Deep Learning
Recurrent Networks:
Stability analysis and LSTMs
Story so far

- **Iterated structures** are good for analyzing time series data with short-time dependence on the past
  - These are “*Time delay*” neural nets, AKA *convnets*
Story so far

• 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+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

• 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
Poll 1

• @920, @921

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
Poll 1

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
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
The behavior of recurrence..

- Returning to an old model..
  \[ Y(t) = f(X(t - i), i = 0 \ldots K) \]
- When will the output “blow up”?
“BIBO” Stability

• 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
The streetlight effect is a type of observational bias where people only look for whatever they are searching by looking where it is easiest.

“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
  - \( z_t = W_h h_{t-1} + W_x x_t, \quad h_t = z_t \)
Linear systems

- \( h_k = W_h h_{k-1} + W_x x_k \)
- \( h_{k-1} = W_h h_{k-2} + W_x x_{k-1} \)

Using index “k” for time
Linear systems

• \( h_k = W_h h_{k-1} + W_x x_k \)

• \( h_{k-1} = W_h h_{k-2} + W_x x_{k-1} \)

• \( h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k \)

Using index “k” for time
Linear systems

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

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

Using index “k” for time

Response to an input $x_0$ at time 0, when there are no other inputs and zero initial condition
Linear systems

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

Using index “k” for time
Linear systems

- \( h_k = W_h h_{k-1} + W_x x_k \)
  - \( h_{k-1} = W_h h_{k-2} + W_x x_{k-1} \)
- \( h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k \)
- \( h_k = W_h^{k+1} h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + W_h^{k-2} W_x x_2 + \cdots \)
- \( h_k = H_k(h_{-1}) + H_k(x_0) + H_k(x_1) + H_k(x_2) + \cdots \)
  - \( = h_{-1} H_k(1_{-1}) + x_0 H_k(1_0) + x_1 H_k(1_1) + x_2 H_k(1_2) + \cdots \)

- Where \( H_k(1_t) \) is the hidden response at time \( k \) when the input is \([0 \ 0 \ 0 \ \ldots \ 1 \ 0 \ \ldots \ 0]\) (where the 1 occurs in the \( t \)-th position) with 0 initial condition
  - The initial condition may be viewed as an input of \( h_{-1} \) at \( t = -1 \)
Linear systems

- \( h_k = W_h h_{k-1} + W_x x_k \)

- \( h_{k-1} = W_h h_{k-2} + W_x x_{k-1} \)

- \( h_k = W_h^2 h_{k-2} + W_h W_x x_{k-1} + W_x x_k \)

- \( h_k = W_h^{k+1} h_{-1} + W_h^k W_x x_0 + W_h^{k-1} W_x x_1 + W_h^{k-2} W_x x_2 + \cdots \)

- \( h_k = H_k(h_{-1}) + H_k(x_0) + H_k(x_1) + H_k(x_2) + \cdots \)

- \( = h_{-1} H_k(1_{-1}) + x_0 H_k(1_0) + x_1 H_k(1_1) + x_2 H_k(1_2) + \cdots \)

Using index ‘k’ for time

For vector systems:

\[
\begin{bmatrix}
H_k(1_{-1}) h_{-1} + H_k(1_0) x_0 + H_k(1_1) x_1 + H_k(1_2) x_2 + \cdots \\
0 & 0 & \ldots & 1 & 0 & \ldots & 0
\end{bmatrix}
\]

(where the 1 occurs in the \( t \)-th position) with 0 initial condition

- The initial condition may be viewed as an input of \( h_{-1} \) at \( t = -1 \)
Streetlight effect

- Sufficient to analyze the response to a single input at $t = 0$
  
  – Principle of superposition in linear systems:
  
  $$h_k = h_{-1}H_k(1_{-1}) + x_0H_k(1_0) + x_1H_k(1_1) + x_2H_k(1_2) + \cdots$$
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
Linear recursions: Vector version

- Vector linear recursion (note change of notation)
  - \( h(t) = Wh(t - 1) + Cx(t) \)
  - \( h_0(t) = W^tCx(0) \)
    - Length of response vector to a single input at 0 is \( |h_0(t)| \)

