Recurrent Neural Networks CS60010: Deep Learning

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- § Get introduced to different recurrent neural architecture *e.g.*, RNNs, LSTMs, GRUs etc.
- § Get introduced to tasks involving sequential inputs and/or sequential outputs.



- § Deep Learning by I. Goodfellow and Y. Bengio and A. Courville. [Link] [Chapter 10]
- § CS231n by Stanford University [Link]
- § Understanding LSTM Networks by Chris Olah [Link]

Why do we Need another NN Model?

- § So far, we focused mainly on prediction problems with fixedsize inputs and outputs.
- § In image classification, input is fixed size image and and output is its class, in video classification, the input is fixed size video and output is its class, in bounding-box regression the input is fixed size region proposal (resized/Rol pooled) and output is bounding box coordinates.



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Why do we Need another NN Model?

§ Suppose, we want our model to write down the caption of this image.



Figure: Several people with umbrellas walk down a side walk on a rainy day.

Image source: COCO Dataset, ICCV 2015

Image: A match a ma

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Why do we Need another NN Model?

§ Will this work?



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Why do we Need another NN Model?

§ Will this work?



§ When the model generates 'people', we need a way to tell the model that 'several' has already been generated and similarly for the other words.

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Why do we Need another NN Model?



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Recurrent Neural Networks: Process Sequences



Image source: CS231n from Stanford -

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- § The fundamental feature of a Recurrent Neural Network (RNN) is that the network contains at least one feedback connection so that activation can flow in a loop.
- § The feedback connection allows information to persist. Remember the generation of people would require the generation of several to be remembered.
- § The simplest form of RNN has the previous set of hidden unit activations feeding back into the network along with the inputs.



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- § Note that the concept of 'time' or sequential processing comes into picture.
- § The activations are updated one time-step at a time.
- § The task of the delay unit is to simply delay the hidden layer activation until the next time-step.

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 \S f, in particular, can be a layer of a neural network.

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- $\S f$, in particular, can be a layer of a neural network.
- § Lets unroll the recurrent connection.



§ Note that all weight matrices are same across timesteps. So, the weights are shared for all the timesteps.

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Recurrent Neural Network: Forward Pass



$$\mathbf{a}^{t} = \mathbf{W}_{h} \mathbf{h}^{t-1} + \mathbf{W}_{i} \mathbf{x}^{t}$$
(1)
$$\mathbf{h}^{t} = \mathbf{g}(\mathbf{a}^{t})$$
(2)
$$\mathbf{x}^{t} - \mathbf{W}_{i} \mathbf{h}^{t}$$
(2)

$$\mathbf{y}^t = \mathbf{W}_o \mathbf{h}^t \tag{3}$$

 \S Note that we can have biases too. For simplicity these are omitted.



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Recurrent Neural Network: BPTT



$$\begin{aligned} \mathbf{a}^t &= \mathbf{W}_h \mathbf{h}^{t-1} + \mathbf{W}_i \mathbf{x}^t \\ \mathbf{h}^t &= \mathbf{g}(\mathbf{a}^t) \\ \mathbf{y}^t &= \mathbf{W}_o \mathbf{h}^t \end{aligned}$$

§ BPTT: Backpropagation through time



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Recurrent Neural Network: BPTT



$$\mathbf{a}^t = \mathbf{W}_h \mathbf{h}^{t-1} + \mathbf{W}_i \mathbf{x}^t$$

 $\mathbf{h}^t = \mathbf{g}(\mathbf{a}^t)$
 $\mathbf{y}^t = \mathbf{W}_o \mathbf{h}^t$

§ BPTT: Backpropagation through time § Total loss $L = \sum_{t=1}^{T} L^t$ and we are after $\frac{\partial L}{\partial \mathbf{W}_o}, \frac{\partial L}{\partial \mathbf{W}_h}$ and $\frac{\partial L}{\partial \mathbf{W}_i}$



