Recurrent Neural Networks: Stability analysis and LSTMs

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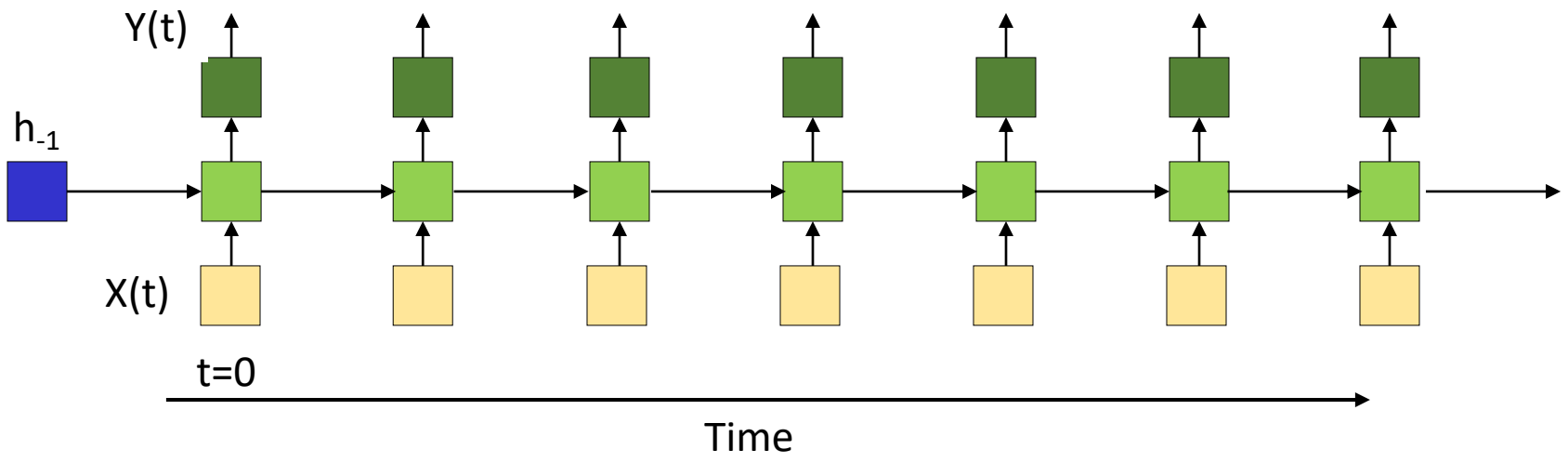
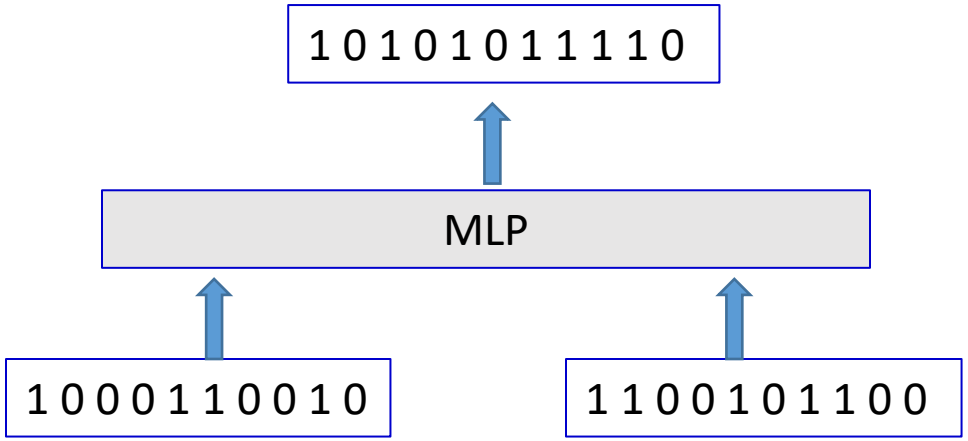
Most slides have been adopted from Bhiksha Raj, 11-785, CMU
and some from Fei Fei Li and colleagues lectures, cs231n, Stanford

Story so far



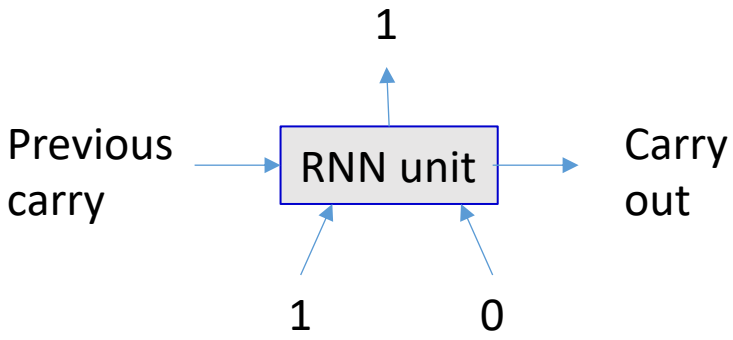
- ***Recurrent structures*** are good for analyzing time series data with ***long-term*** dependence on the past
  - These are ***recurrent*** neural networks

Recurrent structures can do what static structures cannot



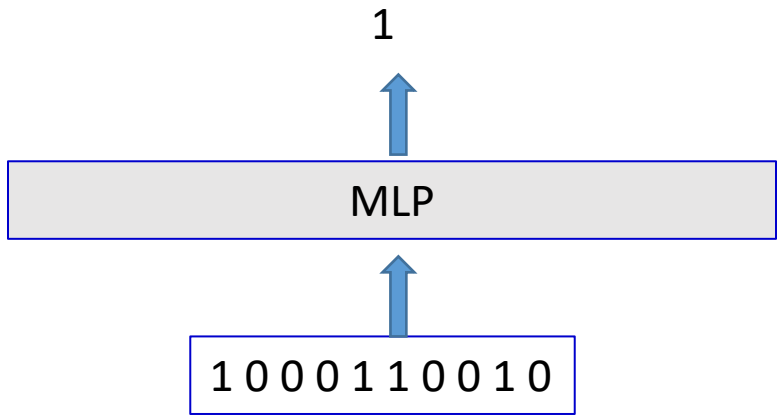
- The addition problem: Add two N-bit numbers to produce a N+1-bit number
  - Input is binary
  - Will require large number of training instances
    - Output must be specified for every pair of inputs
    - Weights that generalize will make errors
  - Network trained for N-bit numbers will not work for N+1 bit numbers

MLPs vs RNNs



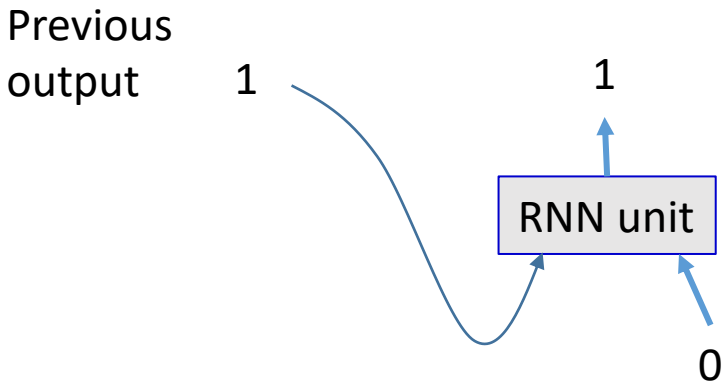
- The addition problem: Add two N-bit numbers to produce a N+1-bit number
- **RNN solution:** Very simple, can add two numbers of any size

MLP: The parity problem



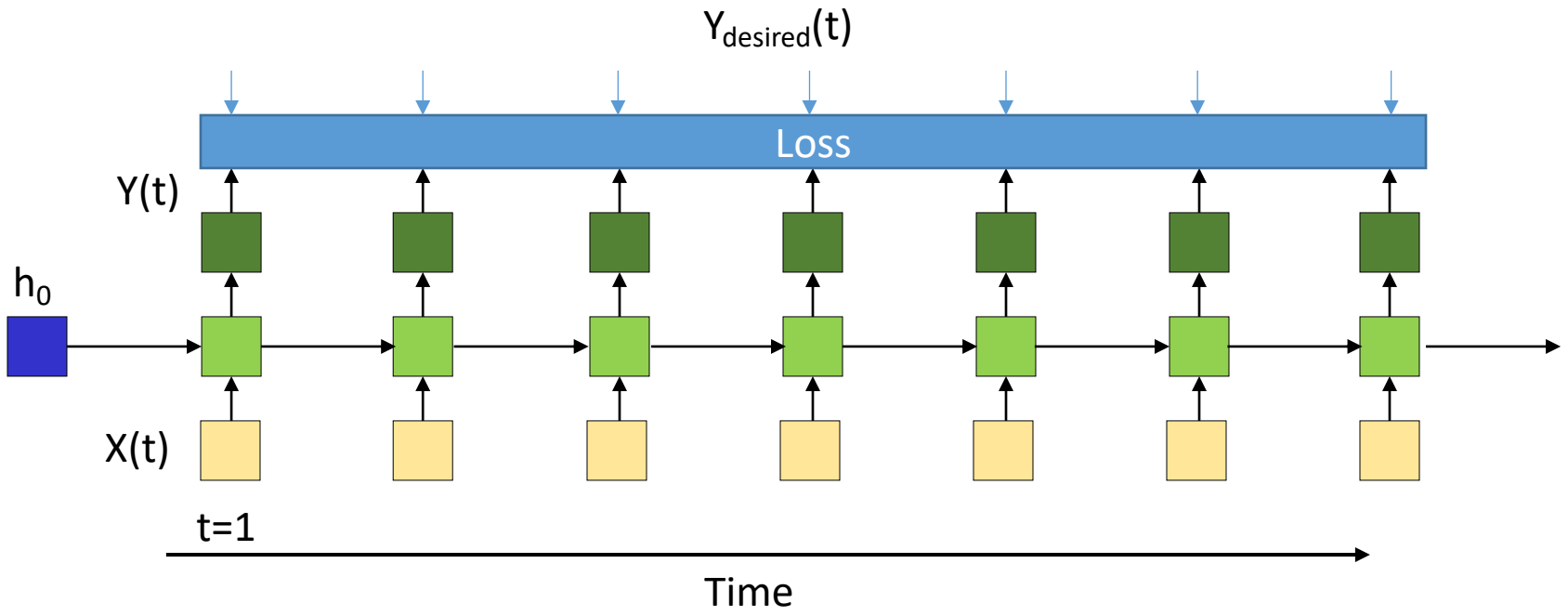
- Is the number of “ones” even or odd
- Network must be complex to capture all patterns
  - XOR network, quite complex
  - Fixed input size

RNN: The parity problem



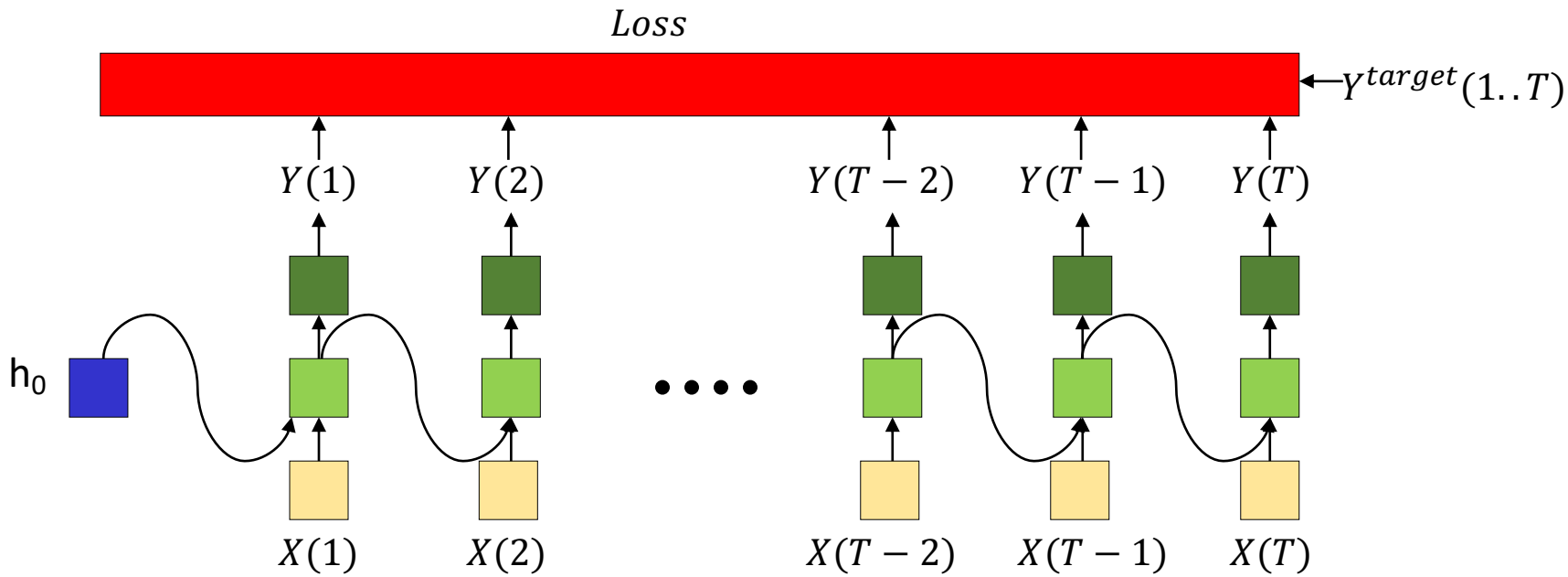
- Trivial solution
- Generalizes to input of any size

Story so far



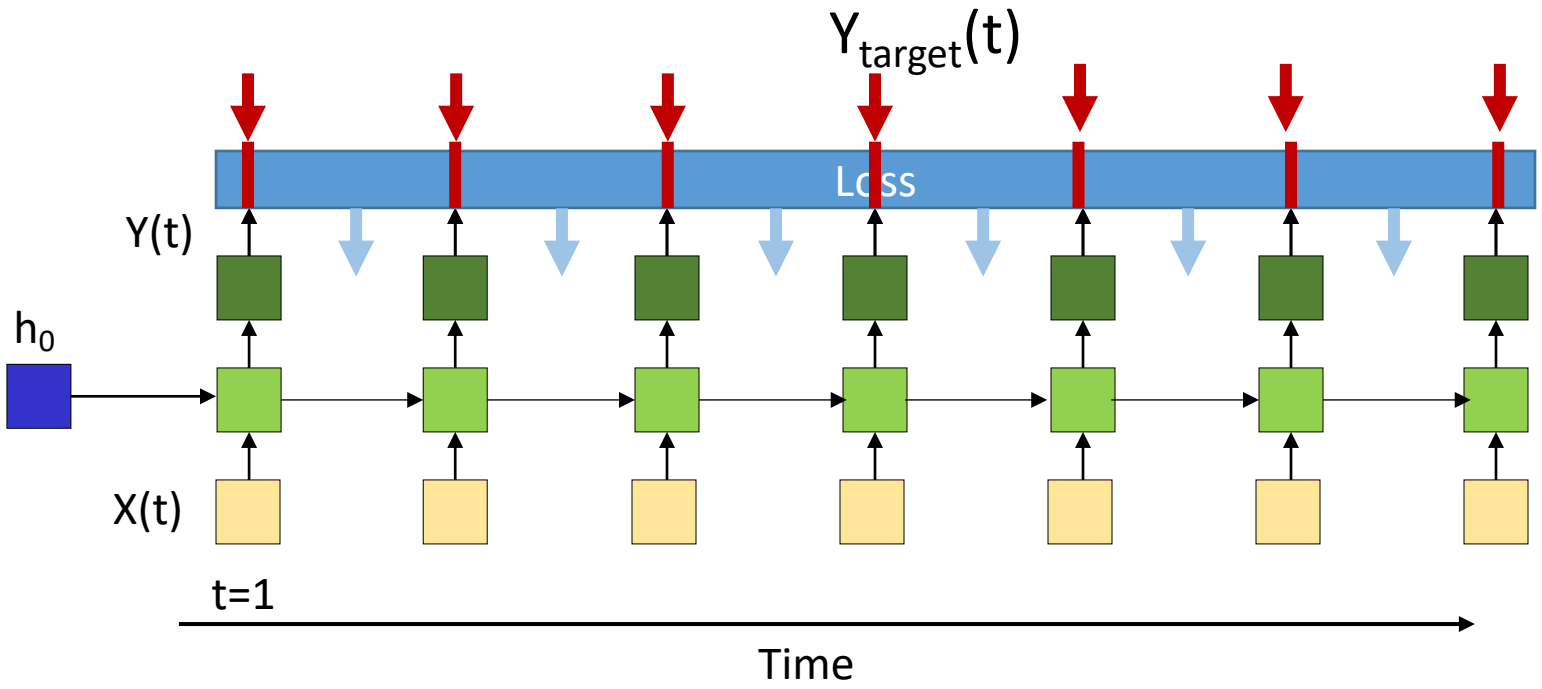
- Recurrent structures can be trained by minimizing the loss between the ***sequence*** of outputs and the ***sequence*** of desired outputs
  - Through gradient descent and backpropagation

Back Propagation Through Time



- The loss computed is between the *sequence of outputs* by the network and the *desired sequence of outputs*
- This is *not* always the sum of the divergences at individual times

Time-synchronous recurrence



- Usual assumption: ***Sequence divergence is the sum of the loss at individual instants***

$$Loss\big(Y_{target}(1 \dots T), Y(1 \dots T)\big) = \sum_t Loss\big(Y_{target}(t), Y(t)\big)$$

$$\nabla_{Y(t)} Loss\big(Y_{target}(1 \dots T), Y(1 \dots T)\big) = \nabla_{Y(t)} Loss\big(Y_{target}(t), Y(t)\big)$$

Long-term behavior of RNNs

- In linear systems, long-term behavior depends entirely on the eigenvalues of the hidden-layer weights matrix
  - If the largest Eigen value is greater than 1, the system will “blow up”
  - If it is lesser than 1, the response will “vanish” very quickly