- We can write \( W = UΛU^{-1} \)
  - \( Wu_i = λ_i u_i \)
  - For any vector \( x' = Cx \) we can write
    - \( x' = a_1 u_1 + a_2 u_2 + \cdots + a_n u_n \)
    - \( Wx' = a_1 λ_1 u_1 + a_2 λ_2 u_2 + \cdots + a_n λ_n u_n \)
    - \( W^tx' = a_1 λ_1^t u_1 + a_2 λ_2^t u_2 + \cdots + a_n λ_n^t u_n \)
  - \( \lim_{t→∞}|W^tx'| = a_m λ_m^t u_m \) where \( m = \arg\max_j λ_j \)
Linear recursions: Vector version

• Vector linear recursion (note change of notation)
  
  – \( h(t) = Wh(t - 1) + Cx(t) \)
  
  – \( h_0(t) = W^t Cx(0) \)

  • 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 eigenvalue of the recurrent weight matrix

• \( W^t x = a_1 \lambda_1 u_1 + a_2 \lambda_2 u_2 + \cdots + a_n \lambda_n u_n \)
  
  – \( \lim_{t \to \infty} |W^t x'| = a_m \lambda_m^t u_m \) where \( m = \arg \max \lambda_j \)
Linear recursions: Vector version

- Vector linear recursion (note change of notation)
  
  - \( h(t) = Wh(t - 1) + Cx(t) \)
  
  - \( h_0(t) = W^tCx(0) \)

- 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..

- \( W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \cdots + a_n \lambda_n^t u_n \)

- \( \lim_{t \to \infty} |W^t x'| = a_m \lambda_m^t u_m \) where \( m = \arg\max_j \lambda_j \)
Linear recursions: Vector version

- Vector linear recursion (note change of notation)
  \[ h(t) = W h(t-1) + f_0(t) \]
  
  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

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- \( W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \cdots + a_n \lambda_n^t u_n \)

\[ \lim_{t \to \infty} |W^t x'| = a_m \lambda_m^t u_m \quad \text{where} \quad m = \arg \max_j \lambda_j \]
Linear recursions: Vector version

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

\[ l(t) = Wl(t-1) + f(t) \]

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 \( |h_n(t)| \)

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..

\[ W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \cdots + a_n \lambda_n^t u_n \]

\[ - \lim_{t \to \infty} |W^t x'| = a_m \lambda_m^t u_m \text{ where } m = \text{argmax}_{j} \lambda_j \]
Linear recursions: Vector version

- Vector linear recursion (note change of notation)
  \[ h(t) = W h(t-1) + \beta(t) \]

If \( |\lambda_{\text{max}}| > 1 \) 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.

- For any vector \( x' = c \lambda \) we can write
  - \( x' = a_1 u_1 + a_2 u_2 + \cdots + a_n u_n \)
  - \( W x' = a_1 \lambda_1 u_1 + a_2 \lambda_2 u_2 + \cdots + a_n \lambda_n u_n \)
  - \( W^t x' = a_1 \lambda_1^t u_1 + a_2 \lambda_2^t u_2 + \cdots + a_n \lambda_n^t u_n \)

- \( \lim_{t \to \infty} |W^t x'| = a_m \lambda_m^t u_m \) where \( m = \arg \max_j \lambda_j \)
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

\[ \lambda_{max} = 0.9 \]
\[ |\lambda_{max}| = 1.1 \]
\[ |\lambda_{max}| = 1 \]
\[ \lambda_{max} = 1 \]
Linear recursions

- Vector linear recursion
  \[ h(t) = Wh(t - 1) + Cx(t) \]
  \[ h_0(t) = W^t cx(0) \]
- Response to a single input \([1 1 1 1]\) at 0

Complex Eigenvalues

<table>
<thead>
<tr>
<th>(\lambda_{\text{max}})</th>
<th>(\lambda_{2\text{nd}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.9</td>
<td>0.5</td>
</tr>
<tr>
<td>1.1</td>
<td>0.1</td>
</tr>
<tr>
<td>1.1</td>
<td>1.0</td>
</tr>
</tbody>
</table>
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

\[ h(t) = \text{sigmoid}(wh(t - 1) + cx(t) + b) \]

- Scalar recurrence with sigmoid activation
- Final value depends only on \( b \) and \( w \) but not \( x \)

\( w = 1.1 \)
\( w = 1.0 \)
\( w = 0.9 \)

\( x(0) = -0.5 \)
\( x(0) = 0 \)
\( x(0) = 0.5 \)
With non-linear activations: Tanh

$$h(t) = \tanh(wh(t-1) + cx(t) + b)$$

- Final value depends only on $b$ and $w$, but not on $x$
- “Remembers” $x$ value much longer than sigmoid

