Deep Learning Recurrent Networks: Stability analysis and LSTMs Fall 2024



 Iterated structures are good for analyzing time series data with short-time dependence on the past

These are "Time delay" neural nets, AKA convolutional nets





- Iterated structures are good for analyzing time series data with short-time dependence on the past
 - These are "Time delay" neural nets, AKA convnets
- 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+1bit 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
- Needs very little training data

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
- Needs a large amount of training data

RNN: The parity problem



- Trivial solution
 - Requires little training data
- Generalizes to input of any size



Some prediction and classification problems that require very large MLPs and a large amount of training data can be solved using small recurrent nets that only require small amounts of training data

- True
- False

Some problems that require large, complicated convolutional neural nets and large amounts of training data could also be solved using much smaller RNNs that only require small amounts of training data

- True
- False



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Story so far



 Recurrent structures can be trained by minimizing the divergence between the *sequence* of outputs and the *sequence* of desired outputs

Through gradient descent and backpropagation

Recap: Types of recursion





• Nothing special about a one step recursion



- Returning to an old model.. $Y(t) = f(X(t - i), i = 0 \dots K)$
- 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
- "Bounded Input Bounded Output" stability
 - This is a highly desirable characteristic

Is this BIBO?



• Will this 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_t since it carries the relevant information
 - Will assume only a single hidden layer for simplicity

Analyzing Recursion



"I'm searching for my keys."

Streetlight effect



- Easier to analyze *linear* systems
 - Will attempt to extrapolate to non-linear systems subsequently
- All activations are identity functions

$$-z_t = W_h h_{t-1} + W_x x_t, \qquad h_t = z_t$$

• $h_k = W_h h_{k-1} + W_x x_k$ - $h_{k-1} = W_h h_{k-2} + W_x x_{k-1}$ Using index "k" for time

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

Using index "k" for time

• $h_k = W_h h_{k-1} + W_x x_k$ - $h_{k-1} = W_h h_{k-2} + W_x x_{k-1}$ Using index "k" for time

- $h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k$
- $h_k = W_h^{k+1}h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + W_h^{k-2} W_x x_2 + \cdots$

Using index "k" for time

- $h_k = W_h h_{k-1} + W_x x_k$ - $h_{k-1} = W_h h_{k-2} + W_x x_{k-1}$
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- $h_k = W_h^{k+1}h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + W_h^{k-2} W_x x_2 + \cdots$

Response at k to an input x0 at time 0, when there are no other inputs and zero initial condition

Using index "k" for time • $h_k = W_h h_{k-1} + W_x x_k$ $- h_{k-1} = W_h h_{k-2} + W_x x_{k-1}$ • $h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k$ • $h_k = W_h^{k+1}h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + W_h^{k-2} W_x x_2 + \cdots$ • $h_k = H_k(h_{-1}) + H_k(x_0) + H_k(x_1) + H_k(x_2) + \cdots$ If this blows up, the entire system blows up If this does not blow up, then responses to later inputs will also not blow up!



• Sufficient to analyze the response to a single input at t = 0

– Principle of superposition in linear systems

Linear recursions

Consider simple, scalar, linear recursion (note change of notation)

$$-h(t) = wh(t - 1) + cx(t)$$
$$-h_0(t) = w^t cx(0)$$

• Response to a single input at 0



• Vector linear recursion (note change of notation)

$$-h(t) = Wh(t-1) + Cx(t)$$

- $h_0(t) = W^t C x(0)$
 - Length of response vector to a single input at 0 is $|h_0(t)|$
- We can write $W = U\Lambda U^{-1}$
 - $-Wu_i = \lambda_i u_i$
 - For any vector x' = Cx we can write
 - $x' = a_1 u_1 + a_2 u_2 + \dots + a_n u_n$
 - $Wx' = a_1\lambda_1u_1 + a_2\lambda_2u_2 + \dots + a_n\lambda_nu_n$
 - $W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \dots + a_n \lambda_n^t u_n$

$$-\lim_{t\to\infty}|W^tx'| = a_m\lambda_m^t u_m \text{ where } m = \underset{j}{\operatorname{argmax}} \lambda_j$$

• Vector linear recursion (note change of notation)

$$-h(t) = Wh(t-1) + Cx(t)$$

- $h_0(t) = W^t C x(0)$
 - Length of response vector to a single input at 0 is $|h_0(t)|$
- We can write $W = U\Lambda U^{-1}$

$$-Wu_i = \lambda_i u_i$$

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 *recurrent* weight matrix

• $W^{\iota}x^{\iota} = \overline{a_1 \lambda_1^{\iota} u_1 + a_2 \lambda_2^{\iota} u_2 + \dots + a_n \lambda_n^{\iota} u_n}$

$$-\lim_{t\to\infty}|W^tx'| = a_m\lambda_m^t u_m \text{ where } m = \underset{j}{\operatorname{argmax}} \lambda_j$$

• Vector linear recursion (note change of notation)

$$-h(t) = Wh(t-1) + Cx(t)$$

 $- h_0(t) = W^t C x(0)$

• Length of response vector to a single input at 0 is $|h_0(t)|$

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 recurrent 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..