“BIBO” Stability

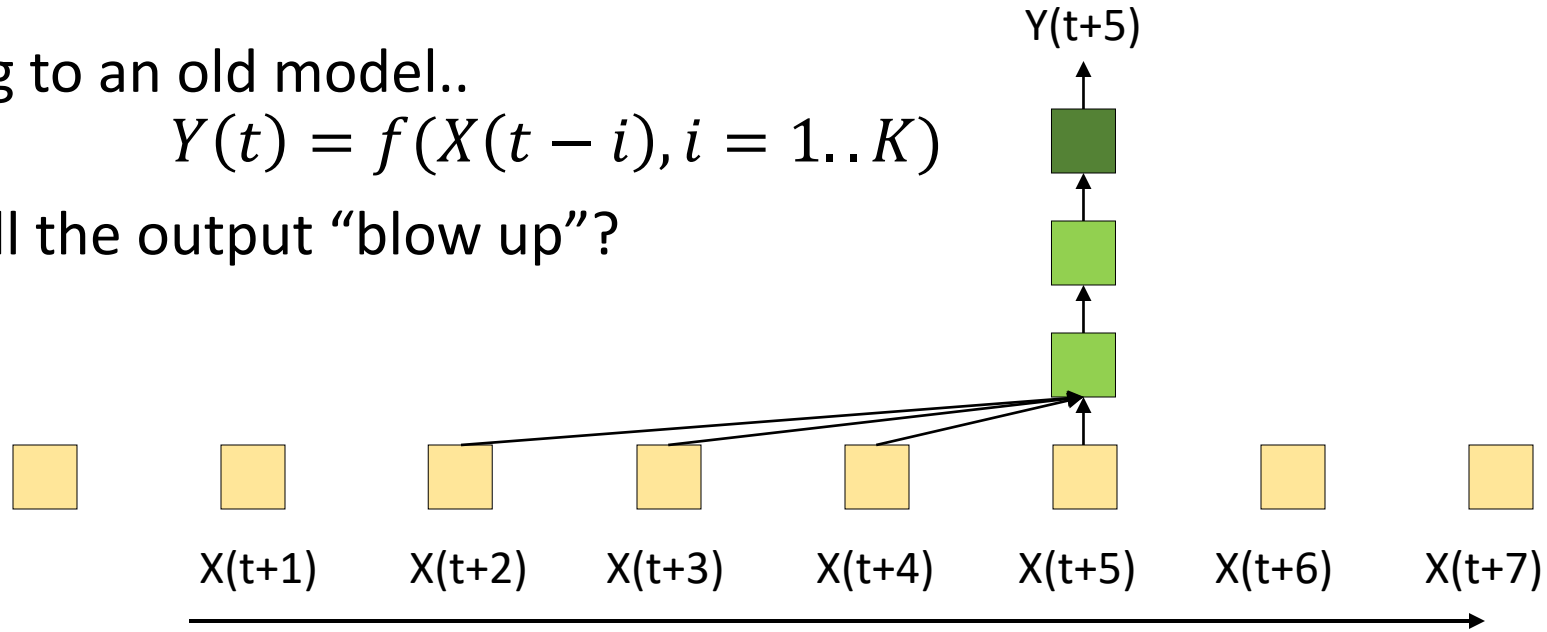
- “Bounded Input Bounded Output” stability
  - This is a highly desirable characteristic

"BIBO" Stability

- Returning to an old model..

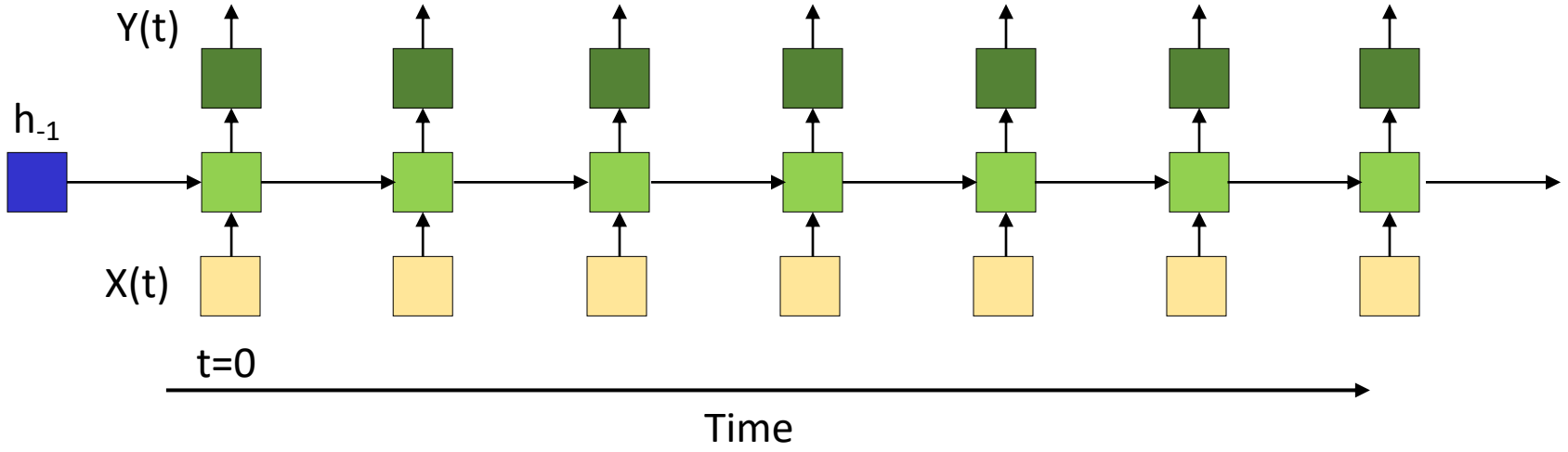
$$Y(t) = f(X(t-i), i = 1..K)$$

- When will the output "blow up"?



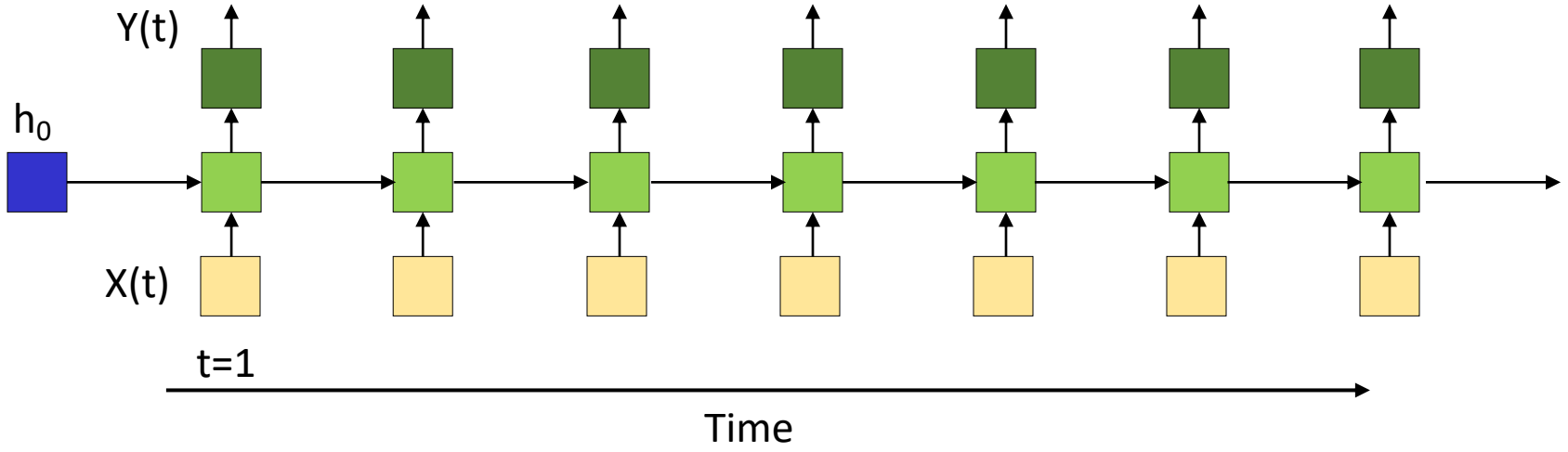
- Time-delay structures have bounded output if
  - The function $f(.)$ has bounded output for bounded input
    - Which is true of almost every activation function
  - $X(t)$ is bounded

Is this BIBO?



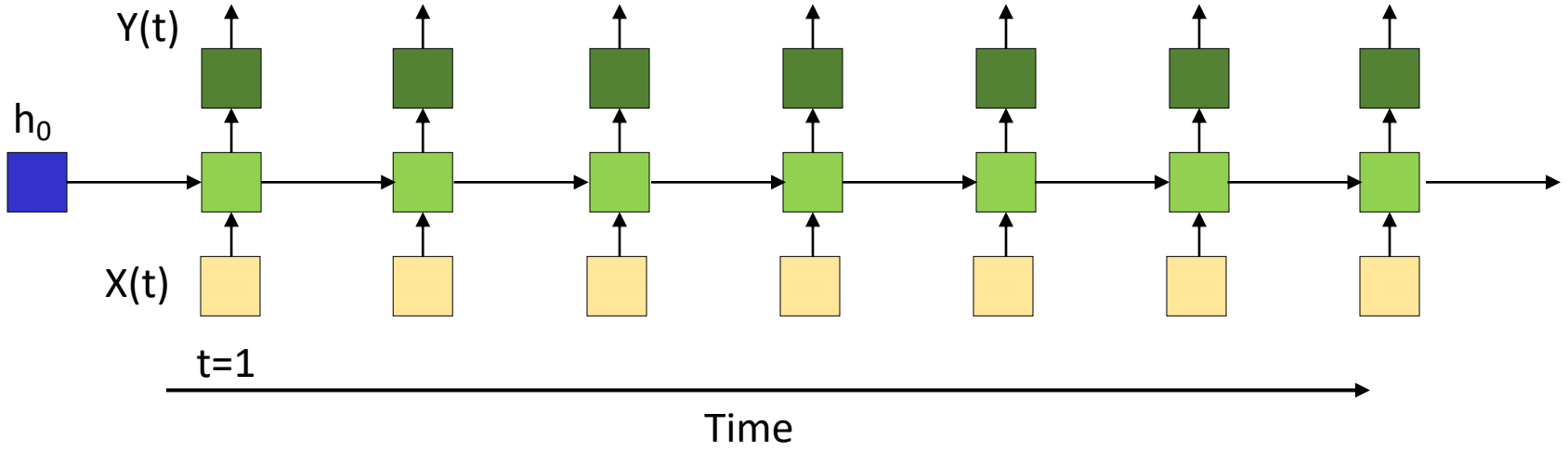
- Will RNN necessarily be BIBO?

Is this BIBO?



- Will this necessarily be BIBO?
  - Guaranteed if output and hidden activations are bounded
    - But will it *saturate* (and where)
  - What if the activations are linear?

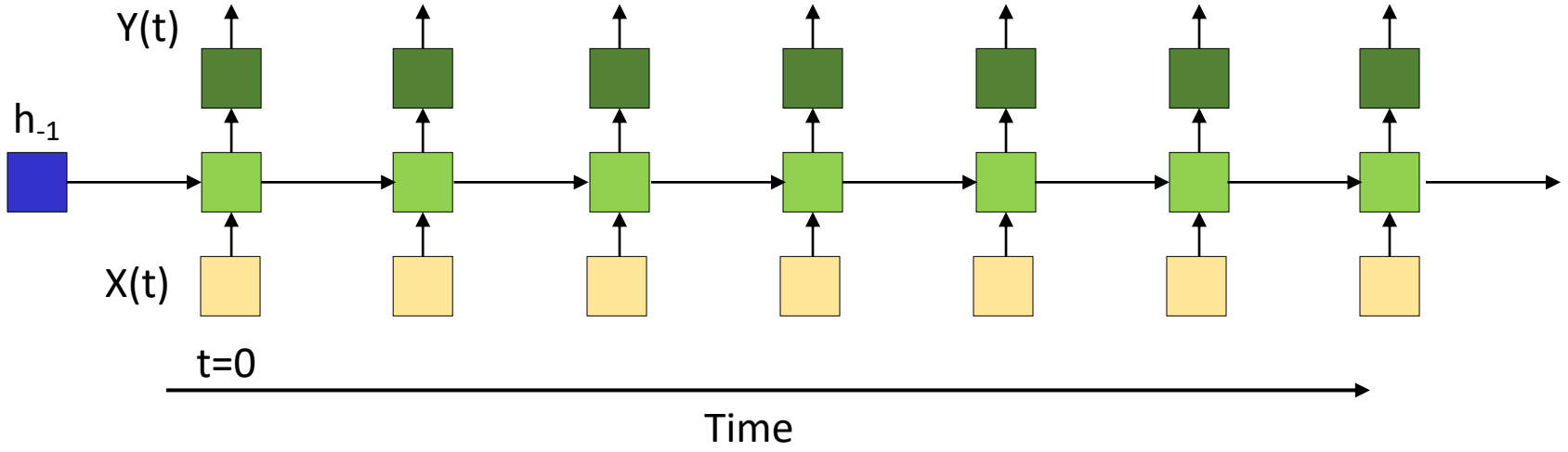
Analyzing recurrence



- Sufficient to analyze the behavior of the hidden layer h_k since it carries the relevant information
  - Will assume only a single hidden layer for simplicity

Analyzing Recursion

Streetlight effect



- Easier to analyze *linear* systems
  - Will attempt to extrapolate to non-linear systems subsequently
- All activations are identity functions
  - $z_k = W_h h_{k-1} + W_x x_k, \qquad h_k = z_k$

Linear systems

- $h_k = W_h h_{k-1} + W_x x_k$

  $- h_{k-1} = W_h h_{k-2} + W_x x_{k-1}$

- $h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k$

Linear systems

- $h_k = W_h h_{k-1} + W_x x_k$

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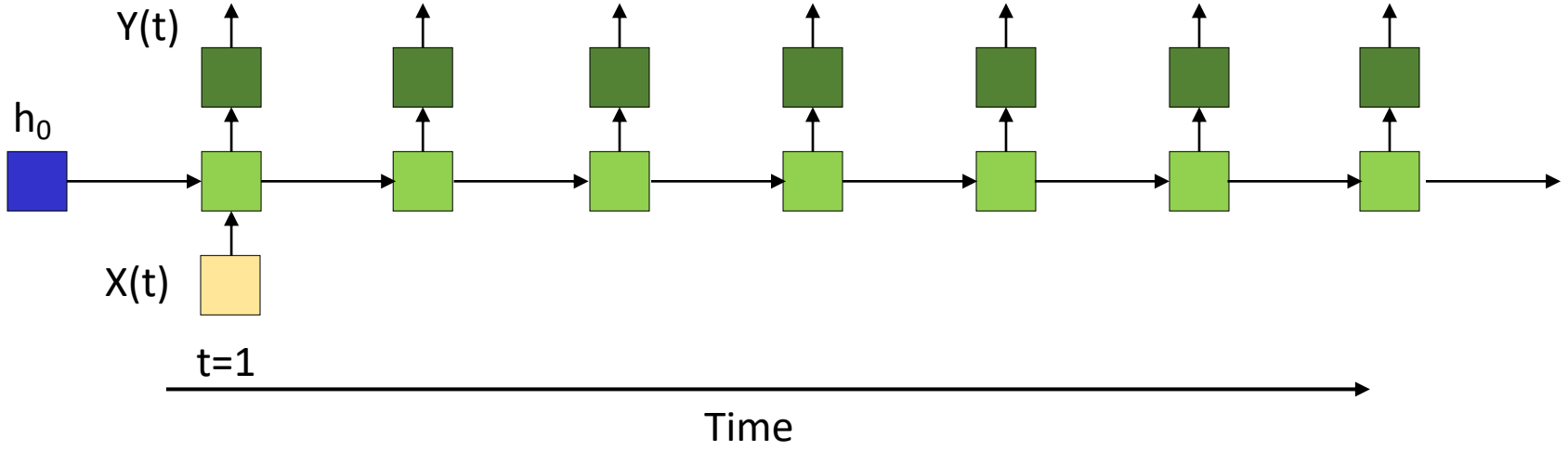
- $h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k$
- $h_k = W_h^{k+1} h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + \cdots$

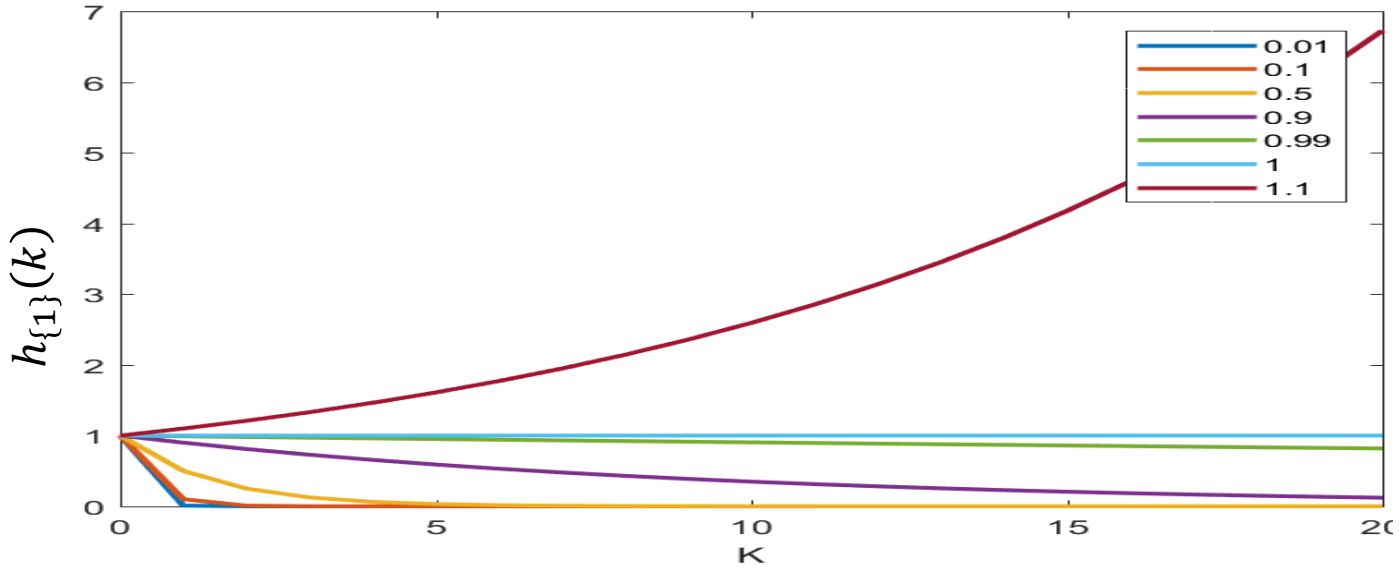
Streetlight effect



- Sufficient to analyze the response to a single input at $t = 1$
  - Principle of superposition in linear systems

Linear recursions

- Consider simple, scalar, linear recursion (note change of notation)
  - $h(t) = W_h h(t-1) + W_x x(t)$
  - $h_{\{1\}}(t) = W_h^t W_x x(1)$
    - Response to a single input appearing at 1



Linear recursions: Vector version

- Vector linear recursion (note change of notation)
  - $h(t) = W_h h(t-1) + W_x x(t)$
  - $h_{\{1\}}(t) = W_h^t W_x x(1)$
    - Length of response vector to a single input appearing at 1 is $|h_{\{1\}}(t)|$

- We can write $W_h = U\Lambda U^{-1}$
  - $W_h u_i = \lambda_i u_i$
  - For any vector v we can write
    - $v = a_1 u_1 + a_2 u_2 + \cdots + a_n u_n$
    - $W_h v = a_1 \lambda_1 u_1 + a_2 \lambda_2 u_2 + \cdots + a_n \lambda_n u_n$
    - $W_h^t v = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \cdots + a_n \lambda_n^t u_n$
  - $\lim_{t\to\infty} W_h^t v = a_m \lambda_m^t u_m$ where $m = \underset{j}{\operatorname{argmax}}\, \lambda_j$

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For any input, for large t the length of the hidden vector will expand or contract according to the t th power of the largest eigen value of the hidden-layer weight matrix

    - $W_h v = a_1\lambda_1 u_1 + a_2\lambda_2 u_2 + \cdots + a_n\lambda_n u_n$
    - $W_h^t v = a_1\lambda_1^t u_1 + a_2\lambda_2^t u_2 + \cdots + a_n\lambda_n^t u_n$
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  - $h_{\{1\}}(t) = W_h^t W_x x(1)$
    - Length of response vector to a single input appearing at 1 is $|h_{\{1\}}(t)|$

For any input, for large t, the length of the hidden vector will expand or contract according to the t th power of the largest eigen value of the hidden-layer weight matrix

Unless it has no component along the eigen vector corresponding to the largest eigen value. In that case it will grow according to the *second* largest Eigen value.. And so on..

