RNN vanishing/exploding gradient problem

Training Deep Networks is hard: Review

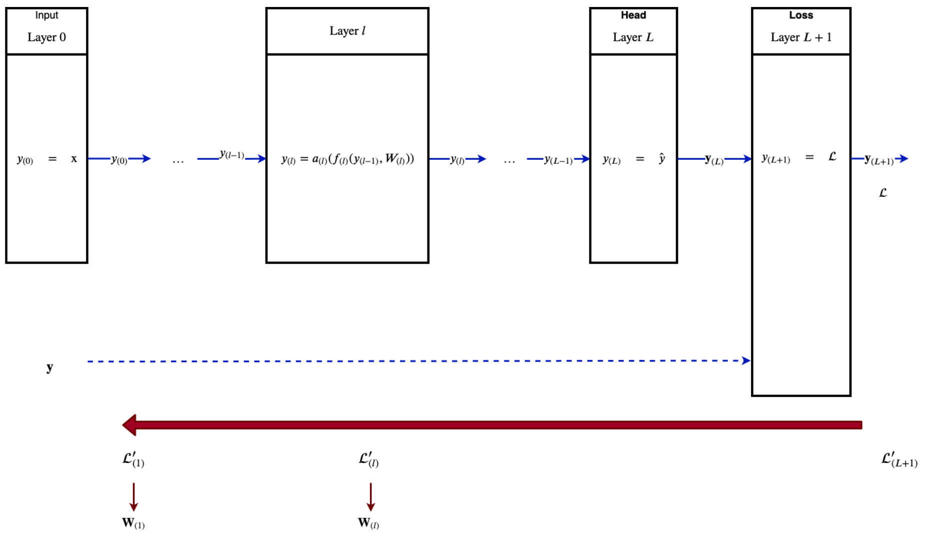
As we learned in the module on Vanishing and Exploding Gradients

- 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

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

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

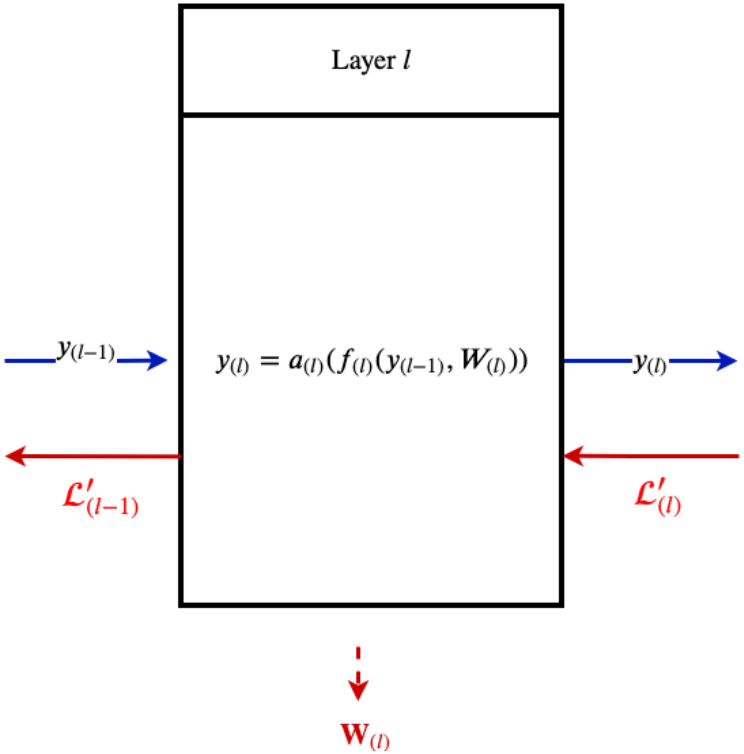
$$\begin{aligned}
\mathcal{L}'_{(l-1)} &= \frac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l-1)}} \\
&= \frac{\partial \mathcal{L}}{\partial \mathbf{y}_{(l)}} \frac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \\
&= \mathcal{L}'_{(l)} \frac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}}
\end{aligned}$$

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

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

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

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

Since

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

The derivative

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

where

$$\begin{aligned}
a'_{(l)} &= \frac{\partial a_{(l)}(f_{(l)}(\mathbf{y}_{(l-1)}, \mathbf{W}_{(l)}))}{\partial f_{(l)}(\mathbf{y}_{(l-1)}, \mathbf{W}_{(l)})} && \text{derivative of } a_{(l)}(\ldots) \text{ wrt } f_{(l)}(\ldots) \\
f'_{(l)} &= \frac{\partial f_{(l)}(\mathbf{y}_{(l-1)}, W_{(l)})}{\partial \mathbf{y}_{(l-1)}} && \text{derivative of } f_{(l)}(\ldots) \text{ wrt } \mathbf{y}_{(l-1)}
\end{aligned}$$