• $W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \dots + a_n \lambda_n^t u_n$

$$-\lim_{t\to\infty}|W^tx'| = a_m\lambda_m^t u_m \text{ where } m = \underset{j}{\operatorname{argmax}} \lambda_j$$

• 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 at 0 is $|h_0(t)|$

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$$-\lim_{t\to\infty}|W^tx'| = a_m\lambda_m^t u_m \text{ where } m = \underset{j}{\operatorname{argmax}} \lambda_j$$

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

• Length of response vector to a single input at 0 is $|h_0(t)|$

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 recurrent 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..

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$$-\lim_{t\to\infty}|W^tx'| = a_m\lambda_m^t u_m \text{ where } m = \underset{j}{\operatorname{argmax}} \lambda_j$$

• Vector linear recursion (note change of notation)

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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 recurrent weight matrix

For any vector x - cx we can write

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- $W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \dots + a_n \lambda_n^t u_n$

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Vector linear recursion (note change of notation)

$$- h(t) = Wh(t-1) + Cx(t)$$

- $h_0(t) = W^t C x(0)$
 - Length of response vector to a single input at 0 is $|h_0(t)|$

• We can write
$$W = U\Lambda U^{-1} = U \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix} U^{-1}$$

$$W^{t} = U\Lambda^{t}U^{-1} = U \begin{bmatrix} \lambda_{1}^{t} & 0 & 0 \\ 0 & \lambda_{2}^{t} & 0 \\ 0 & 0 & \ddots \end{bmatrix} U^{-1} = \lambda_{1}^{t}U \begin{bmatrix} 1 & 0 & 0 \\ 0 & \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{t} & 0 \\ 0 & 0 & \ddots \end{bmatrix} U^{-1}$$

Vector linear recursion (note change of notation)

$$- h(t) = Wh(t-1) + Cx(t)$$

 $- h_0(t) = W^t C x(0) \longleftarrow$

• Length of response vector to a single input at 0 is $|h_0(t)|$

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 λ_1 of the *recurrent* weight matrix

$$W^{t} = U\Lambda^{t}U^{-1} = U \begin{bmatrix} \lambda_{1}^{t} & 0 & 0 \\ 0 & \lambda_{2}^{t} & 0 \\ 0 & 0 & \ddots \end{bmatrix} U^{-1} = \lambda_{1}^{t}U \begin{bmatrix} 1 & 0 & 0 \\ 0 & \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{t} & 0 \\ 0 & 0 & \ddots \end{bmatrix} U^{-1}$$

• Vector linear recursion (note change of notation)

 $\frac{h(t) - Wh(t - 1) + C_{x}(t)}{|\lambda_{1}| > 1 \text{ it will blow up, otherwise it will contract}}$ 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 *recurrent* weight matrix

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Linear recursions

Vector linear recursion

$$-h(t) = Wh(t-1) + Cx(t)$$

$$-h_0(t) = W^t c x(0)$$

• Response to a single input [1 1 1 1] at 0



Linear recursions

Vector linear recursion

$$-h(t) = Wh(t-1) + Cx(t)$$

$$-h_0(t) = W^t c x(0)$$

• Response to a single input [1 1 1 1] at 0


Lesson...

- In linear systems, long-term behavior depends entirely on the eigenvalues of the recurrent 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 but with the same overall trends
 - Magnitudes greater than 1 will cause the system to blow up
- The rate of blow up or vanishing depends only on the Eigen values and not on the input

With non-linear activations: Sigmoid





• Final value depends only on *b* and *w* but not *x*

With non-linear activations: Tanh



• "Remembers" x value much longer than sigmoid

With non-linear activations: RELU





• Relu blows up if w > 1, for x > 0, and "dies" for x < 0

- Unstable or useless

Scalar recurrence

Vector Process: Max eigenvalue 1.1 h(t) = f(Wh(t-1) + Cx(t) + b)**Initial x(0):** Top: [1,1,1,...], Bottom: [-1,-1,-1,...]