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Recurrent Neural Network: BPTT



$$\mathbf{a}^t = \mathbf{W}_h \mathbf{h}^{t-1} + \mathbf{W}_i \mathbf{x}^t$$

 $\mathbf{h}^t = \mathbf{g}(\mathbf{a}^t)$
 $\mathbf{y}^t = \mathbf{W}_o \mathbf{h}^t$

§ BPTT: Backpropagation through time § Total loss $L = \sum_{t=1}^{T} L^{t}$ and we are after $\frac{\partial L}{\partial \mathbf{W}_{o}}, \frac{\partial L}{\partial \mathbf{W}_{h}}$ and $\frac{\partial L}{\partial \mathbf{W}_{i}}$ § Lets compute $\frac{\partial L}{\partial \mathbf{y}^{t}}$.

$$\frac{\partial L}{\partial \mathbf{y}^t} = \frac{\partial L}{\partial L^t} \frac{\partial L^t}{\partial \mathbf{y}^t} = 1 \cdot \left[\frac{\partial L^t}{\partial \mathbf{y}^t} \right]$$
(4)

§ $\frac{\partial L^t}{\partial \mathbf{y}^t}$ is computable depending on the particular form of the loss function.



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Recurrent Neural Network: BPTT



§ Lets compute $\frac{\partial L}{\partial \mathbf{h}^t}$. The subtlety here is that all L^t after timestep t are functions of \mathbf{h}^t . So, let us first consider $\frac{\partial L}{\partial \mathbf{h}^T}$, where T is the last timestep.



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Recurrent Neural Network: BPTT



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$$\frac{\partial L}{\partial \mathbf{h}^T} = \frac{\partial L}{\partial \mathbf{y}^T} \frac{\partial \mathbf{y}^T}{\partial \mathbf{h}^T} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{y}^T} \end{bmatrix} \mathbf{W}_o \tag{5}$$



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Recurrent Neural Network: BPTT



§ Lets compute $\frac{\partial L}{\partial \mathbf{h}^t}$. The subtlety here is that all L^t after timestep t are functions of \mathbf{h}^t . So, let us first consider $\frac{\partial L}{\partial \mathbf{h}^T}$, where T is the last timestep.

$$\frac{\partial L}{\partial \mathbf{h}^T} = \frac{\partial L}{\partial \mathbf{y}^T} \frac{\partial \mathbf{y}^T}{\partial \mathbf{h}^T} = \begin{bmatrix} \frac{\partial L}{\partial \mathbf{y}^T} \end{bmatrix} \mathbf{W}_o$$
(5)

- $\frac{\partial L}{\partial \mathbf{v}^T}$, we just computed last slide (eqn. (4)).
- § For a generic t, we need to compute $\frac{\partial L}{\partial \mathbf{h}^t}$. \mathbf{h}^t affects \mathbf{y}^t and also \mathbf{h}^{t+1} . For this we will use something that we used while studying Backpropagation for feedforward networks.

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Recurrent Neural Network: BPTT



$$\frac{\partial L}{\partial \mathbf{h}^t} = \frac{\partial L}{\partial \mathbf{y}^t} \frac{\partial \mathbf{y}^t}{\partial \mathbf{h}^t} + \frac{\partial L}{\partial \mathbf{h}^{t+1}} \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^t}$$
(6)

Recurrent Neural Network

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Recurrent Neural Network: BPTT



§ If u = f(x, y), where $x = \phi(t), y = \psi(t)$, then $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$

$$\frac{\partial L}{\partial \mathbf{h}^{t}} = \frac{\partial L}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} + \frac{\partial L}{\partial \mathbf{h}^{t+1}} \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}}$$
(6)

 $\frac{\delta}{\partial \mathbf{y}^t}$ we computed in eqn. (4)

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Recurrent Neural Network: BPTT