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

$$\begin{aligned}\mathcal{L}'_{(l-1)} &= \mathcal{L}'_{(l)} \frac{\partial \mathbf{y}_{(l)}}{\partial \mathbf{y}_{(l-1)}} \\ &= \mathcal{L}'_{(l)} a'_{(l)} f'_{(l)}\end{aligned}$$

We see that the backwards step from Loss Gradient of layer l to Loss Gradient of layer $(l-1)$ introduces $a'_{(l)}$ 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 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 $a'_{(l)}$ term that is problematic

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

Recall that

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

so using the sigmoid as the default activation

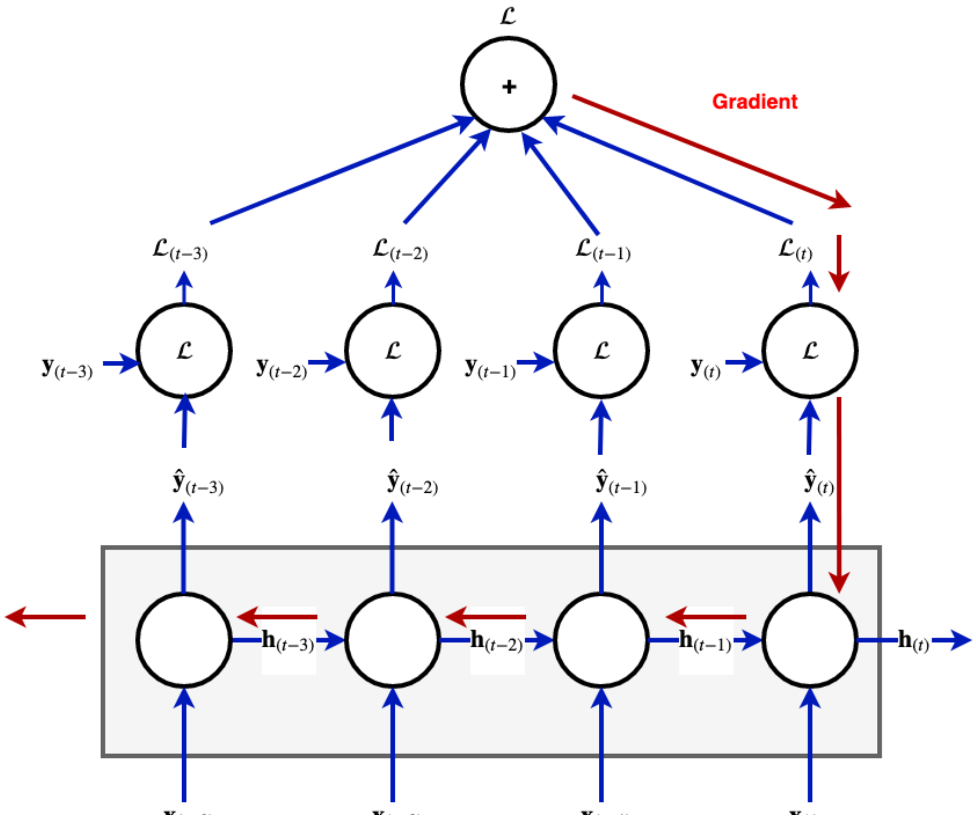
- Made training of deep networks very difficult
- Which stifled progress in Deep Learning

An unrolled RNN is a Deep Network

If we unroll an RNN that has an input sequence of length T

$$\mathbf{x}_{(1)}, \ldots, \mathbf{x}_{(T)}$$

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


$\mathcal{L}$
+
Gradient
$\mathcal{L}_{(t-3)}$
$\mathcal{L}_{(t-2)}$
$\mathcal{L}_{(t-1)}$
$\mathcal{L}_{(t)}$
$\mathbf{y}_{(t-3)}$
$\mathcal{L}$
$\mathbf{y}_{(t-2)}$
$\mathcal{L}$
$\mathbf{y}_{(t-1)}$
$\mathcal{L}$
$\mathbf{y}_{(t)}$
$\mathcal{L}$
$\hat{\mathbf{y}}_{(t-3)}$
$\hat{\mathbf{y}}_{(t-2)}$
$\hat{\mathbf{y}}_{(t-1)}$
$\hat{\mathbf{y}}_{(t)}$
$\mathbf{h}_{(t-3)}$
$\mathbf{h}_{(t-2)}$
$\mathbf{h}_{(t-1)}$
$\mathbf{h}_{(t)}$

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
- Because of the derivative of the activation function (written as ϕ rather than $a_{(l)}$ in the RNN literature)

But it turns out that there is a *second* source of vanishing/exploding gradients for RNN's:

- The weight matrix $\mathbf{W}$ is shared at every step of the unrolled network

Let's see how this can lead to vanishing/exploding gradients.