Scalar recurrence
With non-linear activations: RELU

\[ h(t) = \text{relu}(wh(t - 1) + cx(t) + b) \]

- 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

\[ h(t) = f(W h(t - 1) + C x(t) + b) \]

- **Initial x(0): Top: \([1,1,1,\ldots]\), Bottom: \([-1,-1,-1,\ldots]\)**
Vector Process: Max eigenvalue 0.9

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

- **Initial x(0):** Top: \([1,1,1,...]\), Bottom: \([-1,-1,-1,...]\)
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

\[
h(t) = 0.5h(t-1) + 0.25h(t-5) + x(t)
\]

\[
h(t) = 0.5h(t-1) + 0.25h(t-5) + 0.1h(t-8) + x(t)
\]
Stability Analysis

• Similar analysis of vector functions with non-linear 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

• $\#22$, $\#23$

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
- 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 how long (how many time steps) an RNN can retain some memory of an input pattern

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- It depends on the activation function used in the recurrent layers
- It depends on the actual input being “remembered”
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
  \[ Y = f_N \left( W_N f_{N-1} \left( W_{N-1} f_{N-2} \left( \ldots W_1 X \right) \right) \right) \]
- \( W_k \) is the weights matrix at the \( k^{th} \) layer
- The error for \( X \) can be written as
  \[ \text{Div}(X) = D \left( f_N \left( W_N f_{N-1} \left( W_{N-1} f_{N-2} \left( \ldots W_1 X \right) \right) \right) \right) \]
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

Let $Z = Wg(X)$

\[\nabla_X f = \nabla_Z f \cdot W \cdot \nabla_X g\]

• 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
Training deep networks

- For

\[ \text{Div}(X) = D \left( f_N \left( W_N f_{N-1} \left( W_{N-1} f_{N-2} \left( \ldots W_1 X \right) \right) \right) \right) \]

- We get:

\[ \nabla_{f_k} \text{Div} = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \ldots \nabla f_{k+1} W_{k+1} \]

- Where
  - \( \nabla_{f_k} \text{Div} \) is the gradient \( \text{Div}(X) \) 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 \( W_{k-1} \)
  - \( \nabla f_n \) is jacobian of \( f_N \) w.r.t. to its current input
  - All blue terms are matrices
  - All function derivatives are w.r.t. the (entire, affine) argument of the function
Training deep networks

For

\[ \text{Div}(X) = D \left( f_N \left( W_{N-1} f_{N-1} \left( W_{N-2} f_{N-2} (\ldots W_0 X) \right) \right) \right) \]

We get:

\[ \nabla_{f_k} \text{Div} = \nabla D \left( \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \ldots \nabla f_{k+1} \cdot W_{k+1} \right) \]

Where

- \( \nabla_{f_k} \text{Div} \) is the gradient \( \text{Div}(X) \) 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 \( f_N(X) \) w.r.t. to its current input
- All blue terms are matrices

Let's consider these Jacobians for an RNN (or more generally for any network)
The Jacobian of the hidden layers for an RNN

\[
\begin{align*}
\nabla f_t(z_i) &= \begin{bmatrix}
  f_{t,1}'(z_1) & 0 & \cdots & 0 \\
  0 & f_{t,2}'(z_2) & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & f_{t,N}'(z_N)
\end{bmatrix} \\
X \ h_i^{(1)}(t) &= f_1 \left( z_i^{(1)}(t) \right)
\end{align*}
\]

- \( \nabla f_t() \) is the derivative of the output of the (layer of) hidden recurrent neurons with respect to their input
- 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

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

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

\[ \nabla f_k \text{Div} = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \ldots \nabla f_{k+1} W_{k+1} \]

• In a single-layer RNN, the weight matrices are identical
  – The conclusion below holds for any deep network, though

• The chain product for \( \nabla f_k \text{Div} \) will
  – Expand \( \nabla D \) along directions in which the singular values of the weight matrices are greater than 1
  – Shrink \( \nabla D \) 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

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

- Every blue term is a matrix
- $\nabla D$ is proportional to the actual error
  - Particularly for $L_2$ and KL divergence
- The chain product for $\nabla f_k \text{Div}$ will
  - Expand $\nabla D$ 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

\[ \nabla f_k \text{Div} = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \ldots \nabla f_{k+1} \cdot W_{k+1} \]
Vanishing gradient examples..

