Vanishing Gradients in Vanilla RNNs

Aaron Avram

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Introduction

In this writeup I will describe why Vanilla RNNs suffer from vanishing gradients, then work through the most popular solution: LSTM cells.

Vanishing Gradients

In the basic formulation of a Recurrent Neural Network, we have:

$$
\begin{aligned}
z^{(t)} &= Wh^{(t-1)} + Ux^{(t)} + b \\
h^{(t)} &= \tanh(z^{(t)})
\end{aligned}
$$

Where W and U are matrices and b is a vector. We choose tanh here for convenience but other activation functions may be used, and the next results all follow regardless. For now, only consider W and h discarding U, x and b as this result comes about independently of their influence.

Say we want to find the Jacobian of $h^{(t)}$ with respect to $h(0)$. I claim that the formula is given by $J_t := J(h^{(t)}) = \prod_{k=1}^{t} D_k W$ where $D_k =$diag[$\tanh'(z^{(k)})$], and this is easy to prove by induction:

Proof. **Base Case**: $t = 1$, consider $h^{(1)} = \tanh(Wh^{(0)})$. Clearly, $J(z^1)(h^{(0)}) = W$, and by the chain rule:

$$
\begin{aligned}
(J_t)_{ij} &= \frac{\partial h_i^{(1)}}{\partial z_i^{(1)}} \frac{\partial z_i^{(1)}}{\partial h_{ij}^{(0)}} \\
&= \tanh'(z^{(1)}) W_{ij}
\end{aligned}
$$

So $J_1 = D_1 W$, as required.

Inductive Step. Suppose for some $t \in \mathbb{N}$, $J_t = \prod_{k=1}^{t} D_k W$. Now consider $t + 1$:

$$h^{(t+1)} = \tanh(Wh^{(t)})$$

First let us find $J(h^{(t+1)})(h^{(t)})$:

$$J(h^{(t+1)})(h^{(t)}) = \left[J(h^{(t+1)})(z^{(t+1)}) \right] \left[J(z^{(t+1)})(h^{(t)}) \right]$$

If we let $h^{(t)}$ act as $h^{(0)}$ in the base case, it is clear that:

$$J(h^{(t+1)})(h^{(t)}) = D_{t+1}W$$

And so:

$$J_{t+1} = \prod_{k=1}^{t+1} D_k W$$

As required. $\square$

Now we want to analyze the norm of this Jacobian matrix to understand the behaviour of weight gradients long term. We will let $||.||$ denote the spectral norm. First consider positive W. This means W admits an spectral decomposition, $W = CVC^T$ and $||W|| = ||V|| = \lambda_{max}(V)$. Notice that D_t is a diagonal matrix so its norm is the absolute value of its largest entry. However, since this entry is the product of an elementwise application of the tanh derivative, it is equal to $1 - \tanh^2(x)$ for some $x \in \mathbb{R}$, but since tanh is bounded by $(-1, 1)$, its derivative is bounded by $[0, 1)$. Thus, $0 \leq ||D_t|| < 1$, $\forall t \in \mathbb{N}$. Next consider $D := \{||D_t|| : t \in \mathbb{N}\}$ and define $\delta_i := \inf D$ and $\delta_s := \sup D$. Thus for all t, $0 \leq \delta_i \leq ||D_t|| \leq \delta_s \leq 1$. We can consider $||J_t||$

$$\begin{aligned} ||J_t|| &= ||\prod_{k=1}^{t} D_k W|| \\ &= \prod_{k=1}^{t} (||D_k||)(||W||) \\ &= ||W||^t \prod_{k=1}^{t} (||D_k||) \\ (\delta_i ||W||)^t \leq &||J_t|| \leq (\delta_s ||W||)^t \end{aligned}$$

It is clear that if $(\delta_i||W||)^t$ explodes, so does $||J_t||$ leading to exploding gradients and if $(\delta_s||W||)^t$ vanishes, so does $||J_t||$ leading to vanishing gradients. Now that leaves us a single case. $(\delta_i||W||)^t$ vanishes or goes to 1 and $(\delta_s||W||)^t$ explodes or goes to 1, then: $||W||\delta_i \leq 1$ and $|W||\delta_s \geq 1$. For this we will assume that $\delta_i > 0$ as otherwise this would imply that the hidden states vanish, which is a useless scenario. Then we can bound $||W||$ with $1 \leq \frac{1}{\delta_s} \leq ||W|| \leq \frac{1}{\delta_i}$. In this case, the terms δ_i, δ_s only introduce a bounded multiplicative effect. Thus the size of $||W||$ is ultimately be the major factor that will affect the gradient behaviour. So, we consider a simpler RNN model, with the non-linearities removed. The gradient behaviour here captures the gradient behaviour in the more general case due to the dominating effects of $||W||$. So consider: $h^{(t)} = W^t h^{(0)}$, meaning we now have $J_t = W^t$. And by the spectral decomposition:

$$\begin{aligned} W^t &= (CVC^T)^t \\ &= CV^tC^T \end{aligned}$$

Thus the behaviour of gradient is mostly captured by V^t as C is unitary. But, as t increases, all entries of V that are not equal to 1, either vanish or explode. Thus as t increases the largest eigenvalue of V will dominate gradient behaviour and eigenvalues less than 1 will vanish, which diminishes the expressive power of the network over longer sequences. The only case where V remains stable is if it is also unitary. However, this restricts the space of possible values for W far too much to be used in practice and there is no guarantee that this property will be preserved.

Now in the general case, if W is not positive, we can apply the polar decomposition to see that $W = UR$, and since U is unitary the magnitude of W's gradients will be largerly determined by R, which is the case we have analyzed above. Thus, it is clear that in Vanilla Recurrent Neural Networks, gradient instability easily appears, especially as sequence length increases.