  - For any vector v we can write
    - $v = a_1 u_1 + a_2 u_2 + \cdots + a_n u_n$
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  - $\lim_{t \to \infty} W_h^t v = a_m \lambda_m^t u_m$ where $m = \operatorname{argmax}_j \lambda_j$

Linear recursions: Vector version

- Vector linear recursion (note change of notation)

If $|\lambda_{max}| > 1$ it will blow up, otherwise it will contract and shrink to 0 rapidly

  - Length of response vector to a single input appearing at 1 is $|h_{\{1\}}(t)|$

For any input, for large t the length of the hidden vector will expand or contract according to the t th power of the largest eigen value of the hidden-layer weight matrix

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  - $\lim_{t \to \infty} W_h^t v = a_m \lambda_m^t u_m$ where $m = \underset{j}{\operatorname{argmax}} \lambda_j$

Linear recursions: Vector version

What about at middling values of t? It will depend on the other eigen values

If $|\lambda_{max}| > 1$ it will blow up, otherwise it will contract and shrink to 0 rapidly

For any input, for large t the length of the hidden vector will expand or contract according to the t th power of the largest eigen value of the hidden-layer weight matrix

Unless it has no component along the eigen vector corresponding to the largest eigen value. In that case it will grow according to the *second* largest Eigen value.. And so on..

- For any vector v we can write
  - $v = a_1 u_1 + a_2 u_2 + \cdots + a_n u_n$
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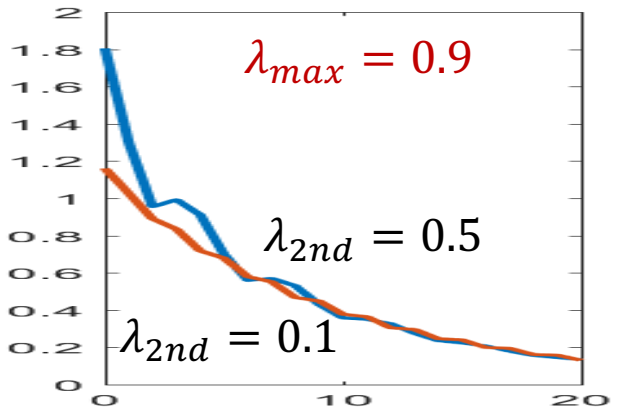
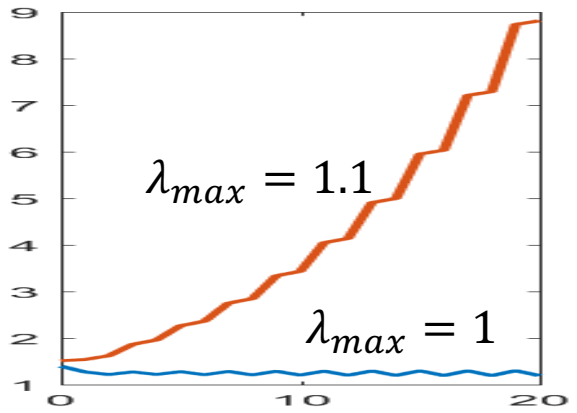
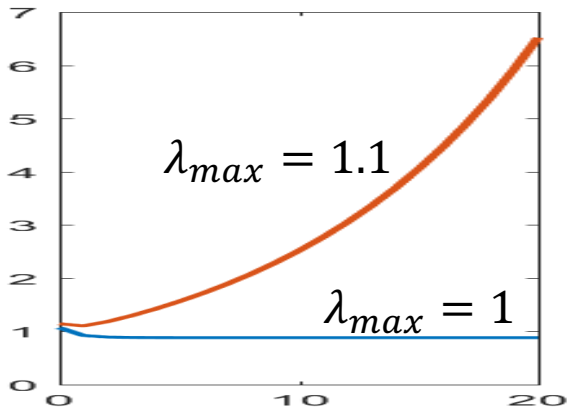
- $\lim_{t \to \infty} W_h^t v = a_m \lambda_m^t u_m$ where $m = \operatorname{argmax}_j \lambda_j$

Linear recursions

- Vector linear recursion
  - $h(t) = W_h h(t-1) + W_x x(t)$
  - $h_{\{1\}}(t) = W_h^t W_x x(1)$
    - Response to a single input [1 1 1 1] appearing at 1







Complex Eigenvalues

Lesson..

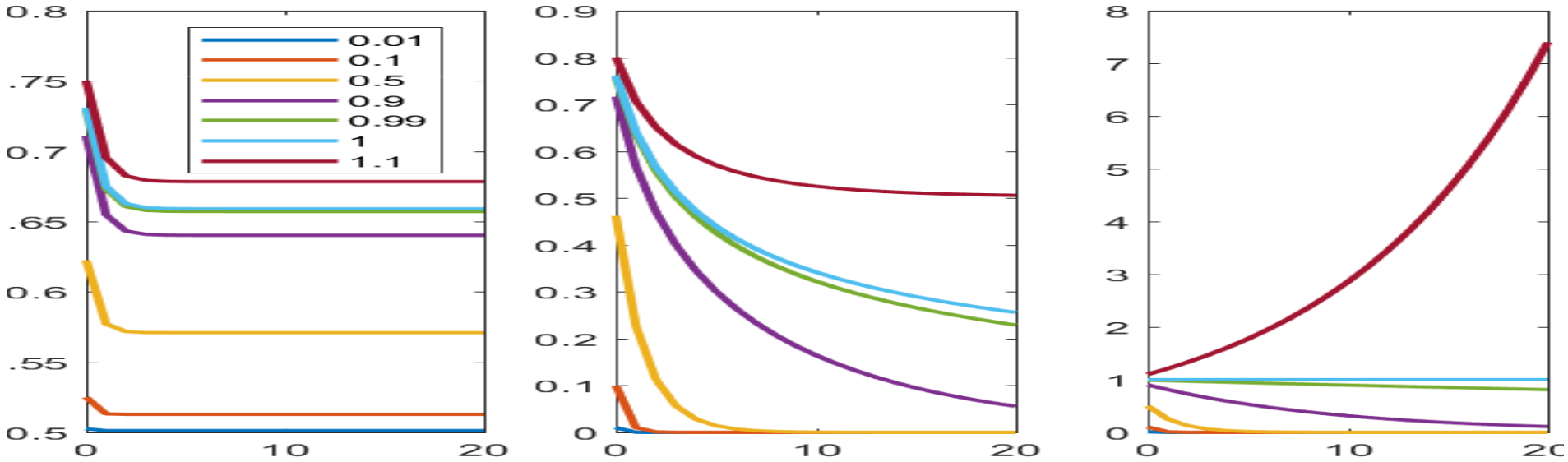
- In linear systems, long-term behavior depends entirely on the eigenvalues of the hidden-layer weights matrix
  - If the largest Eigen value is greater than 1, the system will “blow up”
  - If it is lesser than 1, the response will “vanish” very quickly
  - Complex eigen values cause oscillatory response
    - Which we may or may not want
    - For smooth behavior, must force the weights matrix to have real Eigen values
      - Symmetric weight matrix

How about non-linearities (scalar)

- The behavior of scalar non-linearities

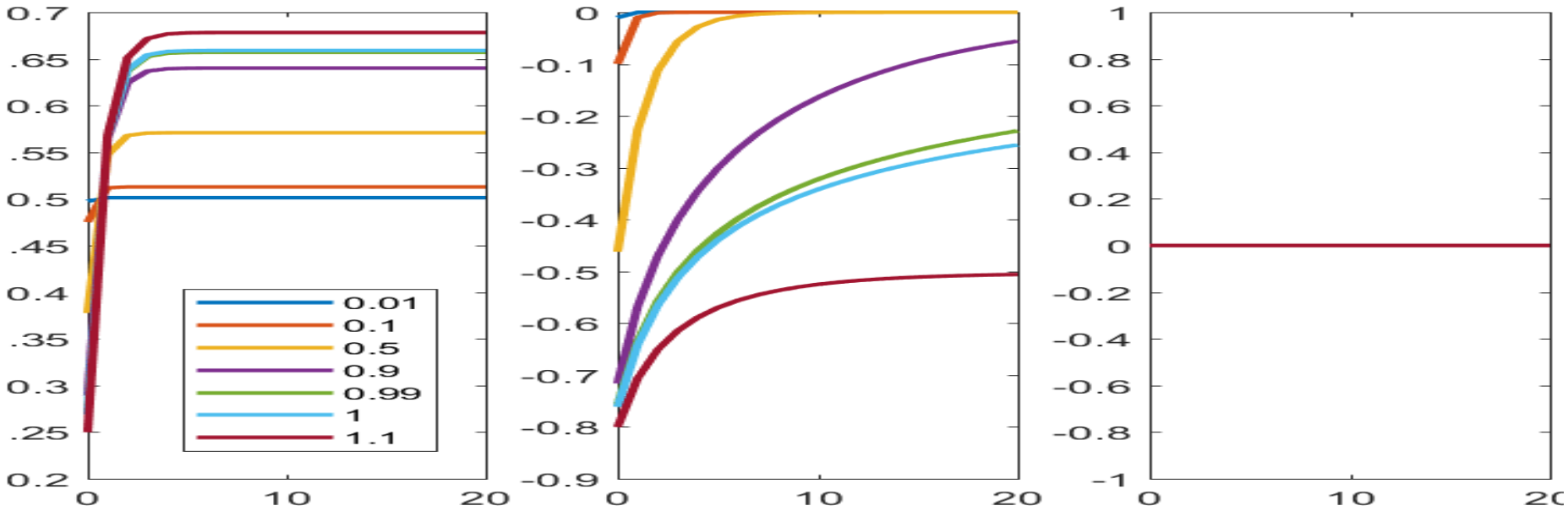
$$h(t) = f(W_h h(t-1) + W_x x(t))$$

- Left: Sigmoid, Middle: Tanh, Right: Relu
  - Sigmoid: Saturates in a limited number of steps, regardless of w_h
  - Tanh: Sensitive to W_h, but eventually saturates
    - "Prefers" weights close to 1.0
  - Relu: Sensitive to W_h, can blow up



How about non-linearities (scalar)

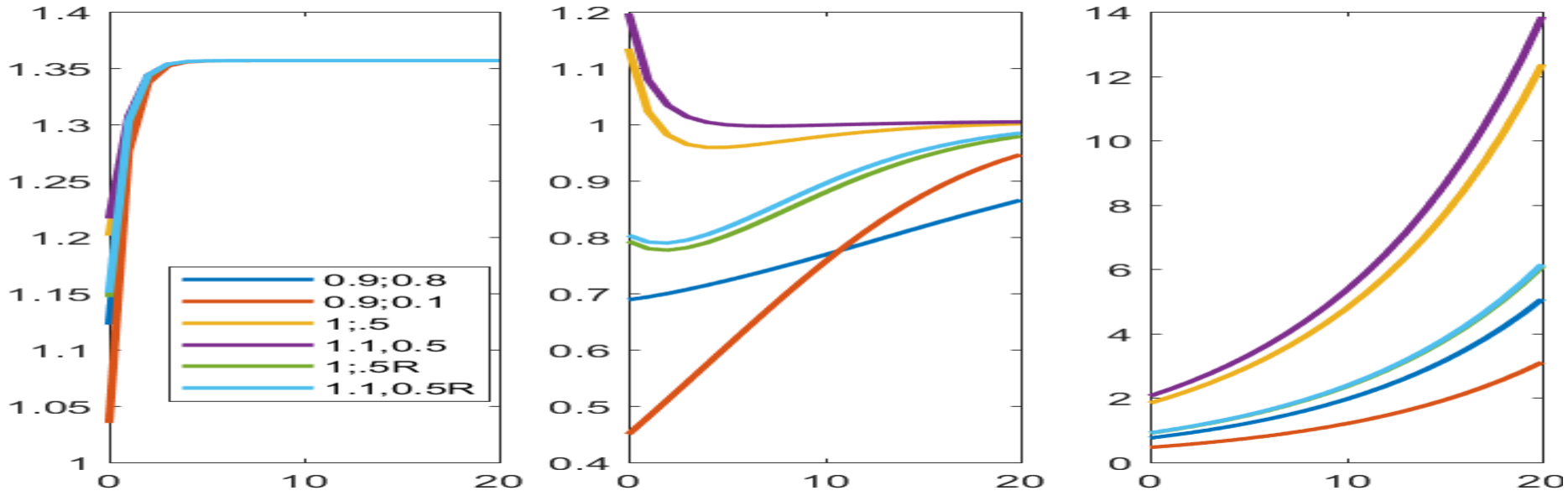
- With a negative start $h(t) = f(w_h h(t-1) + w_x x(t))$
- Left: Sigmoid, Middle: Tanh, Right: Relu
  - Sigmoid: Saturates in a limited number of steps, regardless of w_h
  - Tanh: Sensitive to w_h, but eventually saturates
  - Relu: For negative starts, has no response



Vector Process

- Assuming a uniform unit vector initialization
  - $[1,1,1,\ldots]/\sqrt{N}$
  - Behavior similar to scalar recursion
  - Interestingly, RELU is more prone to blowing up (why?)
- Eigenvalues less than 1.0 retain the most "memory"

$$h(t) = f(W_h h(t-1) + W_x x(t))$$

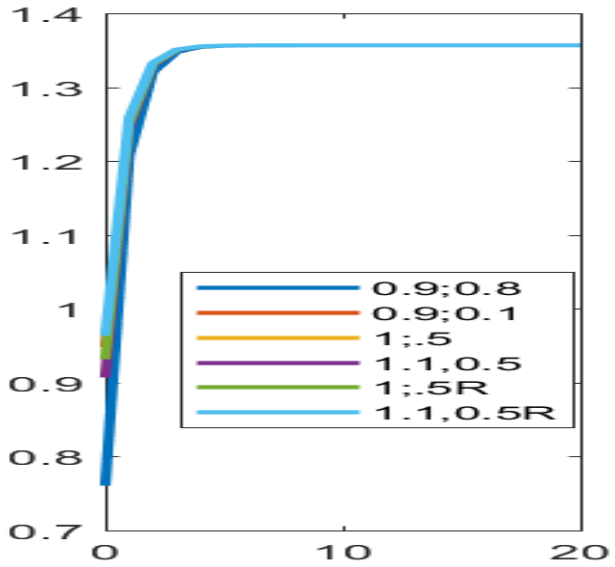


sigmoid tanh relu

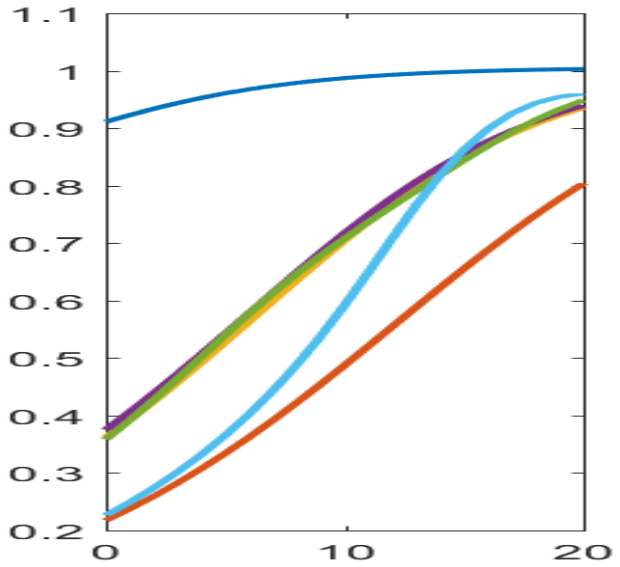
Vector Process

- Assuming a uniform unit vector initialization
  - $[-1, -1, -1, \ldots]/\sqrt{N}$
  - Behavior similar to scalar recursion
  - Interestingly, RELU is more prone to blowing up (why?)