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 $\log |\nabla_{W_{\text{neuron}}} \text{Div}|$ where $W_{\text{neuron}}$ 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 gradient examples...

**RELU activation, Batch gradients**

- 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 $\log|\nabla W_{neuron} \cdot \nabla|$ 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 gradient examples..

Sigmoid activation, Batch gradients

• 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 \( \log |\nabla_{W_{neuron}} \text{Div}| \) 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 gradient examples..

- 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 $\log |\nabla_{W_{\text{neuron}}} \ Div|$ where $W_{\text{neuron}}$ 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 gradient examples..

ELU activation, Individual instances

- 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 $\log|\nabla_{W_{\text{neuron}}} \text{Div}|$ where $W_{\text{neuron}}$ 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

- 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 $t = 0$

$$\nabla f_k Div = \nabla D \cdot \nabla f_N \cdot W_N \cdot \nabla f_{N-1} \cdot W_{N-1} \ldots \nabla f_{k+1} W_{k+1}$$
Recall: Vanishing stuff..

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

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).
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 loss 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)
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
  - 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

\[ h = f_N \left( W_N f_{N-1} \left( W_{N-2} f_{N-1} (\ldots W_1 X) \right) \right) \]

\[ \nabla f_k \text{Div} = \nabla D. \nabla f_N. W_N. \nabla f_{N-1}. W_{N-1} \ldots \nabla f_{k+1} W_{k+1} \]

• The memory retention of the network depends on the behavior of the underlined terms
  – Which in turn depends on the parameters \( W \) 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

\[ h = f_N \left( W_N f_{N-1} \left( W_{N-2} f_{N-1} (\ldots W_1 X) \right) \right) \]

\[ \nabla_{f_k} Div = \nabla D \cdot \nabla f_N W_N \cdot \nabla f_{N-1} W_{N-1} \ldots \nabla f_{k+1} W_{k+1} \]

- 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

- \[ Memory(k) \approx C(x_0). \sigma_1(x_1). \sigma_2(x_2). \ldots \sigma_k(x_k) \]
Enter – the constant error carousel

- History is carried through uncompressed
  - No weights, no nonlinearities
  - Only scaling is through the $\sigma$ “gating” term that captures other triggers
  - E.g. “Have I seen Pattern2”?
Enter – the constant error carousel

- Actual non-linear work is done by other portions of the network
  - Neurons that compute the workable state from the memory
Enter – the constant error carousel

- The gate $\sigma$ depends on current input, current hidden state...
Enter – the constant error carousel

- The gate $\sigma$ depends on current input, current hidden state... and other stuff...
Enter – the constant error carousel

- The gate $\sigma$ 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/](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
• The $\sigma()$ 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

- 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

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

\[ i_t = \sigma (W_i \cdot [h_{t-1}, x_t] + b_i) \]
\[ \tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \]
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 it’s worth remembering
  - If so it’s added to the current memory cell

\[ C_t = f_t \times C_{t-1} + i_t \times \tilde{C}_t \]
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
• The raw memory is informative by itself and can also be input
  – Note, we’re using both $C$ and $h$

\[
\begin{align*}
  f_t &= \sigma \left( W_f \cdot [C_{t-1}, h_{t-1}, x_t] + b_f \right) \\
  i_t &= \sigma \left( W_i \cdot [C_{t-1}, h_{t-1}, x_t] + b_i \right) \\
  o_t &= \sigma \left( W_o \cdot [C_t, h_{t-1}, x_t] + b_o \right)
\end{align*}
\]
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

- 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
LSTM computation: Forward

- Forward rules:

**Gates**

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

**Variables**

\[ \tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \]
\[ C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t \]
\[ h_t = o_t \cdot \tanh(C_t) \]
**LSTM computation: Forward**

![Diagram of LSTM computation](image)

- **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**
  
  $\tilde{C}_t = \tanh \left( W_{\tilde{C}} \cdot [h_{t-1}, x_t] + b_{\tilde{C}} \right)$
  
  $C_t = f_t \cdot C_{t-1} + i_t \cdot \tilde{C}_t$
  
  $h_t = o_t \cdot \tanh \left( C_t \right)$
LSTM Equations

• $i$: input gate, how much of the new information will be let through the memory cell.

