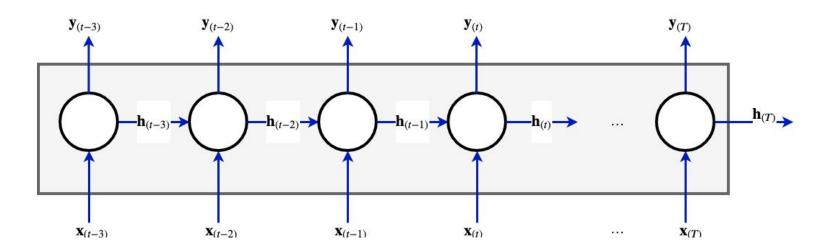
Back propagation through time (BPTT)

A Recurrent Neural Network (RNN)

- Can be viewed as a loop
- That can be unrolled
- Resulting in a multi-layer network
- One layer per time step

Here are the final layers of an unrolled RNN with input sequence

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



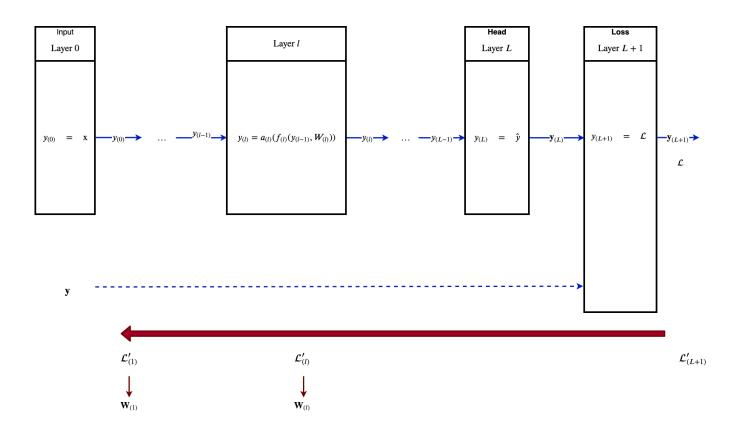
Given enough space: we would continue unrolling on the left to the Input layer

- ullet Resulting in a network with T unrolled layers
- Plus a Loss layer

To compute the derivatives of the Loss with respect to weights

- We could, in theory, use Back Propagation
- Which is the weight update step of Gradient Descent