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Vector Process: Max eigenvalue 0.9

h(t) = f(Wh(t-1) + Cx(t) + b)

• Initial x(0): Top: [1,1,1, ...], Bottom: [−1, −1, −1, ...]



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Stability Analysis

- Formal stability analysis considers convergence of "Lyapunov" functions
 - Alternately, Routh's criterion and/or pole-zero analysis
 - Positive definite functions evaluated at h
 - Conclusions are similar: only the tanh activation gives us any reasonable behavior
 - And still has very short "memory"
- Lessons:
 - Bipolar activations (e.g. tanh) have the best memory behavior
 - Still sensitive to Eigenvalues of W and the bias
 - Best case memory is short
 - Exponential memory behavior
 - "Forgets" in exponential manner

How about deeper recursion

- Consider simple, scalar, linear recursion
 - Adding more "taps" adds more "modes" to memory in somewhat non-obvious ways



Stability Analysis

• Similar analysis of vector functions with nonlinear activations is relatively straightforward

- Linear systems: Routh's criterion

• And pole-zero analysis (involves tensors)

- On board?

- Non-linear systems: Lyapunov functions
- Conclusions do not change

Poll 2

Select all that are true about how long (how many time steps) an RNN can retain some memory of an input pattern

- It depends on the weights of the recurrent layers
- It depends on the bias of the recurrent layers
- It depends on the activation function used in the recurrent layers
- It depends on the actual input being "remembered"

Select all that are true about *what* an RNN remembers about an input pattern

- It depends on the weights of the recurrent layers
- It depends on the bias of the recurrent layers
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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 it's less than one, the response dies down very quickly
- The "memory" of the network also depends on the parameters (and activation) of the hidden units
 - Sigmoid activations saturate and the network becomes unable to retain new information
 - RELU activations blow up or vanish rapidly
 - Tanh activations are the slightly more 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 generation..
 - They can even simplify problems that are difficult for MLPs
- But the memory isn't all that great..
 Also..

The vanishing gradient problem for deep networks

- 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..

Some useful preliminary math: The problem with training deep networks



• A multilayer perceptron is a nested function

$$Y = f_N \left(W_N f_{N-1} (W_{N-1} f_{N-2} (\dots W_1 X)) \right)$$

- W_k is the weights *matrix* at the kth layer
- The *error* for *X* can be written as

$$Div(X) = D\left(f_N\left(W_N f_{N-1}(W_{N-1} f_{N-2}(..., W_1 X))\right)\right)$$

Training deep networks

• Vector derivative chain rule: for any f(Wg(X)):

$$\frac{df(Wg(X))}{dX} = \frac{df(Wg(X))}{dWg(X)} \frac{dWg(X)}{dg(X)} \frac{dg(X)}{dX}$$
Poor notation
$$\text{Let } Z = Wg(X)$$

$$\nabla_X f = \nabla_Z f. W. \nabla_X g$$

- Where
 - $-\nabla_Z f$ is the *jacobian* **matrix** of f(Z)w.r.t Z
 - Using the notation $\nabla_Z f$ instead of $J_f(z)$ for consistency



• Recall the influence diagram

- From the chain rule (right multiplying derivatives):

$$\nabla_{f_1} D = \nabla D \cdot \nabla_{z_3} f_3 \cdot W_3 \cdot \nabla_{z_2} f_2 \cdot W_2$$

Training deep networks

• For

$$Div(X) = D\left(f_N\left(W_N f_{N-1}(W_{N-1} f_{N-2}(..., W_1 X))\right)\right)$$

• We get:

$$\nabla_{f_k} Div = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \dots \nabla f_{k+1} W_{k+1}$$

- Where
 - $V_{f_k}Div$ is the gradient Div(X) of the error w.r.t the output of the kth layer of the network
 - Needed to compute the gradient of the error w.r.t W_{k-1}
 - ∇f_n is *jacobian* of f_N () w.r.t. to its current input
 - (dropping the subscript for brevity)
 - All blue terms are matrices
 - All function derivatives are w.r.t. the (entire, affine) argument of the function

Training deep networks

• For

$$Div(X) = D\left(f_N\left(W_{N-1}f_{N-1}(W_{N-2}f_{N-2}(...W_0X))\right)\right)$$

• We get:

$$\nabla_{f_k} Div = \nabla D (\nabla f_N, W_N, \nabla f_{N-1}, W_{N-1}, \dots, \nabla f_{k+1}, W_{k+1})$$