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$$\frac{\partial L}{\partial \mathbf{h}^{t}} = \frac{\partial L}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} + \frac{\partial L}{\partial \mathbf{h}^{t+1}} \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}}$$
(6)

$$\S \ \frac{\partial \mathbf{y}^t}{\partial \mathbf{h}^t} = \mathbf{W}_o.$$

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Recurrent Neural Network: BPTT



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$$\frac{\partial L}{\partial \mathbf{h}^{t}} = \frac{\partial L}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} + \frac{\partial L}{\partial \mathbf{h}^{t+1}} \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}}$$
(6)

 $\frac{\partial L}{\partial \mathbf{h}^{t+1}}$ is almost same as $\frac{\partial L}{\partial \mathbf{h}^t}$. It is just for the next timestep.



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Recurrent Neural Network: BPTT



§ If u = f(x, y), where $x = \phi(t), y = \psi(t)$, then $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$

$$\frac{\partial L}{\partial \mathbf{h}^{t}} = \frac{\partial L}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} + \frac{\partial L}{\partial \mathbf{h}^{t+1}} \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}}$$
(6)

§
$$\frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}} = \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{a}^{t+1}} \frac{\partial \mathbf{a}^{t+1}}{\partial \mathbf{h}^{t}} = \mathbf{g}' \cdot \mathbf{W}_{h}.$$

§ Since, **g** is an elementwise operation, **g**' will be a diagonal matrix.
§ In particular, if *g* is $tanh$, then
 $\frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^{t}} = diag(1 - (h_{1}^{t})^{2}, 1 - (h_{2}^{t})^{2}, \cdots, 1 - (h_{m}^{t})^{2})$



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Recurrent Neural Network: BPTT



$$\{ \frac{\partial L}{\partial \mathbf{h}^t} = \frac{\partial L}{\partial \mathbf{y}^t} \mathbf{W}_o + \frac{\partial L}{\partial \mathbf{h}^{t+1}} diag \left(1 - (h_1^t)^2, 1 - (h_2^t)^2, \cdots, 1 - (h_m^t)^2 \right) \mathbf{W}_h$$

- § All the other things we can compute, but to compute $\frac{\partial L}{\partial \mathbf{h}^t}$ we need $\frac{\partial L}{\partial \mathbf{h}^{t+1}}$.
- § From eqn. (5), we get $\frac{\partial L}{\partial \mathbf{h}^T}$, which gives $\frac{\partial L}{\partial \mathbf{h}^{T-1}}$ and so on.



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§ Now,
$$\frac{\partial L}{\partial \mathbf{W}_o} = \sum_t \frac{\partial L^t}{\partial \mathbf{W}_o} = \sum_t \frac{\partial L^t}{\partial \mathbf{y}^t} \frac{\partial \mathbf{y}^t}{\partial \mathbf{W}_o} = \sum_t \left[\frac{\partial L^t}{\partial \mathbf{y}^t} \mathbf{h}^t \right]$$

 $\frac{\partial L^t}{\partial \mathbf{y}^t}$ is computable depending on the form of the loss function.



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Recurrent Neural Network: BPTT



$$\{ \frac{\partial L}{\partial \mathbf{h}^t} = \frac{\partial L}{\partial \mathbf{y}^t} \mathbf{W}_o + \frac{\partial L}{\partial \mathbf{h}^{t+1}} diag \left(1 - (h_1^t)^2, 1 - (h_2^t)^2, \cdots, 1 - (h_m^t)^2 \right) \mathbf{W}_h$$

- § All the other things we can compute, but to compute $\frac{\partial L}{\partial \mathbf{h}^t}$ we need $\frac{\partial L}{\partial \mathbf{h}^{t+1}}$.
- § From eqn. (5), we get $\frac{\partial L}{\partial \mathbf{h}^T}$, which gives $\frac{\partial L}{\partial \mathbf{h}^{T-1}}$ and so on.