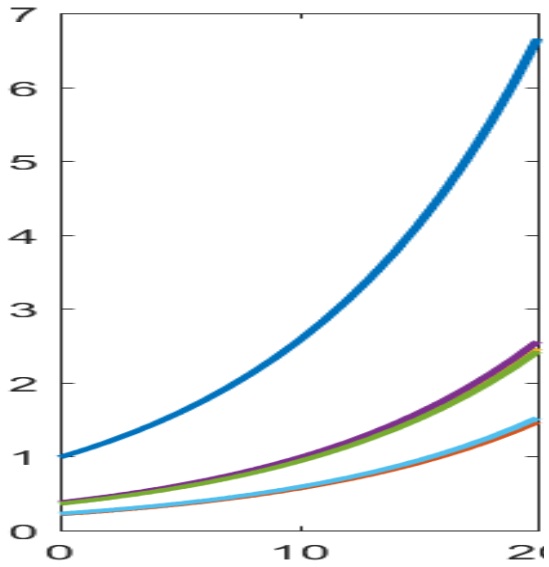
$$h(t) = f(W_h h(t-1) + W_x x(t))$$



sigmoid



tanh



relu

Story so far

- Recurrent networks retain information from the infinite past in principle
- In practice, they tend to blow up or forget
  - If the largest Eigen value of the recurrent weights matrix is greater than 1, the network response may blow up
  - If its less than one, the response dies down very quickly
- The “memory” of the network also depends on the activation of the hidden units
  - Sigmoid activations saturate and the network becomes unable to retain new information
  - RELUs blow up
  - Tanh activations are the most effective at storing memory
    - But still, for not very long

RNNs..

- Excellent models for time-series analysis tasks
  - Time-series prediction
  - Time-series classification
  - Sequence prediction..
  - They can even simplify problems that are difficult for MLPs

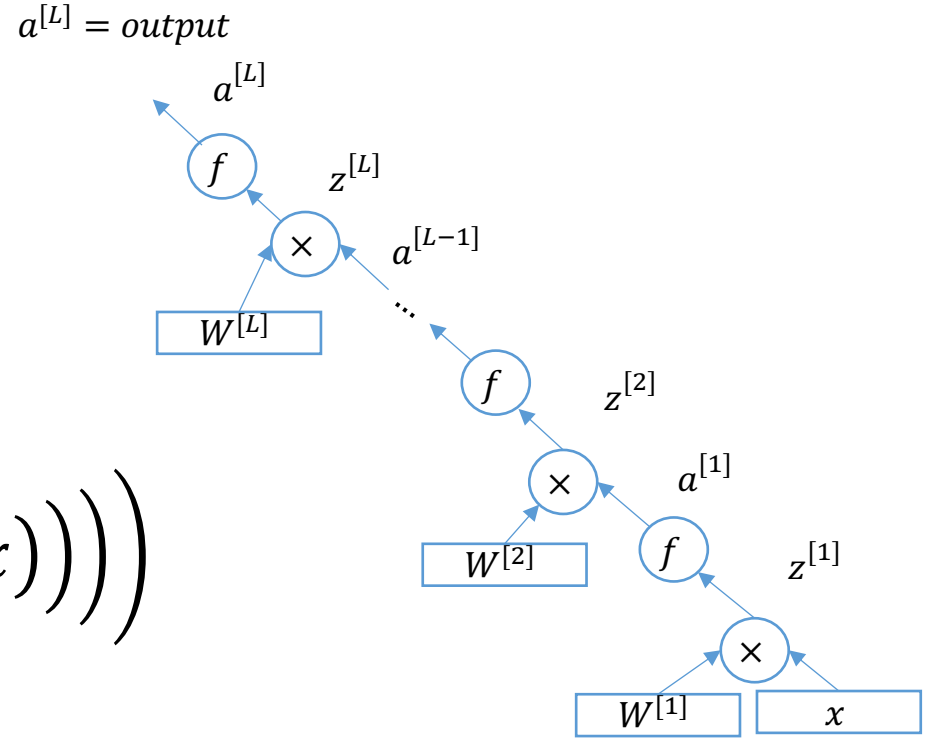
- But the memory isn’t all that great..
  - Also..

The vanishing gradient problem

- A particular problem with training deep networks..
  - (Any deep network, not just recurrent nets)
  - The gradient of the error with respect to weights is unstable..

Recap: Training deep networks

$$Output = a^{[L]}$$
$$= f\left(z^{[L]}\right)$$
$$= f\left(W^{[L]}a^{[L-1]}\right)$$
$$= f\left(W^{[L]}f(W^{[L-1]}a^{[L-2]}\right)$$
$$= f\left(W^{[L]}f\left(W^{[L-1]}\ldots f\left(W^{[2]}f\left(W^{[1]}x\right)\right)\right)\right)$$



For convenience, we use the same activation functions for all layers.

However, output layer neurons most commonly do not need activation function (they show class scores or real-valued targets.)

Recap: Training deep networks

- For

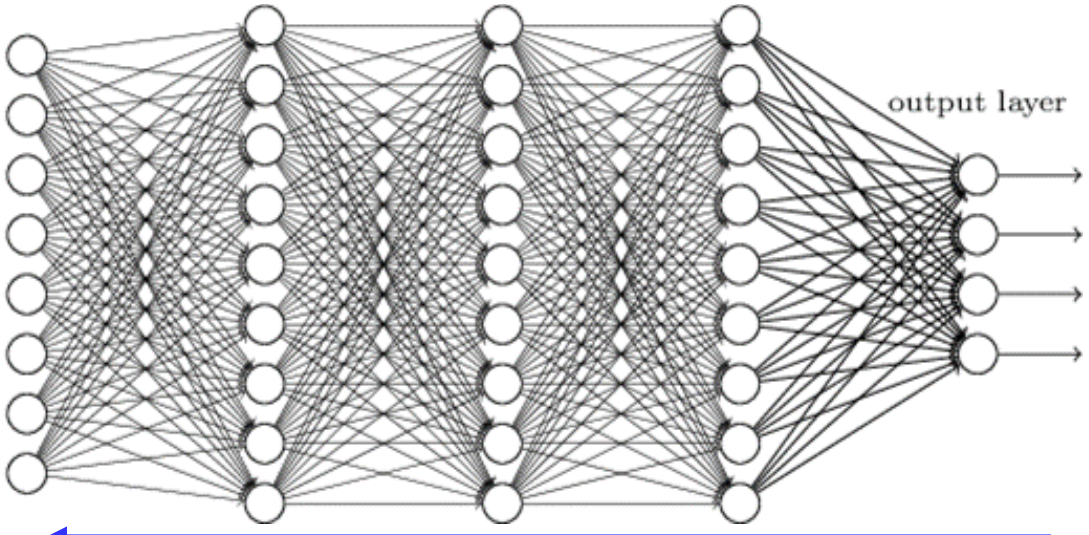
$$Loss(x) = E\left(f^{[L]}\left(W^{[L]}f^{[L-1]}\left(W^{[L-1]}f^{[L-2]}\left(\ldots W^{[1]}x\right)\right)\right)\right)$$

- We get:

$$\nabla_{f^{[l]}}Loss = \nabla_{f^{[L]}}Loss.\nabla f^{[L]}.W^{[L]}.\nabla f^{[L-1]}.W^{[L-1]}\ldots\nabla f^{[l+1]}.W^{[l+1]}$$

- Where
  - $\nabla_{f^{[l]}}Loss$ is the gradient of the error w.r.t the output of the l-th layer of the network
    - Needed to compute the gradient of the error w.r.t $W^{[l]}$
  - $\nabla f^{[l]}$ is *jacobian* of $f^{[l]}$ w.r.t. to its current input
  - All blue terms are matrices

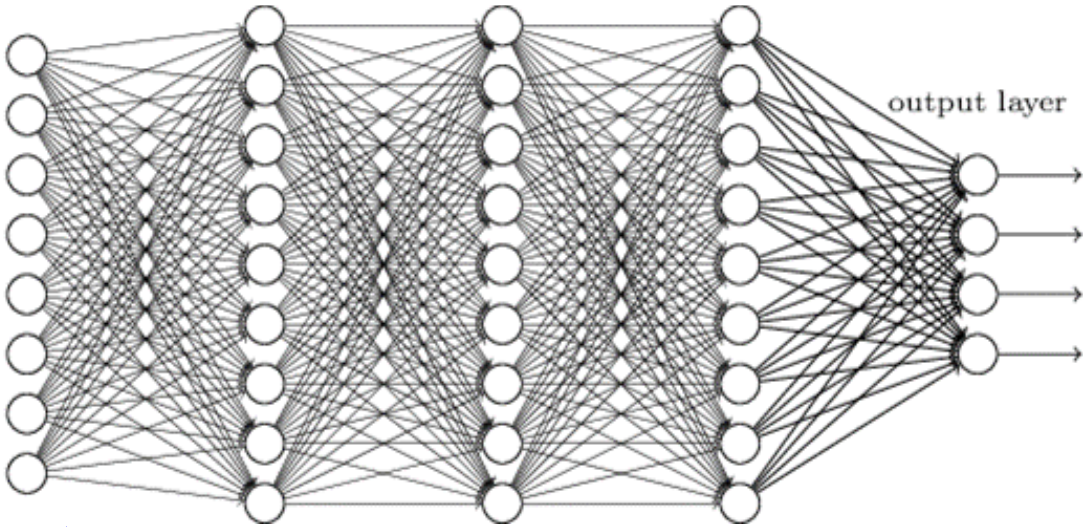
Recap: Gradient problems in deep networks



$$\nabla_{f^{[l]}} Loss = \nabla_{f^{[L]}} Loss . \nabla f^{[L]} . W^{[L]} . \nabla f^{[L-1]} . W^{[L-1]} \ldots \nabla f^{[l+1]} . W^{[l+1]}$$

- The gradients in the lower/earlier layers can *explode* or *vanish*
  - Resulting in insignificant or unstable gradient descent updates
  - Problem gets worse as network depth increases

Recap: Training deep networks



- As we go back in layers, the Jacobians of the activations constantly *shrink* the derivative
  - After a few layers the derivative of the loss at any time is totally "forgotten"

Exploding/Vanishing gradients

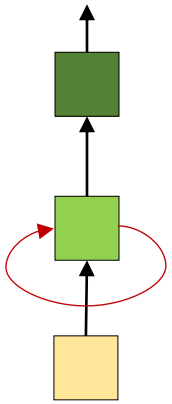
$$\nabla_{f_k} Loss = \nabla Loss . \underline{\nabla f_N . W_{N-1} .} \underline{\nabla f_{N-1} . W_{N-2}} \ \underline{\dots \nabla f_{k+1} W_k}$$

- Every blue term is a matrix
- The chain product for $\nabla_{f_k} Loss$ will
  - E*xpand* $\nabla Loss$ in directions where each stage has singular values greater than 1
  - S*hrink* $\nabla Loss$ in directions where each stage has singular values less than 1

Vanishing gradients

- ELU activations maintain gradients longest
- But in all cases gradients effectively vanish after about 10 layers!
  - Your results may vary
- Both batch gradients and gradients for individual instances disappear
  - In reality a tiny number will actually blow up.

The Jacobian of the hidden layers for an RNN

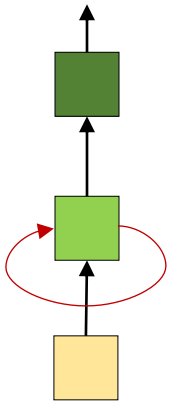


$$h_i(t) = f\big(z_i(t)\big)$$

$$\nabla f(z(t)) = \begin{bmatrix} f'(z_{t,1}) & 0 & \cdots & 0 \\ 0 & f'(z_{t,2}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & f'(z_{t,N}) \end{bmatrix}$$

- $\nabla f(.)$ is the derivative of the output of the (layer of) hidden recurrent neurons with respect to their input
  - For vector activations: A full matrix
  - For scalar activations: A matrix where the diagonal entries are the derivatives of the *activation* of the recurrent hidden layer

The Jacobian



$$h_i(t) = f\big(z_i(t)\big)$$

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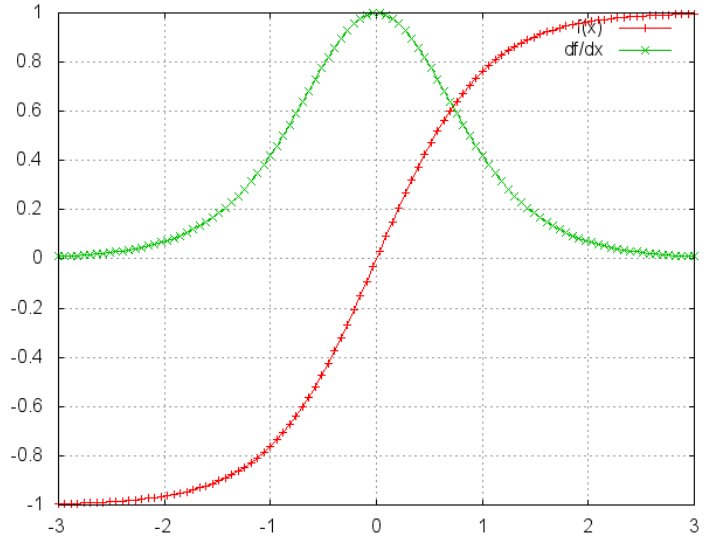
- The derivative (or subgradient) of the activation function is always bounded
  - The diagonals (or singular values) of the Jacobian are bounded
- There is a limit on how much multiplying a vector by the Jacobian will scale it

The derivative of the hidden state activation

$$\nabla f_t(z_i) = \begin{bmatrix} f'_{t,1}(z_1) & 0 & \cdots & 0 \\ 0 & f'_{t,2}(z_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & f'_{t,N}(z_N) \end{bmatrix}$$



- Most common activation functions, such as sigmoid, tanh() and RELU have derivatives that are always no more than 1
- The most common activation for the hidden units in an RNN is the tanh(.)
  - The derivative of $\tanh(.)$ is never greater than 1 (and mostly less than 1)

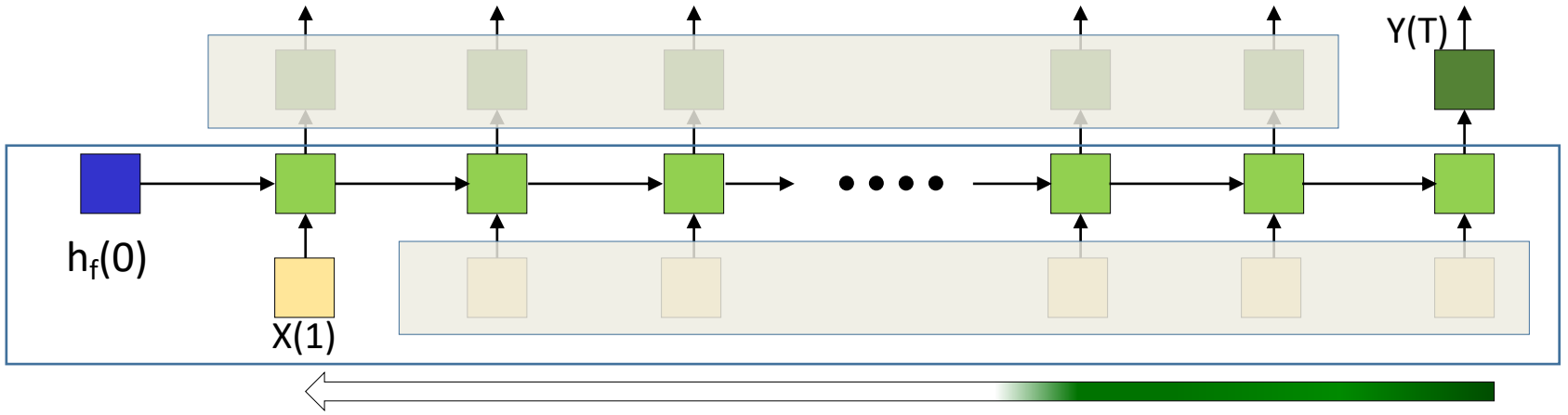
- **Multiplication by the Jacobian is always a *shrinking* operation**

What about the weights

$$\nabla_{f[t]} Loss = \nabla_{f[T]} Loss . \nabla f^{[T]} . W . \nabla f^{[T-1]} . W \ldots \nabla f^{[t+1]} . W$$

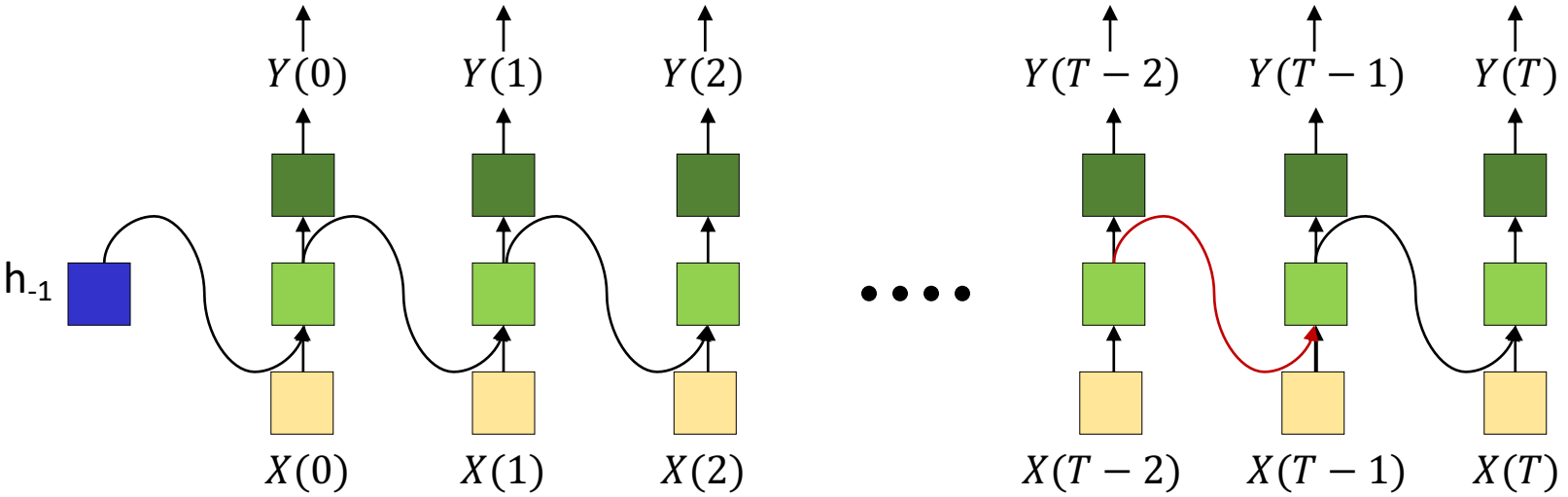
- In a single-layer RNN, the weight matrices are identical
  - The conclusion below holds for any deep network, though
- The chain product for $\nabla_{f[t]} Loss$ will
  - E*xpand* $\nabla_{f[T]} Loss$ along directions in which the singular values of the weight matrices are greater than 1
  - S*hrink* $\nabla_{f[T]} Loss$ in directions where the singular values are less than 1
  - Repeated multiplication by the weights matrix will result in **Exploding** or **vanishing** gradients

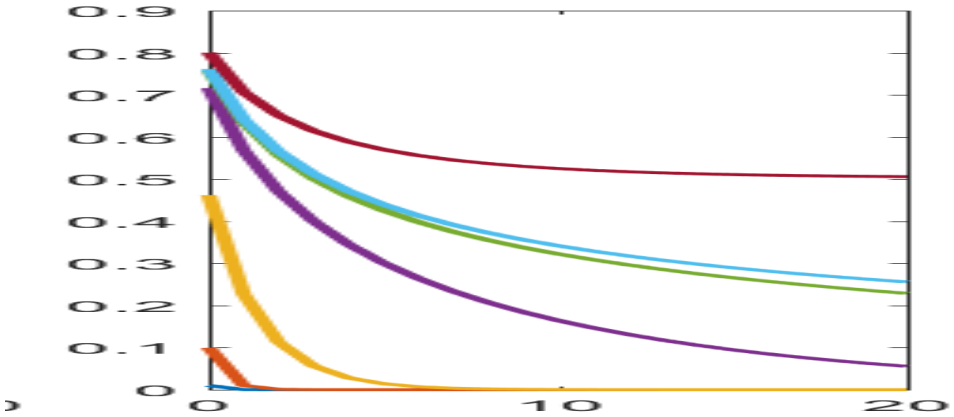
Recurrent nets are very deep nets



- The relation between $X(1)$ and $Y(T)$ is one of a very deep network
  - Gradients from errors at t $= T$ will vanish by the time they're propagated to $t = 1$

Recall: Vanishing stuff..