Backward pass: Loss to Weights



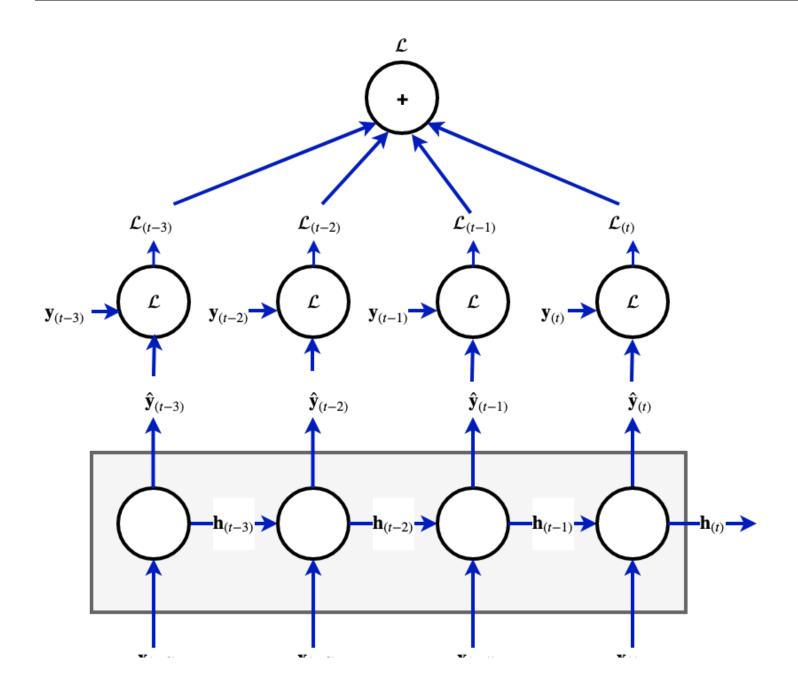
When dealing with unrolled RNN's

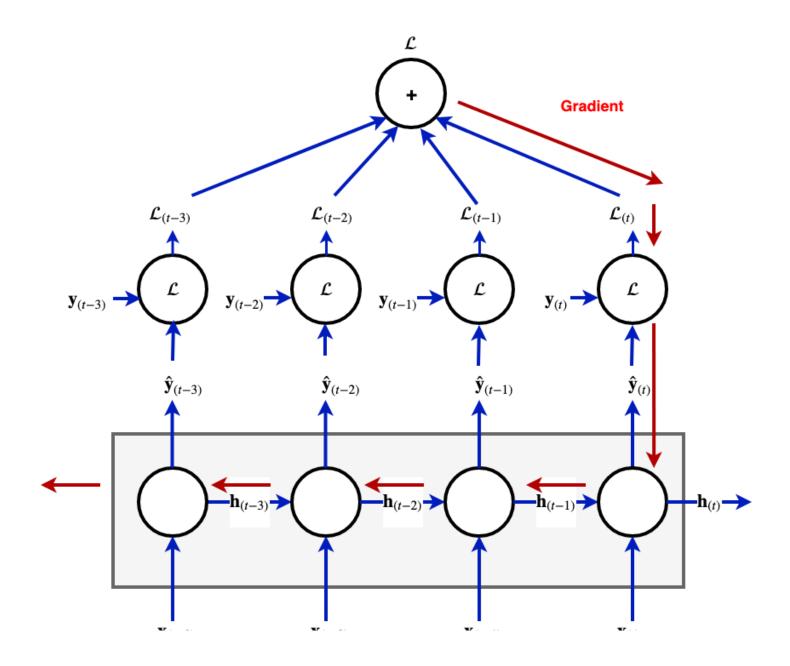
- ullet We will index the "unrolled layers" with time steps, denoted by the label t
- ullet Rather than l, which we use to index layers

This process is called Back Propagation Through Time (BPTT).

The only special thing to note about BPTT is that the Loss function is more complex

- There is a Loss
- Per example (as in non-recurrent layers)
- and Per time-step (unique to recurrent layers)





Truncated back propagation through time (TBPTT)

An unrolled RNN layer turns into a T layer network where T is the number of elements in the input sequence.

For long sequences (large T) this may not be practical.

First, there is the computation time

- ullet t steps to compute $\mathcal{L}_{(t)}^{(\mathbf{i})}$, the loss due to the t^{th} output $\mathbf{y}_{(t)}^{(\mathbf{i})}$ of example i
- $\bullet \ \ {\rm For \, each} \, 1 \leq t \leq T \\$

Less obvious is the *space* requirement

- As we saw in the module "How a Neural Network Toolkit works"
- \bullet We may store information in each layer of the Forward pass (so storage for T layers)
- To facilitate computation of analytical derivatives on the Backward pass
 - For example: the Multiply layer stored the multiplicands in the forward pass
 - Because they are needed for the derivatives

Moreover, as we shall shortly see
 Derivatives may vanish or explode as we proceed further backwards from the Loss layer to the Input layer

So, in theory, the weights $\mathbf{W}_{(t)}$ for small t (close to the input) may not get updated.

- This is certainly a problem in a non-recurrent network
- But is **fatal** in a recurrent layer
- ullet Since there is a **single** weight matrix f W that is shared across *all time steps*

$$\mathbf{W}_{(t)} = \mathbf{W} \text{ for all } 1 \leq t \leq T$$

The solution to these difficulties

- Is to truncate the unrolled RNN
- To a fixed number of time steps
- From the loss layer backwards
- The truncated graph is a suffix of the fully unrolled graph

This process is known as Truncated Back Propagation Through Time (TBPTT).

Note that truncation only occurs in the backward pass.

There is no truncation of the forward pass of the RNN!

Because the unrolled graph is less than T steps

- Gradient computation takes fewer steps
- So weight updates can occur more often

The obvious downside to truncation is that

• Gradients are only approximate

But there is a subtle and more impactful difference

• The RNN layer cannot capture long-term dependencies

Suppose we unrolled the layer for only au time steps (the "window" size)

- The loss for the t^{th} time step ($\mathcal{L}_{(t)}^{(\mathbf{i})}$)
- Flows backwards only to steps

$$(t- au+1),\ldots,t$$

So the "error signal" from time t does not affect time steps t' < (t - au + 1)

Consider a long sentence or document (sequence of words)

- If the gender of the subject is defined by the early words in the sentence
- An incorrect "prediction" late in the sentence
- May not be able to be corrected

"Z was the first woman who ... he said ..."

