} a_{(l)}' &=& rac{\partial a_{(l)}(f_{(l)}(\mathbf{y}_{(l-1)},\mathbf{W}_{(l)}))}{\partial f_{(l)}(\mathbf{y}_{(l-1)},\mathbf{W}_{(l)})} & ext{derivative of } a_{(l)}(\ldots) ext{ wrt } f_{(l)}(\ldots) \ f_{(l)}' &=& rac{\partial f_{(l)}(\mathbf{y}_{(l-1)},W_{(l)})}{\partial \mathbf{y}_{(l-1)}} & ext{derivative of } f_{(l)}(\ldots) ext{ wrt } \mathbf{y}_{(l-1)} \end{array}$$

Substituting the value of the loss gradient into the backward update rule:

$$egin{array}{lll} \mathcal{L}_{(l-1)}' &=& \mathcal{L}_{(l)}' rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \ &=& \mathcal{L}_{(l)}' a_{(l)}' f_{(l)}' \end{array}$$

We see that the backwards step from Loss Gradient of layer l to Loss Gradient of layer (l-1) introduces $a_{(l)}^\prime$ as a multiplicative term.

But as we continue backwards (expanding $\mathcal{L}'_{(l)}$ on the right hand side) we accumulate this multiplicative term

Starting from layer (L+1) and proceeding backwards to layer \emph{l} , the Loss Gradient term looks like

$$\mathcal{L}'_{(l)} = \mathcal{L}'_{(L+1)} \prod_{l'=l+1}^{L} a'_{(l')} f'_{(l')}$$

Specifically: it is the $a_{(l)}^\prime$ term that is problematic

- ullet If the activation functions $a_{(l)}$ is such that $a_{(l)}^{\prime} < 1$:
 - The backwards pass attenuates the Loss Gradient
 - Eventually making it go to 0 (disappear)
- If the activation function $a_{(l)}$ is such that $a_{(l)}^\prime > 1$:
 - The backwards pass amplifies the Loss Gradient
 - \circ Eventually making it go to ∞ (explode)

Recall that

- ullet For $a_{(l)}=\sigma$ (the sigmoid function)
- $\bullet \ \max_z a'_{(l)}(z) = 0.25$

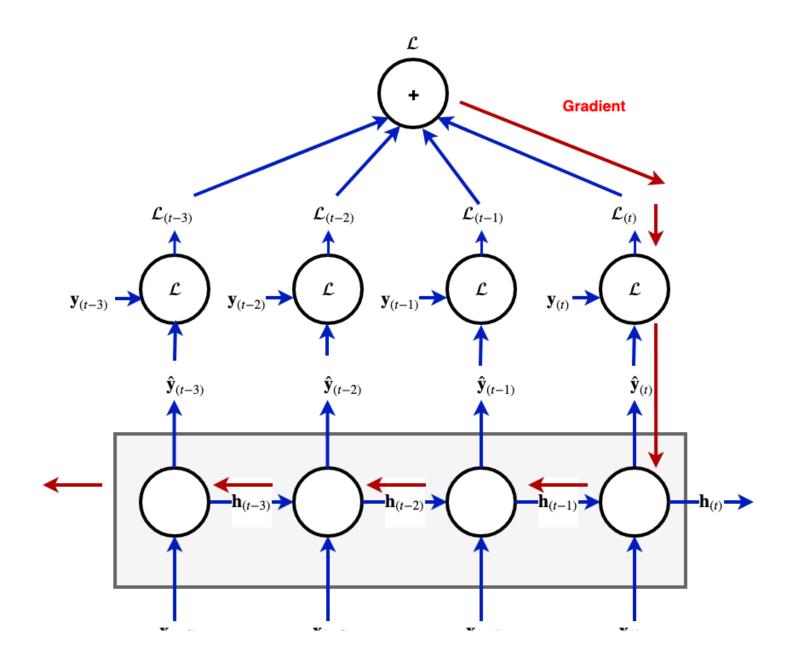
so using the sigmoid as the default activation

- Made training of deep networks very difficult
- Which stifled progress in Deep Learning

An unrolled RNN is a Deep Network

If we unroll an RNN that has an input sequence of length T $\mathbf{x}_{(1)}, \dots, \mathbf{x}_{(T)}$

we wind up with a network of T layers (plus the Loss layer)



As the input sequence length T gets large

- It should be no surprise that training an RNN
- Is exposed to the problem of vanishing and exploding gradients
- \bullet Because of the derivative of the activation function (written as ϕ rather than $a_{(l)}$ in the RNN literature)

But it turns o	out that there is a <i>second</i> sour	rce of vanishing/explo	oding gradients for RNN's:
• The w	veight matrix ${f W}$ is shared at	every step of the unr	olled network
Let's see how	w this can lead to vanishing/e	xploding gradients.	