- Stuff gets forgotten in the forward pass too
  - Each weights matrix and activation can shrink components of the input

Training RNNs is hard

- The unrolled network can be very deep and inputs from many time steps ago can modify output
  - Unrolled network is very deep

- Multiply the same matrix at each time step during forward prop

The vanishing gradient problem: Example

- In the case of language modeling words from time steps far away are not taken into consideration when training to predict the next word

- Example: Jane walked into the room. John walked in too. It was late in the day. Jane said hi to ____

This slide has been adopted from Socher lectures, cs224d, Stanford

The long-term dependency problem

- Must know to “remember” for extended periods of time and “recall” when necessary
  - Can be performed with a multi-tap recursion, but how many taps?
  - Need an alternate way to “remember” stuff

Story so far

- Recurrent networks retain information from the infinite past in principle
- In practice, they are poor at memorization
  - The hidden outputs can blow up, or shrink to zero depending on the Eigen values of the recurrent weights matrix
  - The memory is also a function of the activation of the hidden units
    - Tanh activations are the most effective at retaining memory, but even they don't hold it very long
- Deep networks also suffer from a "vanishing or exploding gradient" problem
  - The gradient of the error at the output gets concentrated into a small number of parameters in the earlier layers, and goes to zero for others

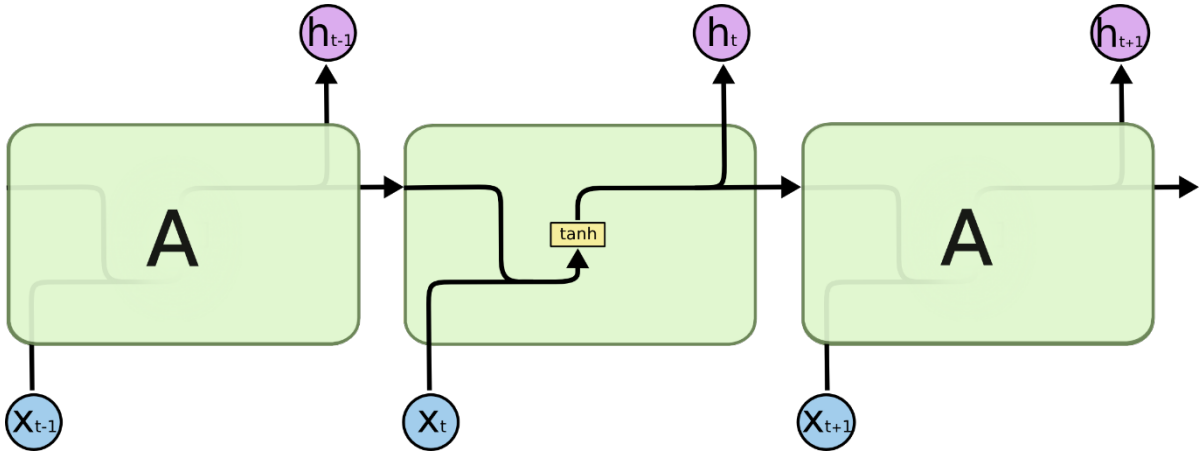
The long-term dependency problem

PATTERN1 [.....] PATTERN 2

Jane had a quick lunch in the bistro. Then *she...*

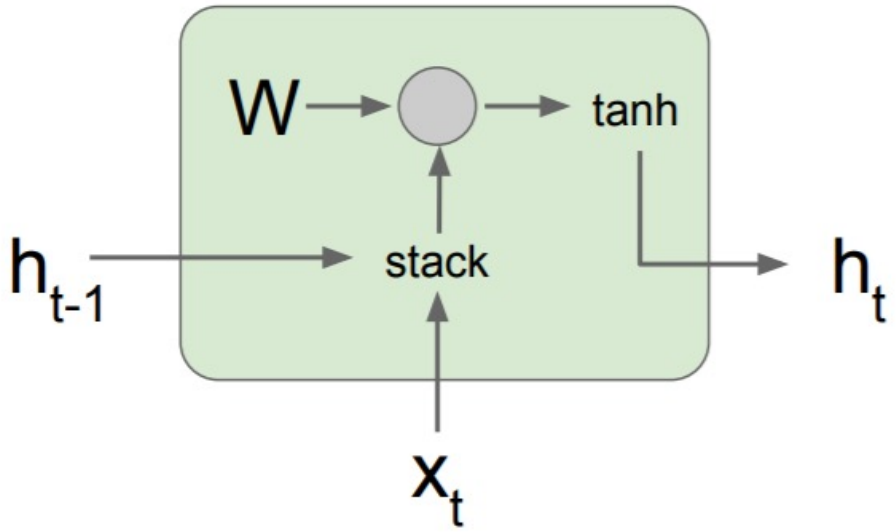
- Any other pattern of any length can happen between pattern 1 and pattern 2
  - RNN will "forget" pattern 1 if intermediate stuff is too long
  - "Jane" → the next pronoun referring to her will be "she"
- Must know to "remember" for extended periods of time and "recall" when necessary
  - Need an alternate way to "remember" stuff

Standard RNN



- Recurrent neurons receive past recurrent outputs and current input as inputs
- Processed through a tanh() activation function
  - As mentioned earlier, tanh() is the generally used activation for the hidden layer
- Current recurrent output passed to next higher layer and next time instant

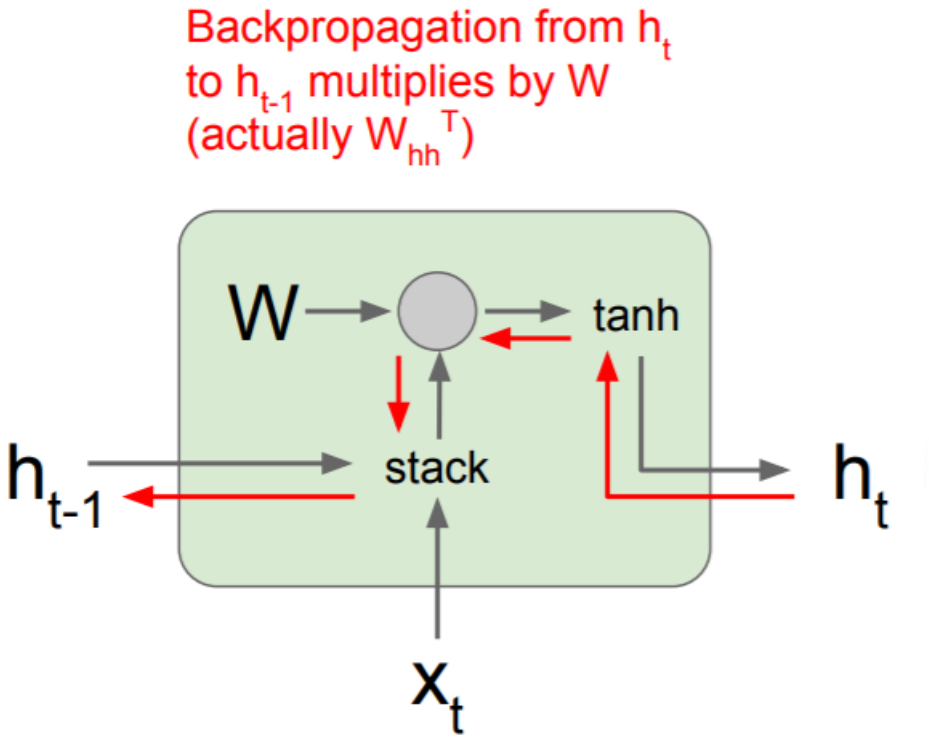
Vanilla RNN Gradient Flow



$$
\begin{aligned}
h_t &= \tanh(W_{hh}h_{t-1} + W_{xh}x_t) \\
&= \tanh\left(\begin{pmatrix} W_{hh} & W_{hx} \end{pmatrix} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} \right) \\
&= \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} \right)
\end{aligned}
$$

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994
Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013

Vanilla RNN Gradient Flow



$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t)$$
$$= \tanh\left((W_{hh} \quad W_{hx})\begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$
$$= \tanh\left(W\begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

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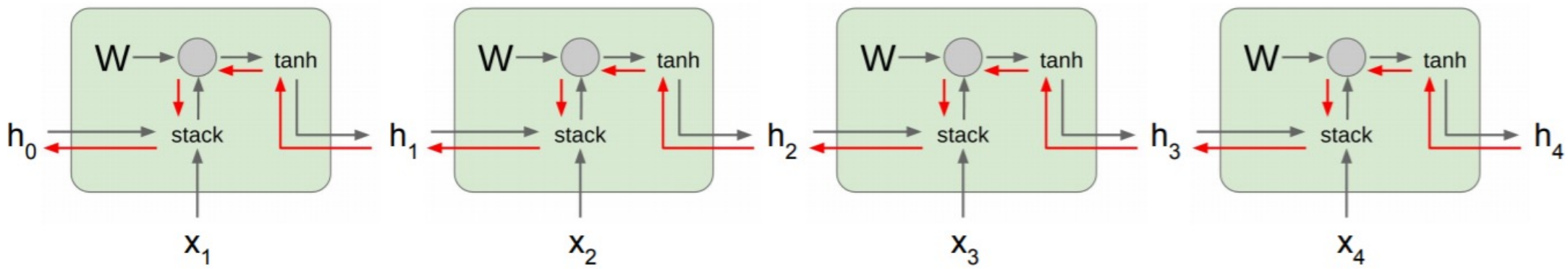
Vanilla RNN Gradient Flow



Largest singular value > 1: Exploding gradients
Largest singular value < 1: Vanishing gradients

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994
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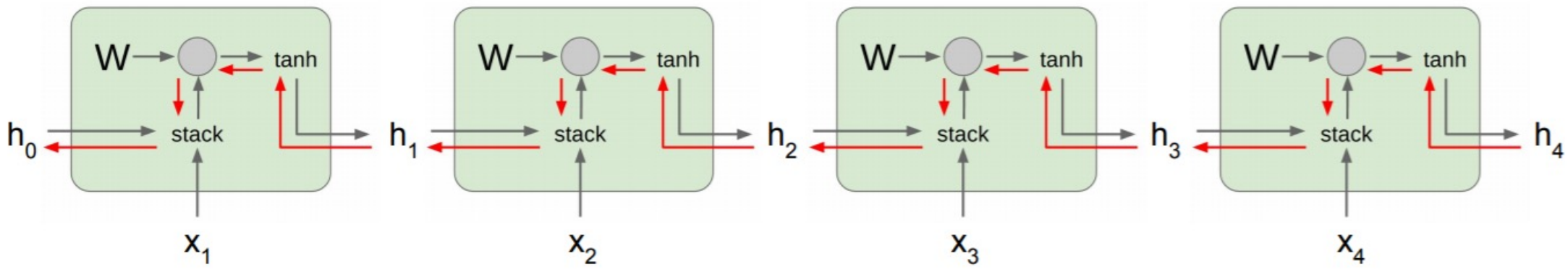
Vanilla RNN Gradient Flow



Computing gradient of h_0 involves many factors of W (and repeated tanh)

Largest singular value > 1: Exploding gradients

Largest singular value < 1: Vanishing gradients

Gradient clipping: Scale Computing gradient if its norm is too big

```
grad_norm = np.sum(grad * grad)
if grad_norm > threshold:
  grad *= (threshold / grad_norm)
```

Change RNN architecture

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994
Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013

Enter the *LSTM*

- *Long Short-Term Memory*
- Explicitly latch information to prevent decay / blowup

- Following notes borrow liberally from
  - http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Better units for recurrent models

- More complex hidden unit computation in recurrence!
  - $h_t = LSTM(x_t, h_{t-1})$
  - $h_t = GRU(x_t, h_{t-1})$
- Main ideas:
  - keep around memories to capture long distance dependencies
  - allow error messages to flow at different strengths depending on the inputs

Exploding/Vanishing gradients

- Can we replace this with something that doesn't fade or blow up?

- Can we have a network that just "remembers" arbitrarily long, to be recalled on demand?
  - Not be directly dependent on vagaries of network parameters, but rather on input-based determination of *whether it must be remembered*
  - Replace them, e.g., by a function of the input that decides if things must be forgotten or not

Long Short Term Memory (LSTM)

Vanilla RNN

$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

LSTM

Four gates

Cell state

Hidden state

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

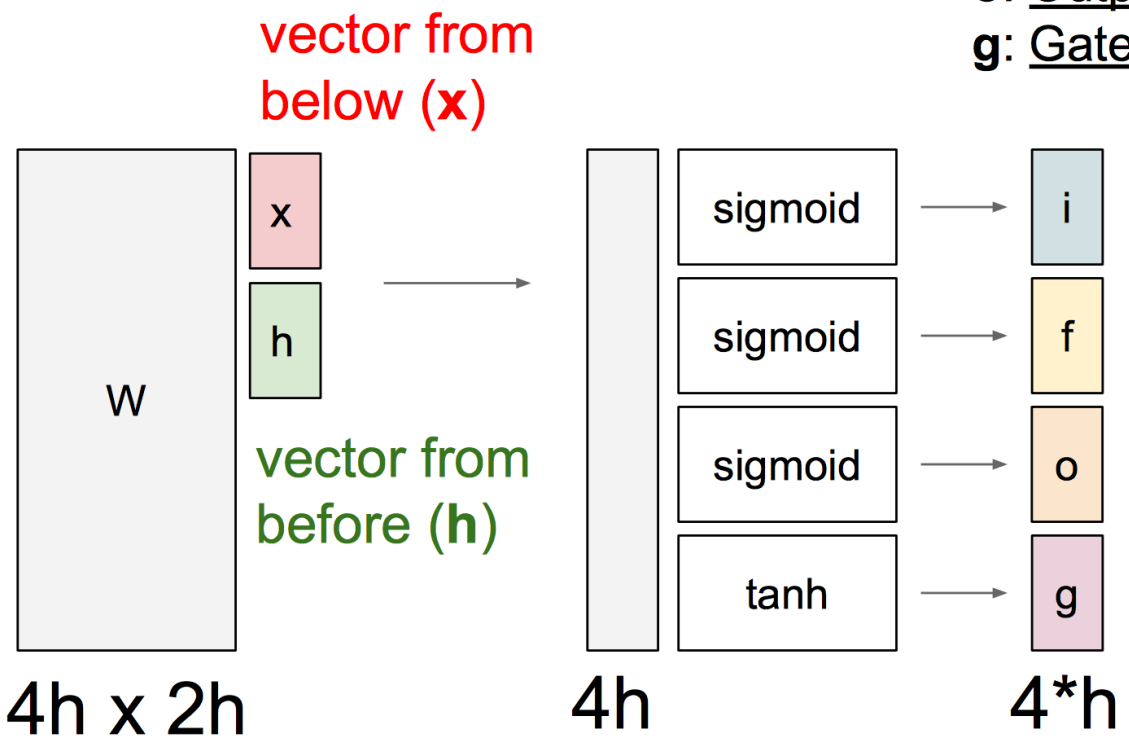
$$h_t = o \odot \tanh(c_t)$$

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation 1997

Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

i: Input gate, whether to write to cell
f: Forget gate, Whether to erase cell
o: Output gate, How much to reveal cell
g: Gate gate (?), How much to write to cell