- Where
 - $\nabla_{f_k} Div$ is the gradient Div(X) of the error w.r.t the output of the kth layer of the network
 - Needed to compute the gradient of the error w.r.t W_k
 - $-\nabla f_n$ is jacobian of f_N () w.r.t. to its current input/
 - All blue terms are matrices

Lets consider these Jacobians for an RNN (or more generally for any network)

The Jacobian of the hidden layers for an RNN



- For recurrent layers with scalar activations, this will be a diagonal matrix
 - The diagonals are the derivatives of the activation function
- There is a limit on how much multiplying a vector by the Jacobian will scale it
 - Bounded by the maximum value that the derivative will take

The derivative of the hidden state activation



- Most common activation functions, such as sigmoid, tanh() and RELU have derivatives that are always less 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

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 divergence at any time is totally "forgotten"

What about the weights

$$\nabla_{f_k} Div = \nabla D. \nabla f_N . V f_{N-1} . \nabla f_{k+1} . W_{k+1}$$

- In a single-layer RNN, the weight matrices are identical
 The conclusion below holds for any deep network, though
- The chain product for $\nabla_{f_k} Div$ will
 - Expand VD along directions in which the singular values of the weight matrices are greater than 1
 - Shrink VD in directions where the singular values are less than 1
 - Repeated multiplication by the weights matrix will result in Exploding or vanishing gradients

Exploding/Vanishing gradients

 $\nabla_{f_k} Div = \nabla D. \, \nabla f_N. W_N. \, \nabla f_{N-1}. W_{N-1} \dots \nabla f_{k+1} W_{k+1}$

- Every blue term is a matrix
- **VD** is proportional to the actual error
 - Particularly for L₂ and KL divergence
- The chain product for $\nabla_{f_k} Div$ will
 - Expand VD in directions where each stage has singular values greater than 1
 - Shrink \(\nabla D\) in directions where each stage has singular values less than 1

Gradient problems in deep networks



- 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

ELU activation, Batch gradients

Output layer

backpropagation Direction of

Input layer

- 19 layer MNIST model •
 - Different activations: Exponential linear units, RELU, sigmoid, tanh
 - Each layer is 1024 units wide
 - Gradients shown at initialization
 - Will actually decrease with additional training
- Figure shows $\log |\nabla_{W_{neuron}} Div|$ where W_{neuron} is the vector of incoming weights to each neuron ٠
 - I.e. the gradient of the loss w.r.t. the entire set of weights to each neuron

RELU activation, Batch gradients





- Input layer
- 19 layer MNIST model
 - Different activations: Exponential linear units, RELU, sigmoid, tanh
 - Each layer is 1024 units wide
 - Gradients shown at initialization
 - Will actually decrease with additional training
- Figure shows $\log |\nabla_{W_{neuron}} Div|$ where W_{neuron} is the vector of incoming weights to each neuron
 - I.e. the gradient of the loss w.r.t. the entire set of weights to each neuron

Sigmoid activation, Batch gradients



Direction of

backpropagation Input layer

- 19 layer MNIST model •
 - Different activations: Exponential linear units, RELU, sigmoid, tanh
 - Each layer is 1024 units wide
 - Gradients shown at initialization
 - Will actually decrease with additional training
- Figure shows $\log |\nabla_{W_{neuron}} Div|$ where W_{neuron} is the vector of incoming weights to each neuron ٠
 - I.e. the gradient of the loss w.r.t. the entire set of weights to each neuron

Tanh activation, Batch gradients

Output layer

backpropagation Direction of

Input layer

- 19 layer MNIST model •
 - Different activations: Exponential linear units, RELU, sigmoid, tanh
 - Each layer is 1024 units wide
 - Gradients shown at initialization
 - Will actually decrease with additional training
- Figure shows $\log |\nabla_{W_{neuron}} Div|$ where W_{neuron} is the vector of incoming weights to each neuron ٠
 - I.e. the gradient of the loss w.r.t. the entire set of weights to each neuron

ELU activation, Individual instances

- 19 layer MNIST model
 - Different activations: Exponential linear units, RELU, sigmoid, tanh
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 - Gradients shown at initialization
 - Will actually decrease with additional training
- Figure shows $\log |\nabla_{W_{neuron}} Div|$ where W_{neuron} is the vector of incoming weights to each neuron
 - I.e. the gradient of the loss w.r.t. the entire set of weights to each neuron

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.

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

Recurrent nets are very deep nets



 $\nabla_{f_k} Div = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \dots \nabla f_{k+1} W_{k+1}$

- The relation between X(0) 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 = 0

Recall: Vanishing stuff..