In other words

- Truncation may affect the ability of an RNN to encode *long-term* dependencies
- Vanishing gradients may cause a similar impact

TBPTT variants

There are several common ways to decide on how many unrolled time steps to keep.

Let t'' denote the index of the *smallest* time step in the unrolled layer for step t.

•
$$t'' = (t - \tau + 1)$$

Plain, untruncated BPTT defines

- t'' = 0
- Unroll all the way to the Input Layer

k-truncated BPTT defines window size au=k

• $t'' = \max(0, t - k)$

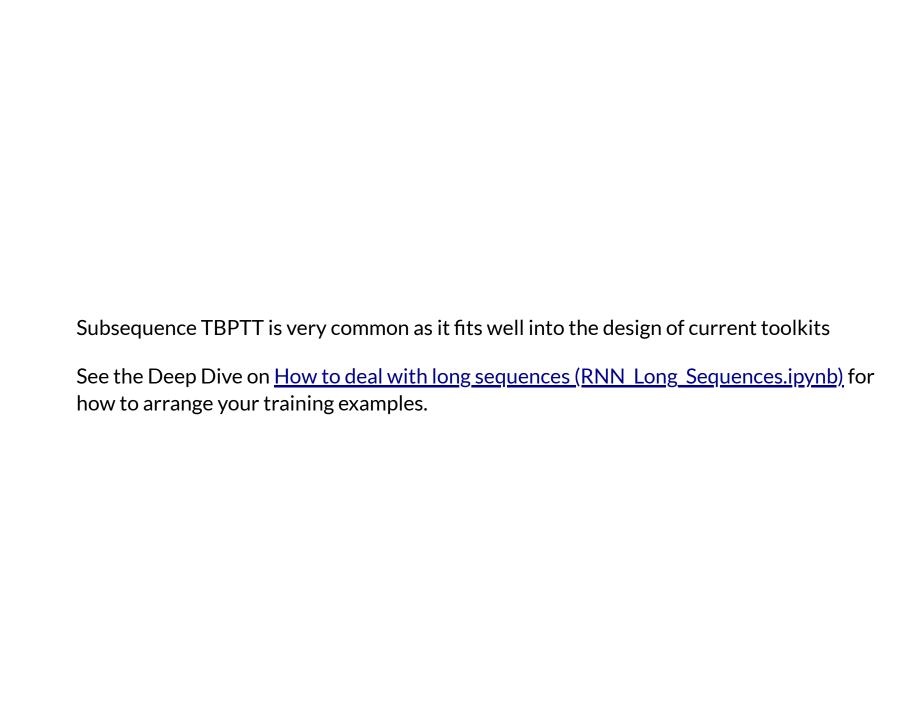
Subsequence truncated BPTT defines

•
$$t'' = k * \lfloor t/k \rfloor$$

That is, it breaks the sequence into "chunks" of size k

$$egin{array}{lll} \mathbf{x}_{(1)}^{(\mathbf{i})}, \dots, \mathbf{x}_{(k)}^{(\mathbf{i})} \ \mathbf{x}_{(k+1)}^{(\mathbf{i})}, \dots, \mathbf{x}_{(2*k)}^{(\mathbf{i})} \ dots \ \mathbf{x}_{((i'*k)+1)}^{(\mathbf{i})}, \dots, \mathbf{x}_{((i'+1)*k)}^{(\mathbf{i})} \ dots \ \end{array}$$

- Gradients flow within chunks
- But not between chunks



Calculating gradients in an RNN

There is an important subtlety we have ignored regarding Back Propagation in an unrolled RNN

• There is a **single** weight matrix W that is shared across all time steps

$$\mathbf{W}_{(t)} = \mathbf{W} \text{ for all } 1 \leq t \leq T$$

This

- Makes the derivative computation slightly more complex
- Creates an *additional* exposure to the problem of vanishing/exploding gradients

A simple picture will illustrate.