$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

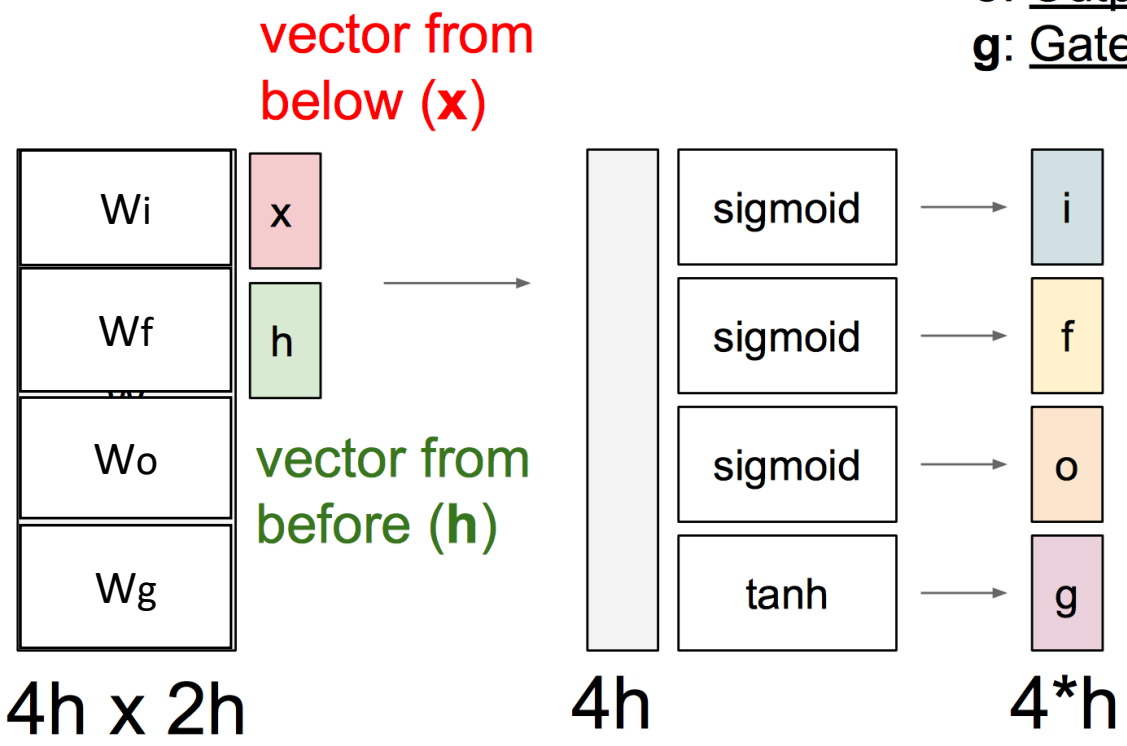
$$h_t = o \odot \tanh(c_t)$$

i, f, o, g, c, and h are vectors of the same length

Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

i: Input gate, whether to write to cell
f: Forget gate, Whether to erase cell
o: Output gate, How much to reveal cell
g: Gate gate (?), How much to write to cell



$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

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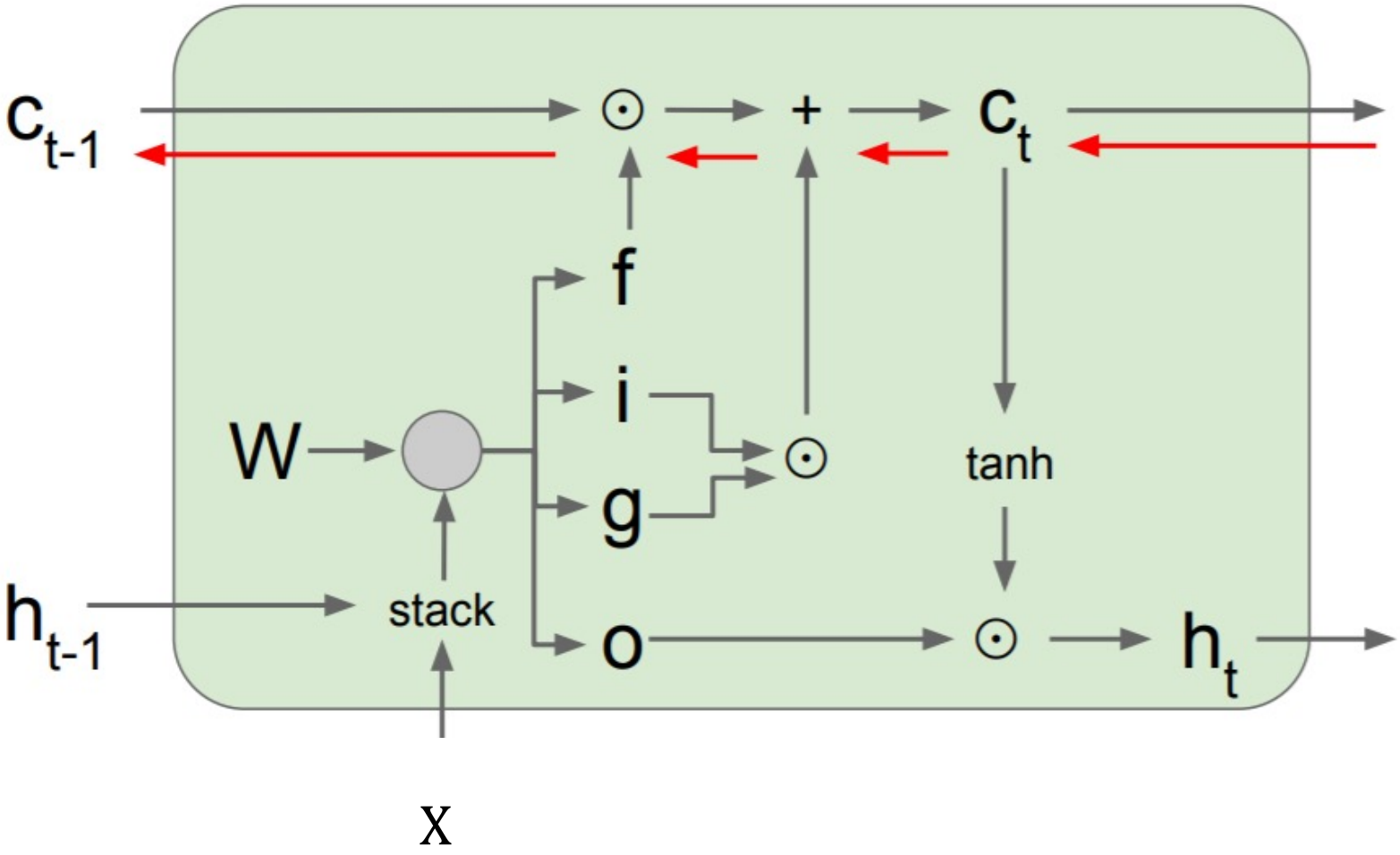
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]



Backpropagation from c_t to c_{t-1} only elementwise multiplication by f, no matrix multiply by W

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

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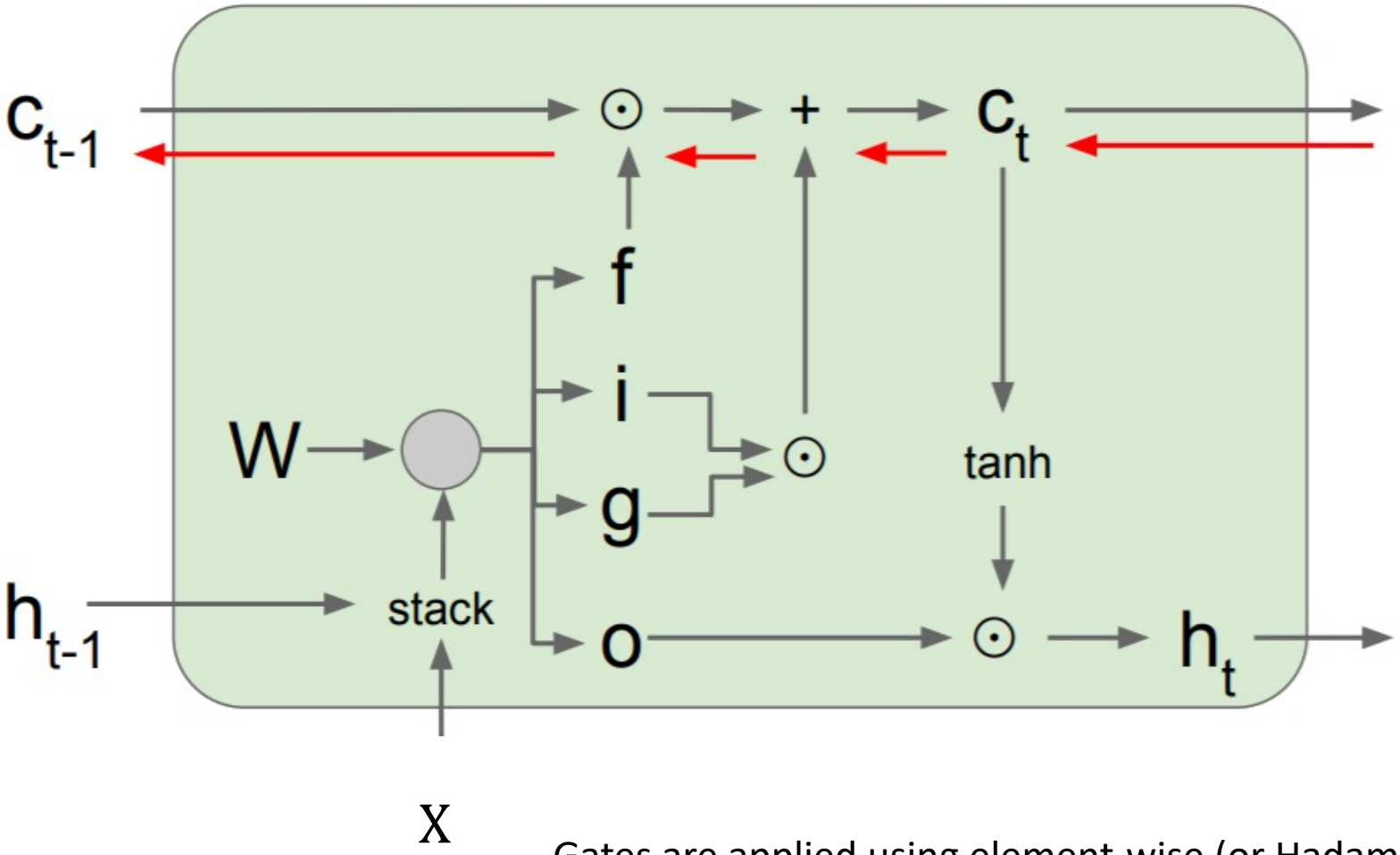
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]



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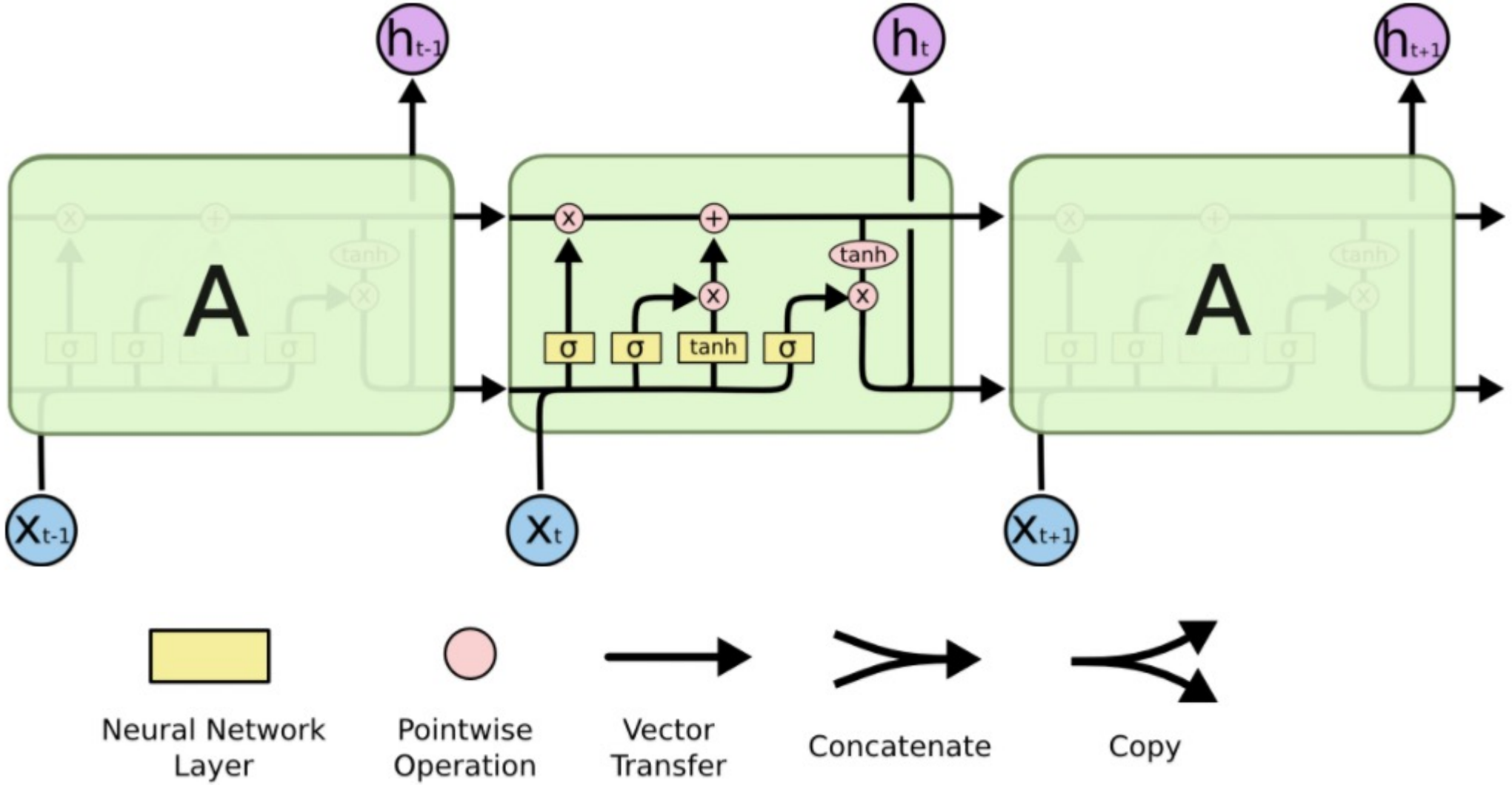
$$c_t = f \odot c_{t-1} + i \odot g$$

$$h_t = o \odot \tanh(c_t)$$

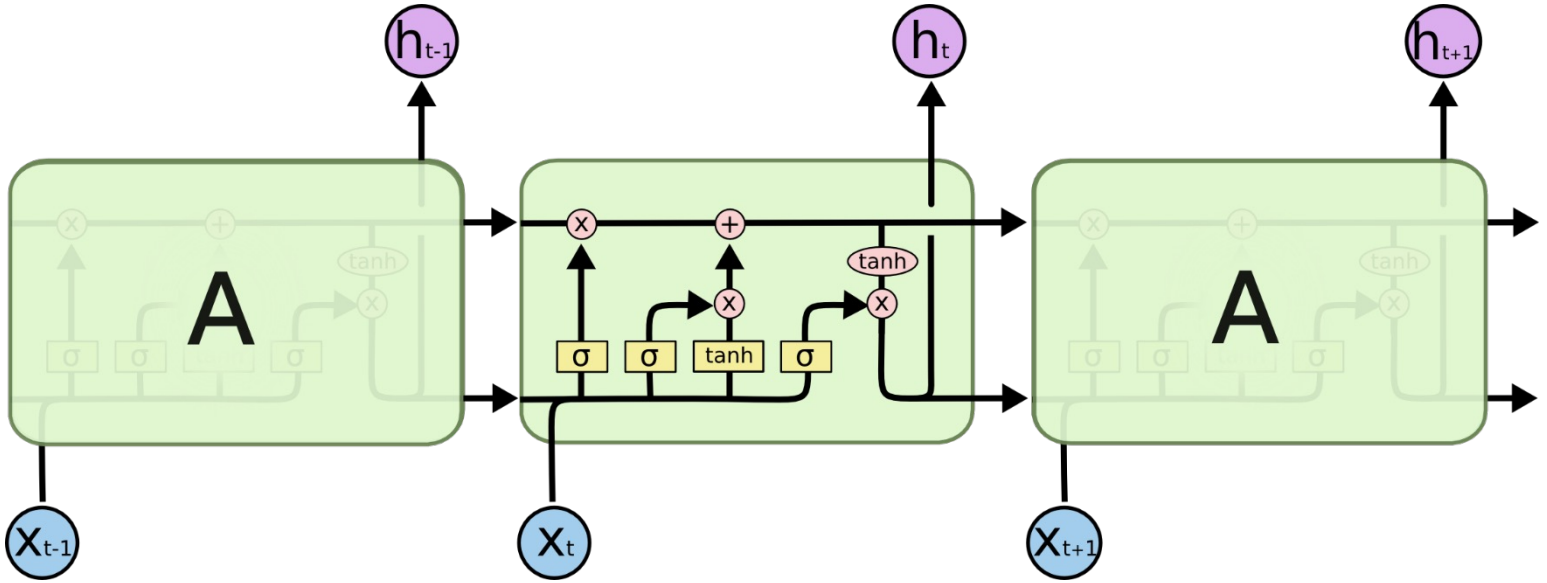
Gates are applied using element-wise (or Hadamard) product

Some visualization



Source: Colah's blog

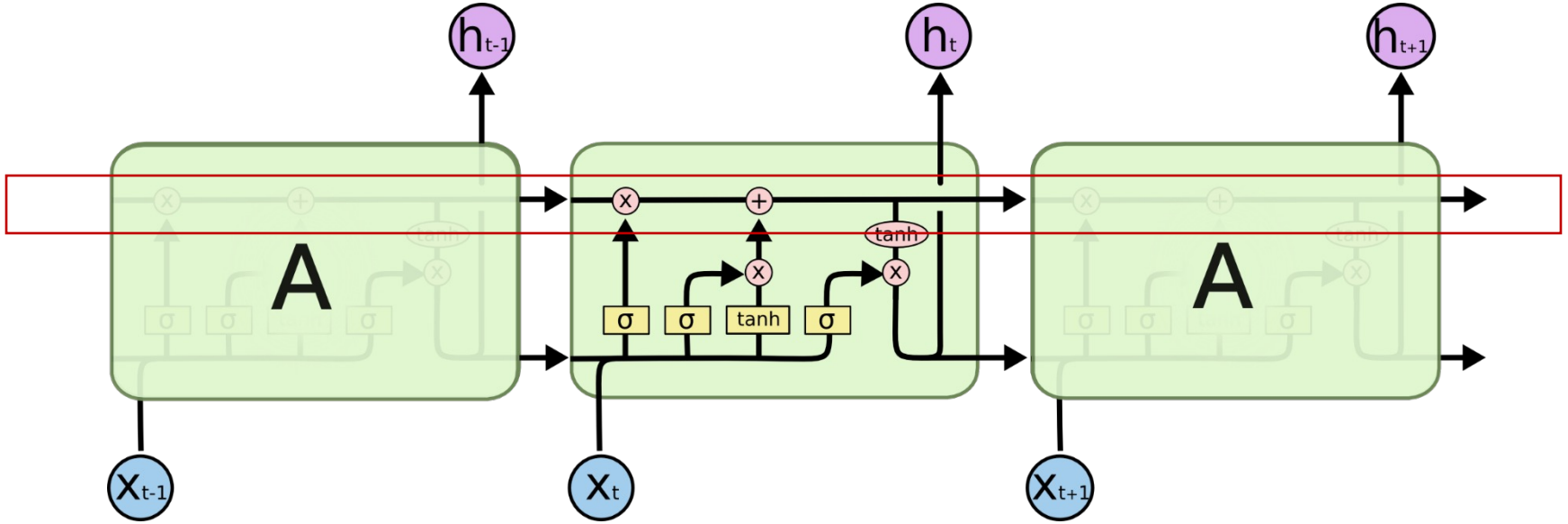
Long Short-Term Memory



- The $\sigma()$ are *multiplicative gates* that decide if something is important or not
- Remember, every line actually represents a *vector*

Source: Colah's blog

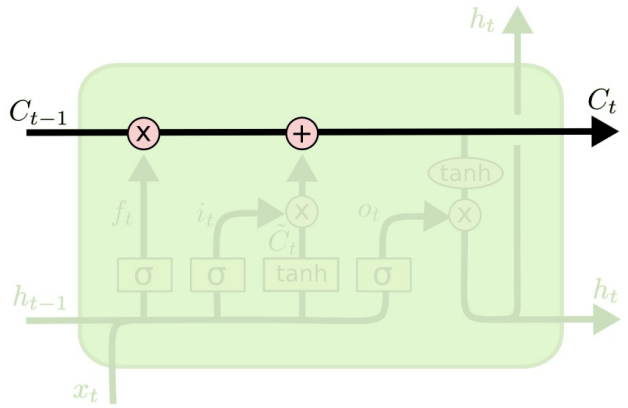
LSTM: Constant Error Carousel



- Key component: a *remembered cell state*

Source: Colah's blog

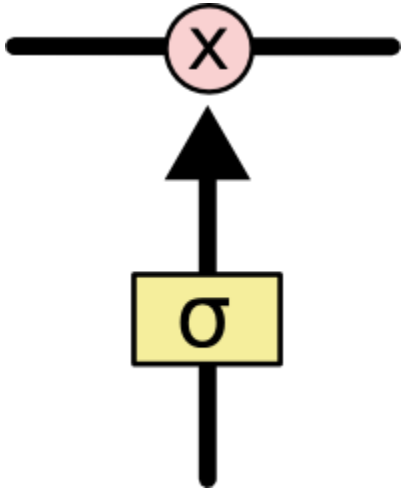
LSTM: CEC



- C_t is the linear history
- Carries information through, only affected by a gate
  - And *addition of history,* which too is gated...