• Stuff gets forgotten in the forward pass too

- Each weights matrix and activation can shrink components of the input



Select all that are true

- The derivatives for most parameters will become vanishingly small as we backpropagate the loss gradient through deep networks
- The derivatives for a small number of parameters will blow up and become large and unstable as we propagate the los gradient through deep networks
- The derivatives would be more stable if the recurrent weight matrices had singular values equal to 1
- The derivatives would be more stable if the recurrent activations were identity transforms (with identity Jacobian matrices)

Select all that are true of recurrent networks

- The memory of the recurrent layer is limited because the recurrent weight matrices are not unitary (with all eigen values equal to 1)
- The memory is also limited by nonlinear activation functions
- The memory would be more stable if the recurrent weight matrix were an identity matrix (i.e. a diagonal matrix with diagonal values equal to "1")
- The memory would be more stable if the recurrent activations were identity transforms (which are linear and do not scale up or shrink the output)

Poll 3

Select all that are true

- The derivatives for most parameters will become vanishingly small as we backpropagate the loss gradient through deep networks
- The derivatives for a small number of parameters will blow up and become large and unstable as we propagate the los gradient through deep networks
- The derivatives would be more stable if the recurrent weight matrices had singular values equal to 1
- The derivatives would be more stable if the recurrent activations were identity transforms (with identity Jacobian matrices)

Select all that are true of recurrent networks

- The memory of the recurrent layer is limited because the recurrent weight matrices are not unitary (with all eigen values equal to 1)
- The memory is also limited by nonlinear activation functions
- The memory would be more stable if the recurrent weight matrix were an identity matrix (i.e. a diagonal matrix with diagonal values equal to "1")
- The memory would be more stable if the recurrent activations were identity transforms (which are linear and do not scale up or shrink the output)


- 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
 - "{" → must be remembered until the closing "}" regardless of the length of the program or how many other braces are opened or closed in-between
- 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

And now we enter the domain of..



Exploding/Vanishing gradients $h = f_N \left(W_N f_{N-1} (W_{N-2} f_{N-1} (... W_1 X)) \right)$ $\nabla_{f_k} Div = \nabla D. \nabla f_N. W_N. \nabla f_{N-1}. W_{N-1} ... \nabla f_{k+1} W_{k+1}$

- The memory retention of the network depends on the behavior of the underlined terms
 - Which in turn depends on the parameters W and the activation function, rather than what it is trying to "remember"
- 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*

Exploding/Vanishing gradients $h = f_N \left(W_N f_{N-1} (W_{N-2} f_{N-1} (... W_1 X)) \right)$ $\nabla_{f_k} Div = \nabla D. \nabla f_N. W_N. \nabla f_{N-1}. W_{N-1} ... \nabla f_{k+1} W_{k+1}$

- Replace this with something that doesn't fade or blow up?
- Network that "retains" *useful* memory arbitrarily long, to be recalled on demand?
 - Input-based determination of *whether it must be remembered*
 - Retain memories until a switch based on the input flags them as ok to forget
 - Or remember less

- *Memory*(*k*) $\approx C(x_0) \cdot \sigma_1(x_1) \cdot \sigma_2(x_2) \cdot \dots \cdot \sigma_k(x_k)$



- History is carried through uncompressed
 - No weights, no nonlinearities
 - Only scaling is through the σ "gating" term that captures other triggers
 - E.g. "Have I seen Pattern2"?



 Actual non-linear work is done by other portions of the network

Neurons that compute the workable state from the memory

Time



• The gate σ depends on current input, current hidden state...



• The gate σ depends on current input, current hidden state... and other stuff...



- The gate σ depends on current input, current hidden state... and other stuff...
- Including, obviously, what is currently in raw memory

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/

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

Long Short-Term Memory



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

LSTM: Constant Error Carousel



• Key component: a *remembered cell state*

LSTM: CEC



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

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

LSTM: Input gate



$$i_t = \sigma \left(W_i \cdot [h_{t-1}, x_t] + b_i \right)$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

- 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 its worth remembering

LSTM: Memory cell update



- 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

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

LSTM: The "Peephole" Connection



$$f_{t} = \sigma \left(W_{f} \cdot [C_{t-1}, h_{t-1}, x_{t}] + b_{f} \right)$$

$$i_{t} = \sigma \left(W_{i} \cdot [C_{t-1}, h_{t-1}, x_{t}] + b_{i} \right)$$

$$o_{t} = \sigma \left(W_{o} \cdot [C_{t}, h_{t-1}, x_{t}] + b_{o} \right)$$

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

The complete LSTM unit



• With input, output, and forget gates and the peephole connection..