Vanishing/Exploding gradients

Let's recall the RNN update equations:

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

For simplicity of presentation:

- we will assume activation function ϕ is the identity function in this section.
- we will identify $\mathbf{y}_{(t)}$ with $\mathbf{h}_{(t)}$

$$\mathbf{y}_{(t)} = \mathbf{h}_{(t)}$$

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

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

Let's focus on the term

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

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

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

$$\frac{\partial \mathbf{y}_{(t)}}{\partial \mathbf{W}_{hh}} \quad = \quad \frac{\partial \mathbf{h}_{(t)}}{\partial \mathbf{W}_{hh}} \quad \text{assume } \mathbf{y}_{(t)} = \mathbf{h}_{(t)}$$

There is a *direct* dependence of $h_{(t)}$ on $\mathbf{W}_{hh}$ via the term

$$\mathbf{W}_{hh}\mathbf{h}_{(t-1)}$$

But there is also the *indirect* dependence via

- $\mathbf{h}_{(t)}$'s dependence on $\mathbf{h}_{(t-1)}$
- which also depends on $\mathbf{W}_{hh}$

So

$$\begin{aligned}\frac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}} &= \frac{d\mathbf{h}_{(t)}^{(\mathbf{i})}}{d\mathbf{W}_{hh}} + \frac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}} \frac{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}} \\ &= \frac{d(\mathbf{W}_{hh}\mathbf{h}_{(t-1)}^{(\mathbf{i})})}{d\mathbf{W}_{hh}} + \frac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}} \frac{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}}\end{aligned}$$

The last term in the derivative

$$\frac{\partial \mathbf{h}^{(\mathbf{i})}_{(t-1)}}{\partial \mathbf{W}_{hh}}$$

is equal to the LHS, offset by one time step

- a recursive call

This term is multiplied by

$$\frac{\partial \mathbf{h}^{(\mathbf{i})}_{(t)}}{\partial \mathbf{h}^{(\mathbf{i})}_{(t-1)}} = \mathbf{W}_{hh}$$

Thus, when we unwind the recursive call

- we wind up with the matrix $\mathbf{W}_{hh}$
- raised to a power
  - power of t when our original LHS is $\frac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}}$

This is similar to a problem we saw before

- vanishing gradient
- raised a' (derivative of the activation function) to a power equal to the depth of the layer in the NN

But this time

- the problem is not the derivative of the activation function
- it is raising a matrix to a power

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

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

In other words:

- 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

Aside

How is raising a matrix to a power related to eigenvalues ?

Consider matrix M. It's eigen decomposition is

$$M = \mathbf{W} \Lambda \mathbf{W}^{-1}$$

where Λ is the *diagonal* matrix of eigenvalues.

$$
\begin{array}{rcll}
M^p & = & M M^{p-1} & \\
 & = & (\mathbf{W}\Lambda\mathbf{W}^{-1}) & M^{p-1} \\
 & = & (\mathbf{W}\Lambda\mathbf{W}^{-1}) & M M^{p-2} \\
 & = & (\mathbf{W}\Lambda\mathbf{W}^{-1}) & (\mathbf{W}\Lambda\mathbf{W}^{-1}) M^{p-2} \\
 & & & \\
 & = & (\mathbf{W}\Lambda\mathbf{W}^{-1}\mathbf{W}\Lambda\mathbf{W}^{-1}) M^{p-2} & \text{associativity of multiplication} \\
 & = & (\mathbf{W}\Lambda^2\mathbf{W}^{-1}) M^{p-2} & \text{since } \mathbf{W}\mathbf{W}^{-1} = I, \Lambda\Lambda = \Lambda^2 \\
 & \vdots & & \\
 & = & (\mathbf{W}\Lambda^p\mathbf{W}^{-1}) M^{p-p} & \text{continuing the expansion of } M \text{ into } (\mathbf{W} \\
 & = & (\mathbf{W}\Lambda^p\mathbf{W}^{-1}) &
\end{array}
$$

So you can see that raising M to the power p results in diagonal matrix Λ being raised to p

- \Which is just a diagonal matrix whose elements are the *scalar* diagonal elements of Λ raised to p

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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
- Due to sharing weights $\mathbf{W}$ across time steps

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

In [2]:

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print("Done")
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Done
```