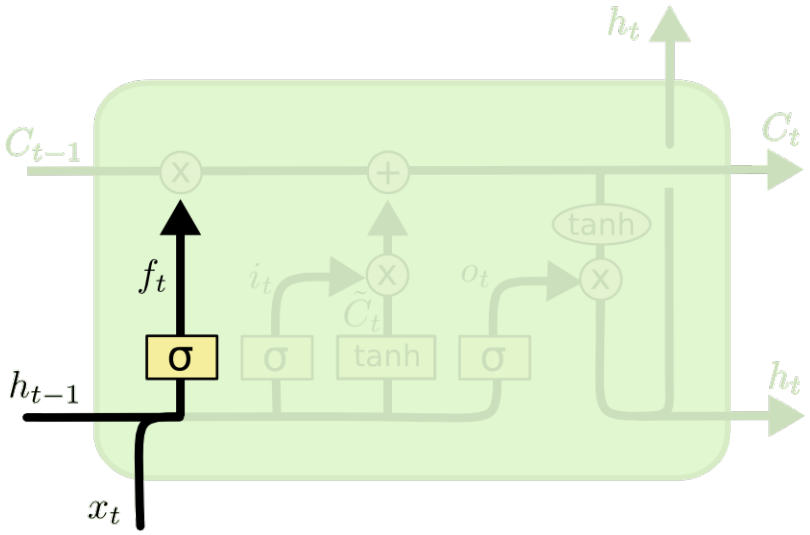
Source: Colah's blog

LSTM: Gates



- Gates are simple sigmoidal units with outputs in the range (0,1)
- Controls how much of the information is to be let through

LSTM: Forget gate

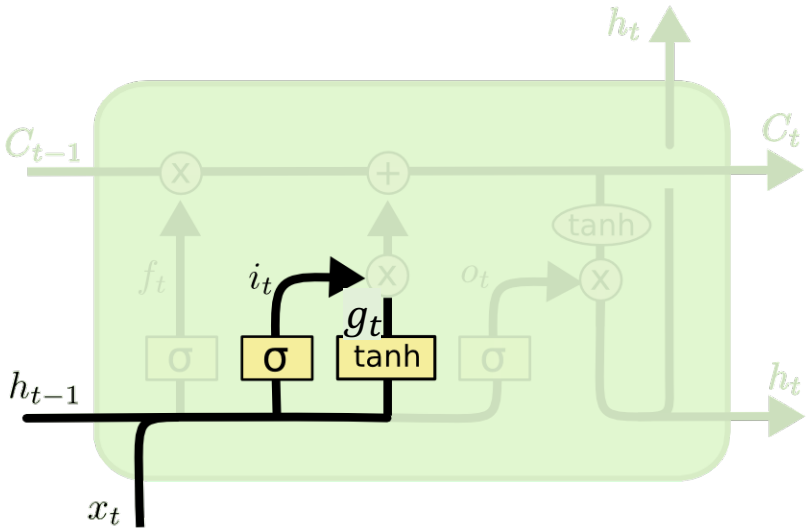


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

- The first gate determines whether to carry over the history or to forget it
  - More precisely, how much of the history to carry over
  - Also called the "forget" gate
  - Note, we're actually distinguishing between the cell memory C and the state h that is coming over time! They're related though

Source: Colah's blog

LSTM: Input gate



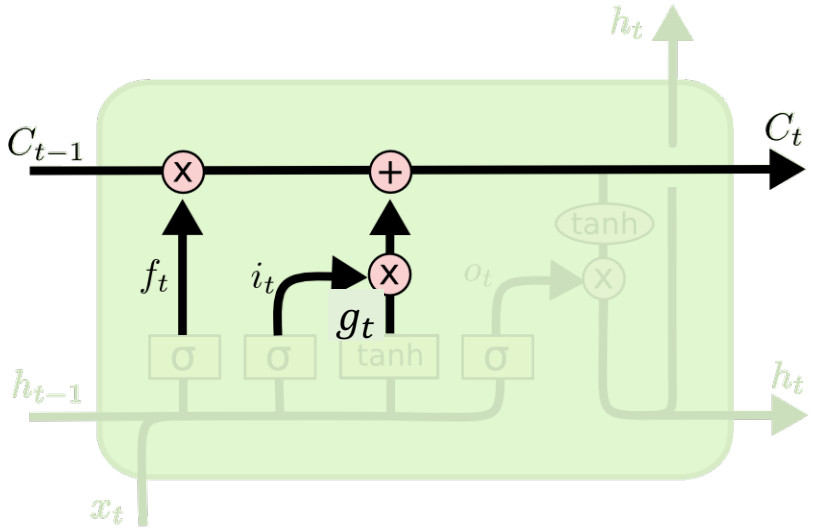
$$i_t = \sigma(W_i[h_{t-1}, x_t] + b_i)$$

$$g_t = \tanh\left(W_g[h_{t-1}, x_t] + b_g\right)$$

- The second input has two parts
  - A perceptron layer that determines if there's something new and interesting in the input
  - A gate that decides if it's worth remembering

Source: Colah's blog

LSTM: Memory cell update

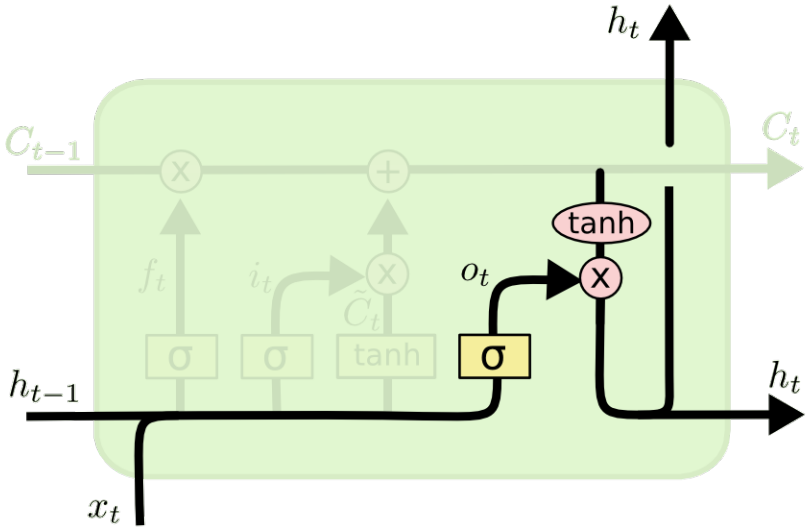


$$C_t = f_t \odot C_{t-1} + i_t \odot g_t$$

- The second input has two parts
  - A perceptron layer that determines if there's something interesting in the input
  - A gate that decides if its worth remembering
  - **If so its added to the current memory cell**

Source: Colah's blog

LSTM: Output and Output gate



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

$$h_t = o_t * \tanh\left(C_t\right)$$

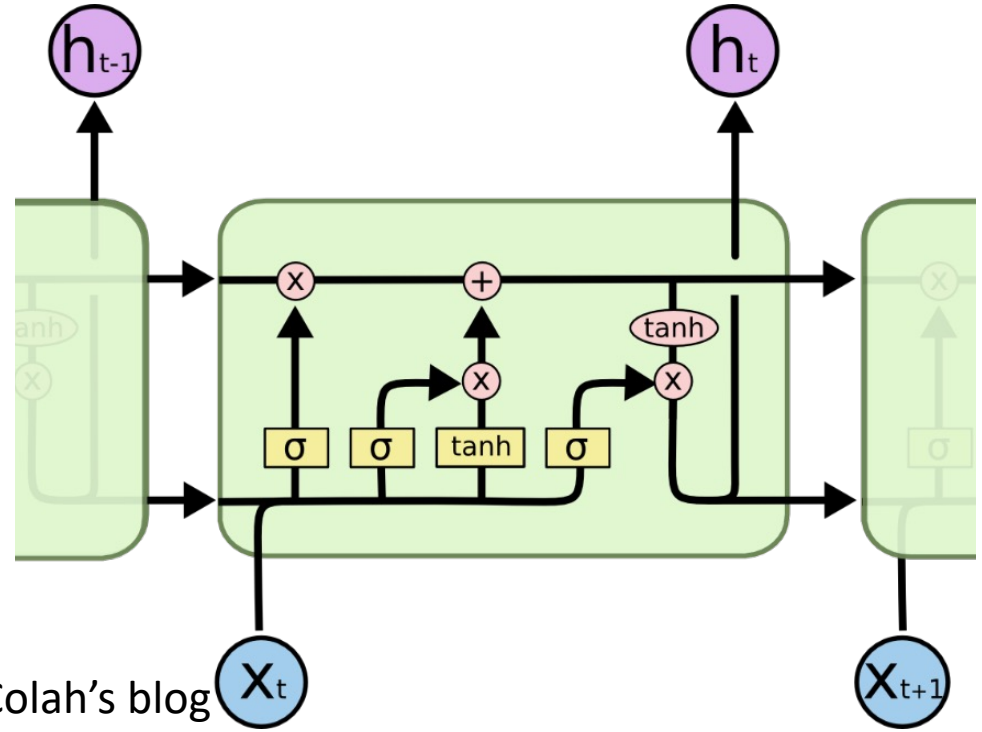
- The *output* of the cell
  - Simply compress it with tanh to make it lie between 1 and -1
    - Note that this compression no longer affects our ability to *carry* memory forward
  - Controlled by an *output* gate
    - To decide if the memory contents are worth reporting at *this* time

Source: Colah's blog

LSTM Equations

- i_t: input gate, how much of the new information will be let through the memory cell.
- f_t: forget gate, responsible for information should be thrown away from memory cell.
- o_t: output gate, how much of the information will be passed to expose to the next time step.
- g_t: self-recurrent which is equal to standard RNN

- c_t: internal memory of the memory cell
- h_t: hidden state

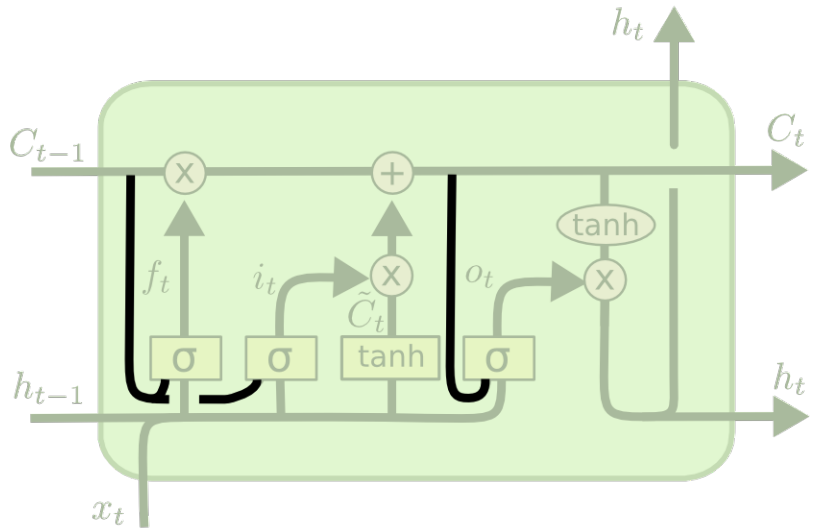


Source: Colah's blog

Long-short-term-memories (LSTMs)

- Gates
  - Input gate (current cell matter): $i_t = \sigma\left(W_i \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_i\right)$
  - Forget (gate 0, forget past): $f_t = \sigma\left(W_f \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_f\right)$
  - Output (how much cell is exposed): $o_t = \sigma\left(W_o \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_o\right)$
- Variables
  - New memory cell: $g_t = \tanh\left(W_c \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_c\right)$
  - Final memory cell: $C_t = i_t \circ g_t + f_t \circ C_{t-1}$
  - Final hidden state: $h_t = o_t \circ \tanh(C_t)$

LSTM: The "Peephole" connection

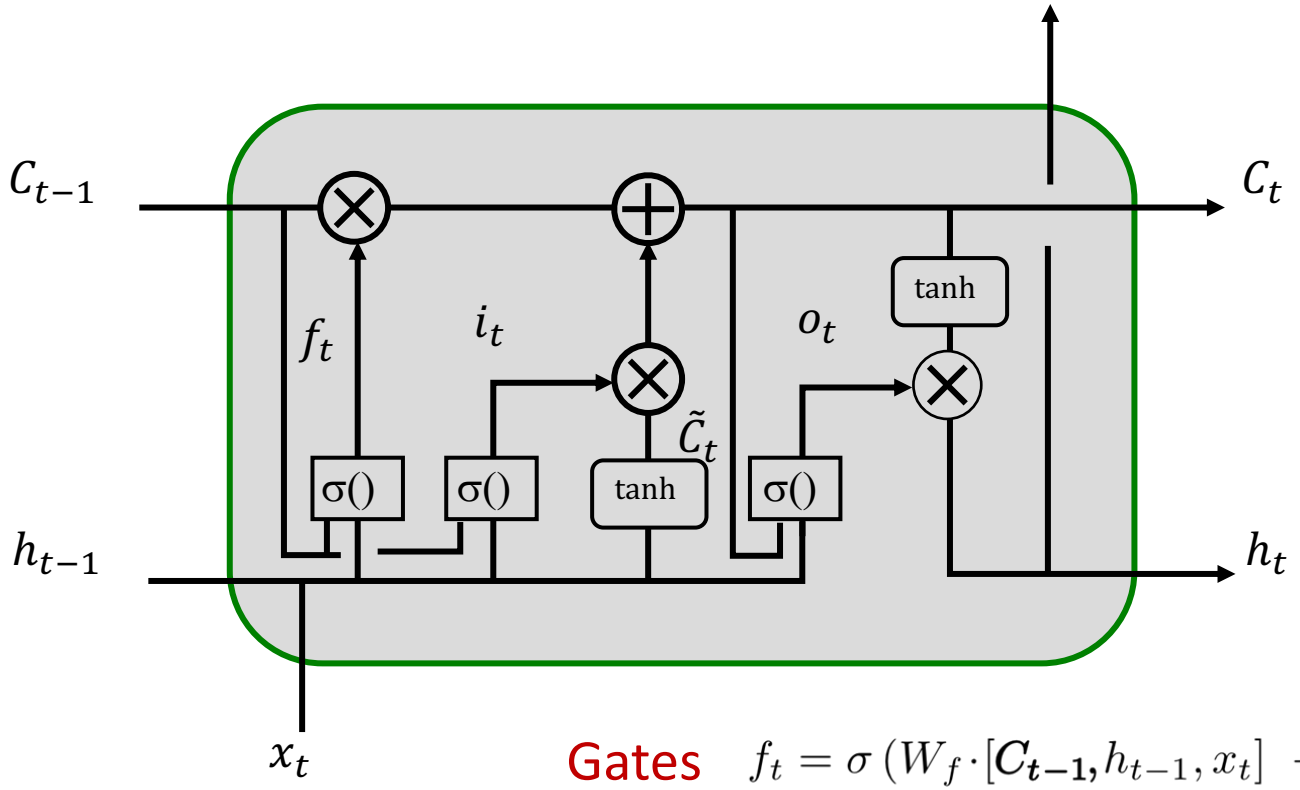


$$f_t = \sigma\left(W_f \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_f\right)$$
$$i_t = \sigma\left(W_i \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_i\right)$$
$$o_t = \sigma\left(W_o \cdot [\boldsymbol{C_t}, h_{t-1}, x_t] \; + \; b_o\right)$$

- The raw memory is informative by itself and can also be input
  - Note, we're using both C and h

Source: Colah's blog

LSTM: The "Peephole" connection



- Forward rules:

Gates

$$f_t = \sigma\left(W_f \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_f\right)$$
$$i_t = \sigma\left(W_i \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_i\right)$$
$$o_t = \sigma\left(W_o \cdot [\boldsymbol{C_t}, h_{t-1}, x_t] \; + \; b_o\right)$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

Variables

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$
$$h_t = o_t * \tanh\left(C_t\right)$$