§ Now,
$$\frac{\partial L}{\partial \mathbf{W}_o} = \sum_t \frac{\partial L^t}{\partial \mathbf{W}_o} = \sum_t \frac{\partial L^t}{\partial \mathbf{y}^t} \frac{\partial \mathbf{y}^t}{\partial \mathbf{W}_o} = \sum_t \left\lfloor \frac{\partial L^t}{\partial \mathbf{y}^t} \right\rfloor \mathbf{h}^t$$

§ $\frac{\partial L^{t}}{\partial \mathbf{y}^{t}}$ is computable depending on the form of the loss function. § (Do it yourself) Similarly for $\frac{\partial L}{\partial \mathbf{W}_{h}}$ and $\frac{\partial L}{\partial \mathbf{W}_{i}}$.

Exploding or Vanishing Gradients

- \S In recurrent nets (also in very deep nets), the final output is the composition of a large number of non-linear transformations.
- § The derivatives through these compositions will tend to be either very small or very large.

$$\S$$
 If $h=(f\circ g)(x)=f(g(x)),$ then $h'(x)=f'(g(x))g'(x)$

- \S If the gradients are small, the product is small.
- § If the gradients are large, the product is large.



 \S Let us see what happens with one learnable weight matrix $oldsymbol{ heta}=\mathbf{W}_h$



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Exploding or Vanishing Gradients



 \S Let us see what happens with one learnable weight matrix $oldsymbol{ heta}=\mathbf{W}_h$

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = \sum_{t=1}^{T} \frac{\partial L^t}{\partial \boldsymbol{\theta}}$$

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Exploding or Vanishing Gradients



 \S Let us see what happens with one learnable weight matrix $oldsymbol{ heta}=\mathbf{W}_h$

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = \sum_{t=1}^{T} \frac{\partial L^{t}}{\partial \boldsymbol{\theta}}$$
$$\frac{\partial L^{t}}{\partial \boldsymbol{\theta}} = \frac{\partial L^{t}}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \boldsymbol{\theta}}$$



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Exploding or Vanishing Gradients



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$$\frac{\partial \mathbf{y}^{t}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} \frac{\partial \mathbf{h}^{t}}{\partial \boldsymbol{\theta}}$$



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Exploding or Vanishing Gradients



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$$\frac{\partial L}{\partial \boldsymbol{\theta}} = \sum_{t=1}^{T} \frac{\partial L^{t}}{\partial \boldsymbol{\theta}}$$
$$\frac{\partial L^{t}}{\partial \boldsymbol{\theta}} = \frac{\partial L^{t}}{\partial \mathbf{y}^{t}} \frac{\partial \mathbf{y}^{t}}{\partial \boldsymbol{\theta}}$$
$$\frac{\partial \mathbf{y}^{t}}{\partial \boldsymbol{\theta}} = \frac{\partial \mathbf{y}^{t}}{\partial \mathbf{h}^{t}} \frac{\partial \mathbf{h}^{t}}{\partial \boldsymbol{\theta}}$$

§ But, \mathbf{h}^t is a function of \mathbf{h}^{t-1} , \mathbf{h}^{t-2} , \cdots , \mathbf{h}^2 , \mathbf{h}^1 and each of these is a function of $\boldsymbol{\theta}$.



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Exploding or Vanishing Gradients



§ Now we will resort to our friend again - If u = f(x, y), where $x = \phi(t), y = \psi(t)$, then $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$



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Exploding or Vanishing Gradients



§ Now we will resort to our friend again - If u = f(x, y), where $x = \phi(t), y = \psi(t)$, then $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$ $\frac{\partial \mathbf{h}^t}{\partial \theta} = \sum_{i=1}^{t-1} \frac{\partial \mathbf{h}^t}{\partial \mathbf{h}^k} \frac{\partial \mathbf{h}^k}{\partial \theta}$



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Exploding or Vanishing Gradients