Select all that are true about LSTMs

- LSTMs "stabilize" the memory by eliminating the problematic recurrent weights and activations
- They update the memory based on patterns detected in the input and the current context of what they already remember
- In the absence of external cues, they can "remember" a pattern forever
- LSTM are suited to building pattern analyzers requiring long-term memory, e.g. code parsers that can verify if an opened brace has been properly closed



Select all that are true about LSTMs

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• Forward rules:

Gates

$$f_{t} = \sigma \left(W_{f} \cdot [C_{t-1}, h_{t-1}, x_{t}] + b_{f} \right)$$

$$i_{t} = \sigma \left(W_{i} \cdot [C_{t-1}, h_{t-1}, x_{t}] + b_{i} \right)$$

$$o_{t} = \sigma \left(W_{o} \cdot [C_{t}, h_{t-1}, x_{t}] + b_{o} \right)$$

Variables

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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



• Forward rules:

LSTM Equations

- *i*: input gate, how much of the new information will be let through the memory cell.
- *f*: forget gate, responsible for information should be thrown away from memory cell.
- *o*: output gate, how much of the information will be passed to expose to the next time step.
- g: self-recurrent which is equal to standard RNN
- c_t : internal memory of the memory cell
- *s_t*: hidden state
- y: final output

•
$$i = \sigma(x_t U^i + s_{t-1} W^i)$$

•
$$f = \sigma \left(x_t U^f + s_{t-1} W^f \right)$$

•
$$o = \sigma(x_t U^o + s_{t-1} W^o)$$

•
$$g = \tanh(x_t U^g + s_{t-1} W^g)$$

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

•
$$s_t = \tanh(c_t) \circ o$$

•
$$y = softmax(Vs_t)$$



LSTM Memory Cell

Notes on the pseudocode

Class LSTM_cell

- We will assume an object-oriented program
- Each LSTM unit is assumed to be an "LSTM cell"
- There's a new copy of the LSTM cell at each time, at each layer
- LSTM cells retain local variables that are not relevant to the computation outside the cell
 - These are static and retain their value once computed, unless overwritten

LSTM cell (single unit) Definitions

```
# Input:
#
    C : previous value of CEC
#
    h : previous hidden state value ("output" of cell)
#
     x: Current input
# [W,b]: The set of all model parameters for the cell
#
       These include all weights and biases
# Output
#
    C : Next value of CEC
#
  h : Next value of h
# In the function: sigmoid(x) = 1/(1+\exp(-x))
#
                    performed component-wise
```

LSTM cell forward



LSTM network forward

Assuming h(-1,*) is known and C(-1,*)=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 lth hidden layer
W_o and b_o are output layer weights and biases

Training the LSTM

- Identical to training regular RNNs with one difference
 - Commonality: Define a sequence divergence and backpropagate its derivative through time
- Difference: Instead of backpropagating gradients through an RNN unit, we will backpropagate through an LSTM cell



 $\nabla_{C_t} Div =$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ o_t \circ tanh'(.)$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{Co})$



$$\begin{split} \nabla_{C_t} Div &= \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{Co}) + \\ \nabla_{C_{t+1}} Div \circ f_{t+1} + \end{split}$$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.)W_{Co}) +$ $\nabla_{C_{t+1}} Div \circ (f_{t+1} + C_t \circ \sigma'(.)W_{Cf})$


 $\begin{aligned} \nabla_{C_t} Div &= \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{Co}) + \\ \nabla_{C_{t+1}} Div \circ \left(f_{t+1} + C_t \circ \sigma'(.) W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{Ci} \dots \right) \end{aligned}$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.)W_{Co}) +$ $\nabla_{C_{t+1}} Div \circ \left(f_{t+1} + C_t \circ \sigma'(.)W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{Ci} \dots \right)$

 $\nabla_{h_t} Div = \nabla_{z_t} Div \nabla_{h_t} z_t$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.)W_{Co}) + \\ \nabla_{C_{t+1}} Div \circ (f_{t+1} + C_t \circ \sigma'(.)W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{Ci} \dots)$

 $\nabla_{h_t} Div = \nabla_{Z_t} Div \nabla_{h_t} Z_t + \nabla_{C_{t+1}} Div \circ C_t \circ \sigma'(.) W_{hf}$



 $\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.)W_{Co}) + \nabla_{C_{t+1}} Div \circ (f_{t+1} + C_t \circ \sigma'(.)W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{Ci} \dots)$