LSTM network forward

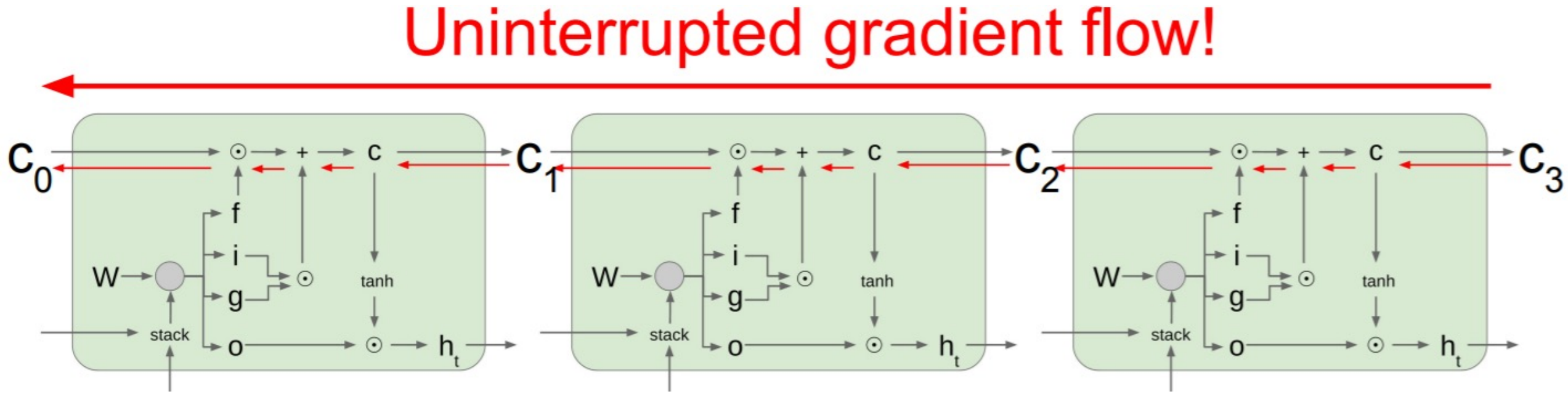
```
# Assuming h(0,*) is known and C(0,*)=0
# Assuming L hidden-state layers and an output layer
# Note: LSTM_cell is an indexed class with functions
# [W{l},b{l}] are the entire set of weights and biases
#                for the l^th hidden layer
# W_o and b_o are output layer weights and biases

for t = 1:T  # Including both ends of the index
    h(t,0) = x(t) # Vectors. Initialize hidden layer h(0) to input
    for l = 1:L  # hidden layers operate at time t
        [C(t,l),h(t,l)] = LSTM_cell(t,l).forward(C(t-1,l),h(t-1,l)
                                    ,h(t,l-1)[W{l},b{l}])
    z_o(t) = W_o h(t,L) + b_o
    Y(t) = softmax( z_o(t) )
```

LSTM cell forward

```
# Continuing from previous slide
# Note: [W,h] is a set of parameters, whose individual elements are
#       shown in red within the code.  These are passed in

# Static local variables which aren't required outside this cell
static local z_f, z_i, z_c, f, i, o, C_i
function [C_o, h_o] = LSTM_cell.forward(C,h,x, [W,h])
    z_f = W_fc C + W_fh h + W_fx x + b_f
    f = sigmoid(z_f) # forget gate

    z_i = W_ic C + W_ih h + W_ix x + b_i
    i = sigmoid(z_i) # input gate

    z_c = W_cc C + W_ch h + W_cx x + b_c
    C_i = tanh(z_c)  # Detecting input pattern

    C_o = f∘C + i∘C_i # "∘" is component-wise multiply

    z_o = W_oc C_o + W_oh h + W_ox x + b_o
    o = sigmoid(z_o) # output gate

    h_o = o∘tanh(C) # "∘" is component-wise multiply

    return C_o,h_o
```

Long Short Term Memory (LSTM)

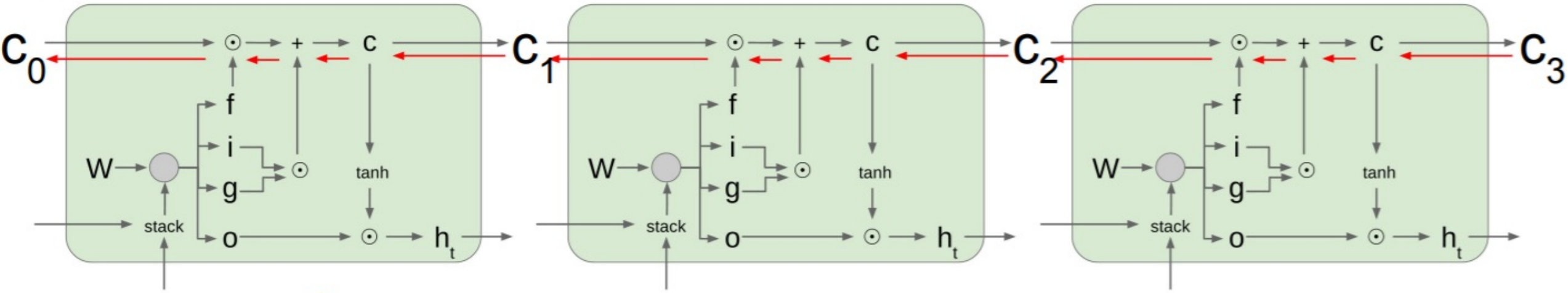
[Hochreiter et al., 1997]



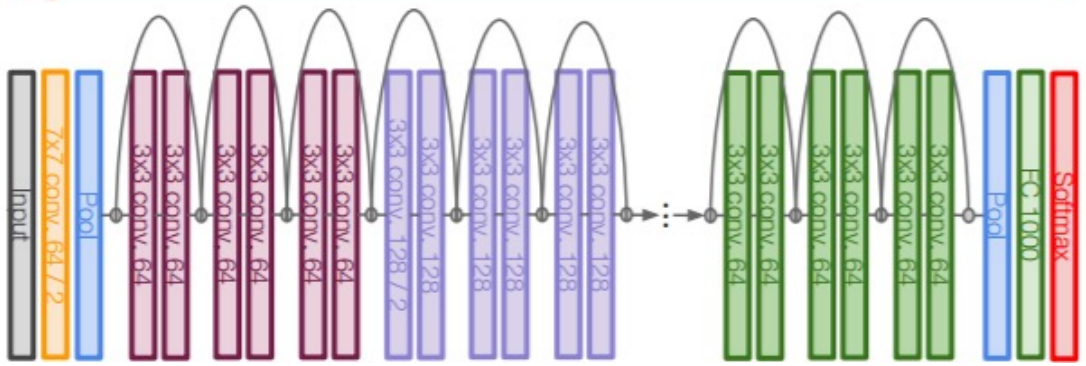
Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

Uninterrupted gradient flow!



Similar to ResNet!



In between:

Highway Networks

$$g = T(x, W_T)$$

$$y = g \odot H(x, W_H) + (1 - g) \odot x$$

Srivastava et al, "Highway Networks", ICML DL Workshop 2015

Gated Recurrent Units: Lets simplify the LSTM

- Don’t bother to separately maintain compressed and regular memories
  - Pointless computation!
- But compress it before using it to decide on the usefulness of the current input!

GRUs

- Gated Recurrent Units (GRU) introduced by Cho et al. 2014
- **Update gate**

$$z_t = \sigma\left(W_z \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_z\right)$$

- **Reset gate**

$$r_t = \sigma\left(W_r \begin{bmatrix} h_{t-1} \\ x_t \end{bmatrix} + b_r\right)$$

- **Memory**

$$\hat{h}_t = \tanh\left(W_m \begin{bmatrix} r_t \circ h_{t-1} \\ x_t \end{bmatrix} + b_m\right)$$

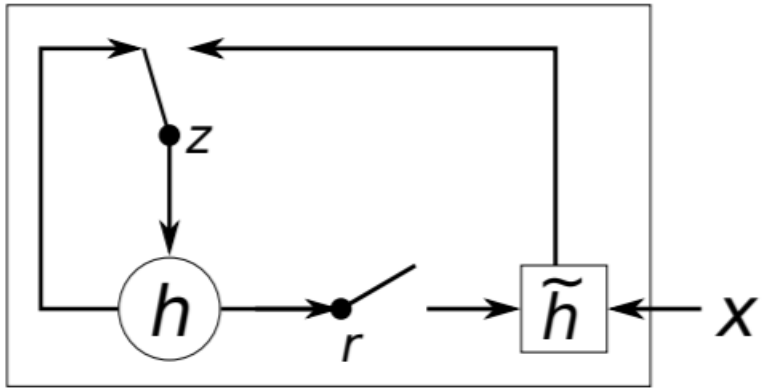
- **Final Memory**

$$h_t = z_t \circ h_{t-1} + (1 - z_t) \circ \hat{h}_t$$

If reset gate unit is ~0, then this ignores previous memory and only stores the new input

GRU intuition

- Units with long term dependencies have active update gates z
- Illustration:



This slide has been adopted from Socher lectures, cs224d, Stanford

GRU intuition

- If reset is close to 0, ignore previous hidden state
  →Allows model to drop information that is irrelevant in the future

- Update gate z controls how much of past state should matter now.
  – If z close to 0, then we can copy information in that unit through many time steps! Less vanishing gradient!

- Units with short-term dependencies often have reset gates very active

This slide has been adopted from Socher lectures, cs224d, Stanford

Other RNN Varients

GRU [*Learning phrase representations using rnn encoder-decoder for statistical machine translation*, Cho et al. 2014]

$$r_t = \sigma(W_{xr}x_t + W_{hr}h_{t-1} + b_r)$$
$$z_t = \sigma(W_{xz}x_t + W_{hz}h_{t-1} + b_z)$$
$$\tilde{h}_t = \tanh(W_{xh}x_t + W_{hh}(r_t \odot h_{t-1}) + b_h)$$
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t$$

[*LSTM: A Search Space Odyssey*, Greff et al., 2015]

[*An Empirical Exploration of Recurrent Network Architectures*, Jozefowicz et al., 2015]

MUT1:

$$\begin{aligned} z &= \text{sigm}(W_{xz}x_t + b_z) \\ r &= \text{sigm}(W_{xr}x_t + W_{hr}h_t + b_r) \\ h_{t+1} &= \tanh(W_{hh}(r \odot h_t) + \tanh(x_t) + b_h) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT2:

$$\begin{aligned} z &= \text{sigm}(W_{xz}x_t + W_{hz}h_t + b_z) \\ r &= \text{sigm}(x_t + W_{hr}h_t + b_r) \\ h_{t+1} &= \tanh(W_{hh}(r \odot h_t) + W_{xh}x_t + b_h) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT3:

$$\begin{aligned} z &= \text{sigm}(W_{xz}x_t + W_{hz}\tanh(h_t) + b_z) \\ r &= \text{sigm}(W_{xr}x_t + W_{hr}h_t + b_r) \\ h_{t+1} &= \tanh(W_{hh}(r \odot h_t) + W_{xh}x_t + b_h) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

Which of these variants is best?

- Do the differences matter?
  - Greff et al. (2015), perform comparison of popular variants, finding that they're all about the same.
  - Jozefowicz et al. (2015) tested more than ten thousand RNN architectures, finding some that worked better than LSTMs on certain tasks.

LSTM Achievements

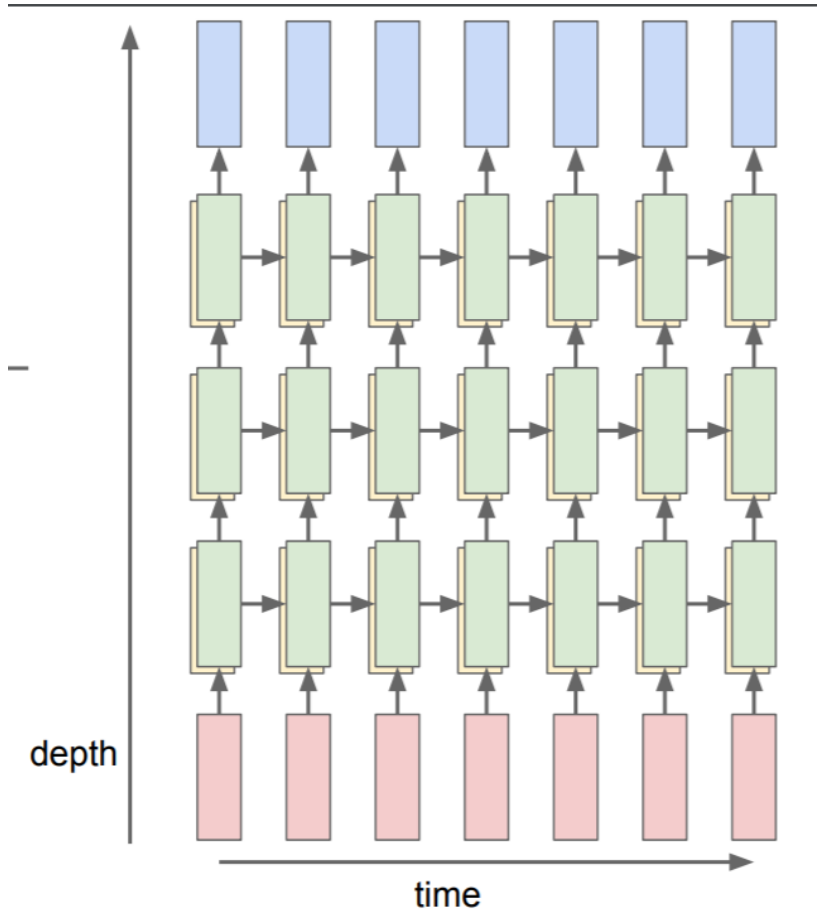
- In 2013–2015, LSTMs started achieving state-of-the-art results
  - LSTMs have essentially replaced n-grams as language models for **speech**.
  - **Image captioning** and other multi-modal tasks which were very difficult with previous methods became feasible with LSTMs.
  - **Neural MT**: broken away from plateau of SMT, especially for grammaticality (partly because of characters/subwords), but not yet industry strength.
  - Many **traditional NLP tasks** work very well with LSTMs, but not necessarily the top performers: e.g., POS tagging and NER: Choi 2016.

[Ann Copestake, Overview of LSTMs and word2vec, 2016.]
https://arxiv.org/ftp/arxiv/papers/1611/1611.00068.pdf

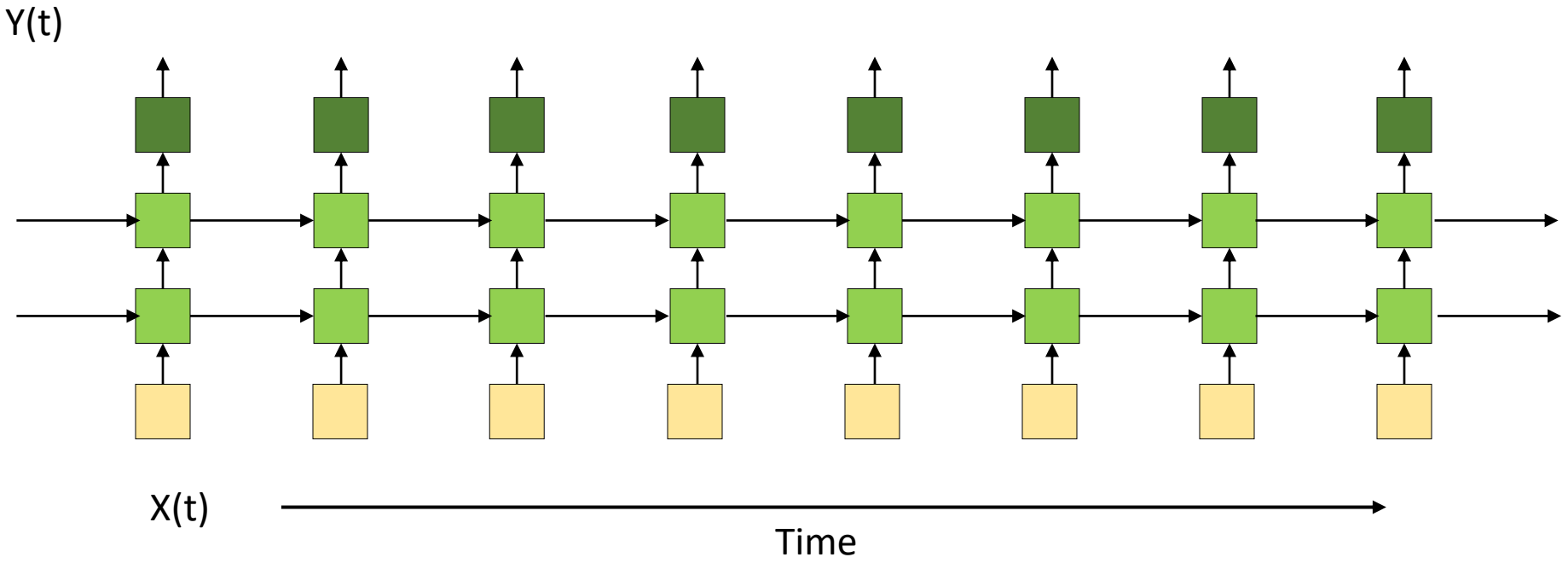
Multi-layer RNN

$$h_t^l = \tanh W^l \begin{pmatrix} h_t^{l-1} \\ h_{t-1}^l \end{pmatrix}$$

$h \in \mathbb{R}^n$ W^l $[n \times 2n]$



Multi-layer LSTM architecture



- Each green box is now an entire LSTM or GRU unit
- Also keep in mind each box is an *array* of units

Story so far

- Recurrent networks are poor at memorization
  - Memory can explode or vanish depending on the weights and activation
- They also suffer from the vanishing gradient problem during training
  - Error at any time cannot affect parameter updates in the too-distant past
  - E.g. seeing a “close bracket” cannot affect its ability to predict an “open bracket” if it happened too long ago in the input
- LSTMs are an alternative formalism where memory is made more directly dependent on the input, rather than network parameters/structure
  - Through a memory structure with no weights or activations, but instead direct switching and “increment/decrement” from pattern recognizers
  - Do not suffer from a vanishing gradient problem but ***do* suffer from *exploding* gradient issue**

RNN: Summary

- RNNs allow a lot of flexibility in architecture design
- Vanilla RNNs are simple but don’t work very well
- Backward flow of gradients in RNN can explode or vanish.
  - Exploding is controlled with gradient clipping.
  - Vanishing is controlled with additive interactions (LSTM)
- Common to use LSTM or GRU: their additive interactions improve gradient flow