§ Now we will resort to our friend again - If u = f(x, y), where $x = \phi(t), y = \psi(t)$, then $\frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial t}$ $\frac{\partial \mathbf{h}^t}{\partial \theta} = \sum_{k=1}^{t-1} \frac{\partial \mathbf{h}^t}{\partial \mathbf{h}^k} \frac{\partial \mathbf{h}^k}{\partial \theta}$

$$\begin{cases} \text{And} \\ \frac{\partial \mathbf{h}^{t}}{\partial \mathbf{h}^{k}} = \frac{\partial \mathbf{h}^{t}}{\partial \mathbf{h}^{t-1}} \frac{\partial \mathbf{h}^{t-1}}{\partial \mathbf{h}^{t-2}} \cdots \frac{\partial \mathbf{h}^{k+1}}{\partial \mathbf{h}^{k}} \\ = diag[\{1 - (h_{1}^{t-1})^{2}\}\{1 - (h_{1}^{t-2})^{2}\} \cdots, \{1 - (h_{2}^{t-1})^{2}\}\{1 - (h_{2}^{t-2})^{2}\} \cdots,] \end{cases}$$

Exploding or Vanishing Gradients

§ Exploding Gradients

- Easy to detect
- Clip the gradient at a threshold
- § Vanishing Gradients
 - More difficult to detect
 - Architectures designed to combat the problem of vanishing gradients.
 Example: LSTMs by Schmidhuberet *et. al.*



Long Short Term Memory (LSTM)

- § Hochreiter & Schmidhuber(1997) solved the problem of getting an RNN to remember things for a long time (*e.g.*, hundreds of time steps).
- § They designed a memory cell using logistic and linear units with multiplicative interactions.
- § Information is handled using three gates, namely forget, input and output.



Recall: Vanilla RNNs

§ In a standard RNN the repeating module has a simple structure.



Source: Chris Olah's blog

Image: A math a math

Introduction
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LSTMs

- § LSTMs also have this chain like structure, but the repeating module has a different structure.
- § Instead of having a single neural network layer, there are four, interacting in a very special way.





LSTM Memory/Cell State

- § The key to LSTMs is the cell state, the horizontal line running through the top of the diagram.
- § The cell state is kind of like a conveyor belt. Its very easy for information to just flow along it unchanged.



§ The LSTM does have the ability to remove or add information to the cell state, carefully regulated by gates. Source: Chris Olah's blog





- § Composed of a sigmoid neural net layer and a pointwise multiplication operation.
- § Sigmoid: outputs numbers between
 - Zero: "let nothing through" and
 - One: "let everything through"



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Image: Image:





§ And LSTM has three such gates.



Source: Chris Olah's blog

Image: A math a math

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Forget Gate

- § The first step is to decide what information is going to be throw away from the cell state. This decision is made by the "forget gate layer".
- § It looks at h_{t-1} and x_t , and outputs a number between 0 and 1 for each number in the cell state C_{t-1} . A 1 represents "completely keep this" while a 0 represents "completely get rid of this".



 $f_t = \sigma \left(W_f \cdot [h_{t-1}, x_t] + b_f \right)$

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 Source: Chris Olah's blog

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Input Gate

- § The next step is to decide what new information is going to be stored in the cell state. This has two parts.
- § First, a sigmoid layer called the "input gate layer" decides which values to update. Next, a tanh layer creates a vector of new candidate values, \tilde{C}_t , that could be added to the state.



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Input Gate

- $\$ Its now time to update the old cell state, C_{t-1} , into the new cell state $C_t.$
- § This is done by multiplying the old state by f_t , forgetting the things that were decided to forget earlier and adding $i_t * \tilde{C}_t$.



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Output Gate

- § Finally, we need to decide what is going to be the output. This output will be based on the cell state.
- § First a sigmoid layer is run which decides what parts of the cell state are going to be output.
- § Then, the cell state is put through tanh (to push the values to be between 1 and 1) and this is multiplied by the output of the sigmoid gate.



$$o_t = \sigma \left(W_o \left[h_{t-1}, x_t \right] + b_o \right)$$
$$h_t = o_t * \tanh \left(C_t \right)$$

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