 $\nabla_{h_t} Div = \nabla_{Z_t} Div \nabla_{h_t} Z_t + \nabla_{C_{t+1}} Div \circ \left(C_t \circ \sigma'(.) W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{hi}\right)$



 $\begin{aligned} \nabla_{C_t} Div &= \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{Co}) + \\ \nabla_{C_{t+1}} Div \circ \left(f_{t+1} + C_t \circ \sigma'(.) W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{Ci} \dots \right) \end{aligned}$

$$\nabla_{h_t} Div = \nabla_{Z_t} Div \nabla_{h_t} Z_t + \nabla_{C_{t+1}} Div \circ \left(C_t \circ \sigma'(.) W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{hi}\right) + \nabla_{C_{t+1}} Div \circ i_{t+1} \circ tanh'(.) W_{hi}$$



 $\begin{aligned} \nabla_{C_t} Div &= \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{Co}) + \\ \nabla_{C_{t+1}} Div \circ \left(f_{t+1} + C_t \circ \sigma'(.) W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{Ci} \dots \right) \end{aligned}$

$$\nabla_{h_t} Div = \nabla_{Z_t} Div \nabla_{h_t} Z_t + \nabla_{C_{t+1}} Div \circ \left(C_t \circ \sigma'(.) W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{hi}\right) + \nabla_{C_{t+1}} Div \circ o_{t+1} \circ tanh'(.) W_{hi} + \nabla_{h_{t+1}} Div \circ tanh(.) \circ \sigma'(.) W_{ho}$$



$$\nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.)W_{Co}) + \nabla_{C_{t+1}} Div \circ (f_{t+1} + C_t \circ \sigma'(.)W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{Ci} \dots)$$

$$\nabla_{h_t} Div = \nabla_{Z_t} Div \nabla_{h_t} Z_t + \nabla_{C_{t+1}} Div \circ \left(C_t \circ \sigma'(.) W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{hi}\right) + \nabla_{C_{t+1}} Div \circ o_{t+1} \circ tanh'(.) W_{hi} + \nabla_{h_{t+1}} Div \circ tanh(.) \circ \sigma'(.) W_{ho}$$

Notes on the backward pseudocode

Class LSTM_cell

- We first provide backward computation *within a cell*
- For the backward code, we will assume the static variables computed during the forward are still available
- The following slides first show the forward code for reference
- Subsequently we will give you the backward, and explicitly indicate which of the forward equations each backward equation refers to
 - The backward code for a cell is long (but simple) and extends over multiple slides

LSTM cell forward (for reference)



LSTM cell backward

```
# Static local variables carried over from forward
static local z_f, z_i, z_c, z_o, f, i, o, C_i
function [dC,dh,dx,d[W, b]]=LSTM cell.backward(dC, dh, C, h, C, h, x, [W,b])
     # First invert h_o = o \circ tanh(C)
     do = dh<sub>o</sub> \circ tanh (C<sub>o</sub>)<sup>T</sup>
     d \tanh C_o = dh_o \circ o
     dC_{o} += dtanhC_{o} \circ (1-tanh^{2}(C_{o}))^{T} # (1-tanh^{2}) is the derivative of tanh
     # Next invert o = sigmoid(z_o)
     dz_{o} = do \circ sigmoid(z_{o})^{T} \circ (1-sigmoid(z_{o}))^{T} # do x derivative of sigmoid(z_{o})
     # Next invert z_0 = W_{00}C_0 + W_{0h}h + W_{0x}x + b_0
     dC_{o} += dz_{o}W_{oc} \# Note - this is a regular matrix multiply
     dh = dz_0 W_{ob}
     dx = dz W_{ox}
     dW_{oc} = C_{o}dz_{o} \# Note - this multiplies a column vector by a row vector
     dW_{oh} = h dz_{o}
     dW_{ox} = x dz_{o}
     db_0 = dz_0
     # Next invert C_0 = f \circ C + i \circ C_1
     dC = dC_0 \circ f
     dC_i = dC_o \circ i
     di = dC_0 \circ C_i
     df = dC_0 \circ C
```