Vanishing/Exploding gradients

Let's recall the RNN update equations:

$$egin{array}{lll} \mathbf{h}_{(t)} &=& \phi(\mathbf{W}_{xh}\mathbf{x}_{(t)} + \mathbf{W}_{hh}\mathbf{h}_{(t-1)} + \mathbf{b}_h) \ \mathbf{y}_{(t)} &=& \mathbf{W}_{hy}\mathbf{h}_{(t)} + \mathbf{b}_y \end{array}$$

For simplicity of presentation: we will assume activation function ϕ is the identity function in this section.

Returning to the equation that derives the derivative of the Loss with respect to weights \mathbf{W} :

$$rac{\partial \mathcal{L}}{\partial \mathbf{w}_{(l)}} \;\;\; = \;\;\; rac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l)}} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{w}_{(l)}} \;\;\; = \;\;\; \mathcal{L}'_{(l)} rac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{w}_{(l)}}$$

Let's focus on the term

$$rac{\partial \mathbf{y}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}}$$

(replacing l as the index of the layer with t, the time step)

We will focus on the part of ${f W}$ that is ${f W}_{hh}$

$$rac{\partial \mathbf{y}_{(t)}}{\partial \mathbf{W}_{hh}} = rac{\partial \mathbf{y}_{(t)}}{\partial \mathbf{h}_{(t)}} rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{W}_{hh}}$$

This term comes about due to the RNN update equation

$$\mathbf{y}_{(t)} = \mathbf{W}_{hy}\mathbf{h}_{(t)} + \mathbf{b}_y$$

• And $\mathbf{h}_{(t)}$ is a function of \mathbf{W}_{hh}

$$rac{\partial \mathbf{y}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}} = rac{\partial \mathbf{y}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hy}} + rac{\partial \mathbf{y}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{h}_{(t)}} rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{W}_{hh}}$$

Let's expand the term

$$rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{W}_{hh}}$$

Since

$$\mathbf{h}_{(t)} = \mathbf{W}_{xh}\mathbf{x}_{(t)} + \mathbf{W}_{hh}\mathbf{h}_{(t-1)} + \mathbf{b}_h$$

 ${f h}_{(t)}$ depends on ${f h}_{(t-1)}$, which by recursion depends on ${f h}_{(t-2)}$ which \dots depends on ${f h}_{(0)}.$

• and all $\mathbf{h}_{(t)}$ share the same \mathbf{W}_{hh} .

This means that $\mathbf{h}_{(t)}$ depends on \mathbf{W}_{hh} through each $\mathbf{h}_{(t-k)}$ for $k=1,\ldots,t.$

$$rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{W}_{hh}} = \sum_{k=1}^t rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{h}_{(t-k)}} rac{\partial \dot{\mathbf{h}}_{(t-k)}}{\partial \mathbf{W}_{hh}}$$

The problematic term for us is

$$rac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{h}_{(t-k)}}$$

It can be computed by
$$k$$
 applications of the Chain Rule as
$$\frac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{h}_{(t-k)}} \ = \ \frac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{h}_{(t-1)}} \frac{\partial \mathbf{h}_{(t-1)}}{\partial \mathbf{h}_{(t-2)}} \dots \frac{\partial \mathbf{h}_{(t-k+1)}}{\partial \mathbf{h}_{(t-k)}}$$
$$= \ \prod_{u=0}^{k-1} \frac{\partial \mathbf{h}_{(t-u)}}{\partial \mathbf{h}_{(t-u-1)}}$$

Each term

$$rac{\partial \mathbf{h}_{(t-u)}}{\partial \mathbf{h}_{(t-u-1)}}$$

results in a term \mathbf{W}_{hh} because

$$\mathbf{h}_{(t)} = \mathbf{W}_{xh}\mathbf{x}_{(t)} + \mathbf{W}_{hh}\mathbf{h}_{(t-1)} + \mathbf{b}_h$$

So the repeated product is equal to the matrix \mathbf{W}_{hh} raised to the power \pmb{k}

For simplicity, suppose \mathbf{W}_{hh} were a scalar (in general: use eigenvalues of matrices and matrix algebra)

Raising \mathbf{W}_{hh} to the power of k

- ullet Approaches 0 as k increases, when $\mathbf{W}_{hh} < 1$
- ullet Approaches ∞ as k increases, when $\mathbf{W}_{hh}>1$

In other words:

- ullet As the distance k between time steps increases
- The Loss Gradient tends to either vanish or explode
- Inhibiting weight updates and learning

If updates do occur, they will either be

- Erratic (large loss gradients)
- Slow (small loss gradients)

Remember that this cause of vanishing/exploding gradients is particular to recurrent layers

• Because of the sharing of weights between time steps

Controlling exploding gradients by clipping

In theory, we can control the explosion by clipping the gradient $\frac{\partial \mathcal{L}}{\partial W_i}$.

We are still left with the vanishing gradient problem.

This means that "vanilla" RNN's have difficulty learning long-term dependencies (i.e., too many steps backward).

Conclusion

Recurrent layers are especially exposed to the problem of Vanishing and Exploding gradients

- As potentially very deep networks in the unrolled form
- ullet Due to sharing weights ${f W}$ across time steps

We will introduce some architectural innovations in Recurrent layers to ameliorate this problem.

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