Consider the loss at time step t of example i

$$oldsymbol{ullet} oldsymbol{\mathcal{L}_{(t)}^{(i)}} = L(\hat{\mathbf{y}}_{(t)}^{(i)}, \mathbf{y}_{(t)}^{(i)}; \mathbf{W})$$

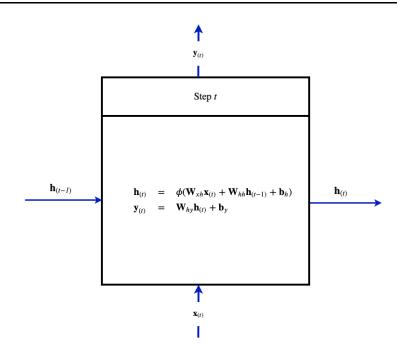
- The loss is a function of
 - ullet $\hat{f y}_{(t)}^{({f i})}$: The t^{th} element of the output sequence $\hat{f y}^{({f i})}={f y}_{(T)}$ for example i
 - The $\mathbf{y}_{(t)}^{(\mathbf{i})}$: The t^{th} element of the **target** sequence $\mathbf{y}^{(\mathbf{i})}$ for example i

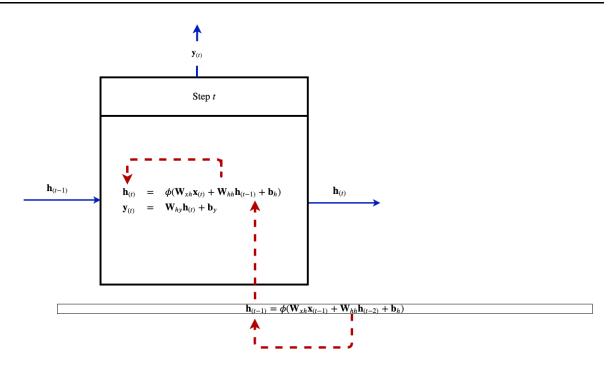
The derivative

$$rac{\partial \mathcal{L}_{(t)}}{\partial \mathbf{W}}$$

- ullet Which is used in Gradient Descent to update the estimate for weights ${f W}$
- ullet Is the sensitivity of $\mathcal{L}_{(t)}$ to a change in old W

RNN Time step





The red lines show **two** different ways that ${f W}$ affects ${f h}_{(t)}$

- ullet And thus $\hat{\mathbf{y}}_{(t)} = \mathbf{W}_{hy}\mathbf{h}_{(t)} + \mathbf{b}_y$
- ullet By its indirect effect on ${f h}_{(t)}$ through ${f h}_{(t-1)}$ (lower line)
- ullet By its direct effect on ${f h}_{(t)}$ (upper line)
- ullet Both using the part of ${f W}$ denoted by ${f W}_{hh}$

So

$$egin{array}{lll} rac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}} &=& rac{d \mathbf{h}_{(t)}^{(\mathbf{i})}}{d \mathbf{W}_{hh}} + rac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}} rac{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}} \ &=& rac{d (\mathbf{W}_{hh} \mathbf{h}_{(t-1)}^{(\mathbf{i})})}{d \mathbf{W}_{hh}} + rac{\partial \mathbf{h}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}} rac{\partial \mathbf{h}_{(t-1)}^{(\mathbf{i})}}{\partial \mathbf{W}_{hh}} \end{array}$$

(Each addend reflect a different path through which \mathbf{W}_{hh} affects $\mathbf{h}_{(t)}$)

So

$$rac{\partial \mathcal{L}_{(t)}^{(\mathbf{i})}}{\partial \mathbf{W}} = \mathcal{L}_{(t)}^{\prime} rac{\partial \mathbf{y}_{(t)}^{(\mathbf{i})}}{\partial W}$$

and

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

depends on all time steps from 1 to t.

Thus, the derivative update for \mathbf{W} cannot be computed without the gradient (for each time step t) flowing all the way back to time step 0.

Conclusion

Updating the weights of a Recurrent layer appears, at first glance, to be straight forward

- Unroll the loop
- Use ordinary Back Propagation

We have discovered some complexity

- Full unrolling is expensive
- Gradient computation is complicated by shared weights

Fortunately, we have solutions to these complexities.

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In [3]: print("Done")
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Done