LSTM cell backward (continued)

```
# Next invert C_i = tanh(z_c)
dz_c = dC_i \circ (1-tanh^2(z_c))^T
# Next invert z_c = W_{cc}C + W_{ch}h + W_{cx}x + b_c
dC += dz_{c}W_{cc}
dh += dz_{c} W_{ch}
dx += dz_{c} W_{cx}
dW_{cc} = C dz_{c}
dW_{ch} = h dz_{c}
dW_{cx} = x dz_{c}
db_c = dz_c
# Next invert i = sigmoid(z;)
dz_i = di \circ sigmoid(z_i)^T \circ (1-sigmoid(z_i))^T
# Next invert z_i = W_{ic}C + W_{ib}h + W_{iv}x + b_i
dC += dz_i W_{ic}
dh += dz_i W_{ih}
dx += dz, W_{ix}
dW_{ic} = C dz_{i}
dW_{ih} = h dz_i
dW_{ix} = x dz_i
db_i = dz_i
```

LSTM cell backward (continued)

Next invert f = sigmoid(z_f) d z_f = df \circ sigmoid(z_f)^T \circ (1-sigmoid(z_f))^T

Finally invert $z_f = W_{fc}C + W_{fh}h + W_{fx}x + b_f$ dC += $dz_f W_{fc}$ dh += $dz_f W_{fh}$ dx += $dz_f W_{fx}$

$$dW_{fc} = C dz_{f}$$
$$dW_{fh} = h dz_{f}$$
$$dW_{fx} = x dz_{f}$$
$$dW_{fx} = dz_{f}$$

return dC, dh, dx, d[W, b]
d[W,b] is shorthand for the complete set
 of weight and bias derivatives

LSTM network forward (for reference)

Assuming h(-1,*) is known and C(-1,*)=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 1th hidden layer
W_o and b_o are output layer weights and biases

LSTM network backward

```
# Assuming h(-1,*) is known and C(-1,*)=0
# Assuming L hidden-state layers and an output layer
# Note: LSTM_cell is an indexed class with functions
# [W{1},b{1}] are the entire set of weights and biases
# for the 1<sup>th</sup> hidden layer
# W<sub>o</sub> and b<sub>o</sub> are output layer weights and biases
# Y is the output of the network
# Assuming dW<sub>o</sub> and db<sub>o</sub> and d[W{1} b{1}] (for all 1) are
# all initialized to 0 at the start of the computation
```

```
for t = T-1:0 # Including both ends of the index
dz_o = dY(t) o Softmax_Jacobian(zo(t))
dW_o += h(t,L) dz_o(t)
dh(t,L) = dz_o(t)W_o
db_o += dz_o(t)
for l = L-1:0
```

```
[dC(t,l),dh(t,l),dx(t,l),d[W, b]] = ...
... LSTM_cell(t,l).backward(...
... dC(t+1,l), dh(t+1,l)+dx(t,l+1), C(t-1,l), h(t-1,l), ...
... C(t,l), h(t,l), h(t,l-1), [W(l),b(l)])
d[W{l} b{l}] += d[W,b]
```

Gated Recurrent Units: Lets simplify the LSTM



$$z_t = \sigma \left(W_z \cdot [h_{t-1}, x_t] \right)$$
$$r_t = \sigma \left(W_r \cdot [h_{t-1}, x_t] \right)$$
$$\tilde{h}_t = \tanh \left(W \cdot [r_t * h_{t-1}, x_t] \right)$$
$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

 Simplified LSTM which addresses some of your concerns of *why*

Gated Recurrent Units: Lets simplify the LSTM



$$z_t = \sigma \left(W_z \cdot [h_{t-1}, x_t] \right)$$

$$r_t = \sigma \left(W_r \cdot [h_{t-1}, x_t] \right)$$

$$\tilde{h}_t = \tanh \left(W \cdot [r_t * h_{t-1}, x_t] \right)$$

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

- Combine forget and input gates
 - If new input is to be remembered, then this means old memory is to be forgotten
 - Why compute twice?

Gated Recurrent Units: Lets simplify the LSTM



$$z_t = \sigma \left(W_z \cdot [h_{t-1}, x_t] \right)$$
$$r_t = \sigma \left(W_r \cdot [h_{t-1}, x_t] \right)$$
$$\tilde{h}_t = \tanh \left(W \cdot [r_t * h_{t-1}, x_t] \right)$$
$$h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$$

- Don't bother to separately maintain compressed and regular memories
 - Pointless computation!
 - Redundant representation

LSTM architectures example



- Each green box is now a (layer of) LSTM or GRU cell(s)
 - Keep in mind each box is an *array* of units
 - For LSTMs the horizontal arrows carry both C(t) and h(t)

Bidirectional LSTM



- Like the BRNN, but now the hidden nodes are LSTM units.
 - Or layers of LSTM 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 "Constant Error Carousel" 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

Significant issues

- The Divergence
- How to use these nets..
- This and more in next couple of classes..