• $f$: forget gate, responsible for information that 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

\[
\begin{align*}
i &= \sigma(x_t U^i + s_{t-1} W^i) \\
f &= \sigma(x_t U^f + s_{t-1} W^f) \\
o &= \sigma(x_t U^o + s_{t-1} W^o) \\
g &= \tanh(x_t U^g + s_{t-1} W^g) \\
c_t &= c_{t-1} \circ f + g \circ i \\
s_t &= \tanh(c_t) \circ o \\
y &= \text{softmax}(Vs_t)
\end{align*}
\]
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

# Static local variables to the cell
static local z_f, z_i, z_c, z_o, f, i, o, C_i

function [C,h] = LSTM_cell.forward(C,h,x,[W,b])
  code on next slide
# 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 \(z_f, z_i, z_c, z_o, f, i, o, C_i\)

function \([C_o, h_o] = LSTM\_cell\_forward(C, h, x, [W, b])\)

\[
\begin{align*}
    z_f &= W_{fc}C + W_{fh}h + W_{fx}x + b_f \\
    f &= \text{sigmoid}(z_f) \quad \# \text{forget gate} \\

    z_i &= W_{ic}C + W_{ih}h + W_{ix}x + b_i \\
    i &= \text{sigmoid}(z_i) \quad \# \text{input gate} \\

    z_c &= W_{cc}C + W_{ch}h + W_{cx}x + b_c \\
    C_i &= \text{tanh}(z_c) \quad \# \text{Detecting input pattern} \\

    C_o &= f \circ C + i \circ C_i \quad \# \text{“} \circ \text{“ is component-wise multiply} \\

    z_o &= W_{oc}C_o + W_{oh}h + W_{ox}x + b_o \\
    o &= \text{sigmoid}(z_o) \quad \# \text{output gate} \\

    h_o &= o \circ \text{tanh}(C_o) \quad \# \text{“} \circ \text{“ is component-wise multiply} \\
    \text{return } C_o, h_o
\end{align*}
\]
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 l^{th} hidden layer
# W_ω and b_ω are output layer weights and biases

for t = 0:T-1  # Including both ends of the index
    \( h(t,0) = x(t) \)  # Vectors. Initialize h(0) to input
for l = 1:L  # hidden layers operate at time t
    \[ [C(t,l),h(t,l)] = \text{LSTM}\_\text{cell}(t,l).\text{forward}(...\text{...C}(t-1,l),h(t-1,l),h(t,l-1)[W{l},b{l}]) \]
    \( z_ω(t) = W_ω h(t,L) + b_ω \)
    \( Y(t) = \text{softmax}( z_ω(t) ) \)
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
Backpropagation rules: Backward

\[ \nabla_{C_t} \text{Div} = \]
\[ \nabla_c D_i v = \nabla_{h_t} D_i v \circ o_t \circ \tanh'(.) \]
\[ \nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(\cdot) + tanh(\cdot) \circ \sigma'(\cdot)W_{Co}) \]
Backpropagation rules: Backward

\( \nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ \tanh'(.) + \tanh(.) \circ \sigma'(.) W_{Co}) + \\
\nabla_{C_{t+1}} Div \circ f_{t+1} + 
\)
Backpropagation rules: Backward

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

\[ C_{t-1} \]
\[ f_t \]
\[ i_t \]
\[ \sigma(.) \]
\[ \tanh \]
\[ C_t \]
\[ h_{t-1} \]
\[ x_t \]
\[ C_t \]
\[ C_{t+1} \]
\[ f_{t+1} \]
\[ \tilde{C}_{t+1} \]
\[ \sigma(.) \]
\[ \tanh \]
\[ h_{t+1} \]
\[ x_{t+1} \]
Backpropagation rules: Backward

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

\[ \nabla_{C_t} \text{Div} = \nabla_{h_t} \text{Div} \circ (o_t \circ \tanh'(.) + \tanh(.) \circ \sigma'(.) W_{CO}) + \\
\nabla_{C_{t+1}} \text{Div} \circ (f_{t+1} + C_t \circ \sigma'(.) W_{Cf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{Ci} \ldots) \\

\nabla_{h_t} \text{Div} = \nabla_{z_t} \text{Div} \nabla_{h_t} z_t \]
Backpropagation rules: Backward

\[
\nabla_{C_t} \text{Div} = \nabla_{h_t} \text{Div} \odot (o_t \odot \text{tanh}'(.)) + \text{tanh}(.) \odot \sigma'(.)W_{Co} + \\
\n\nabla_{C_{t+1}} \text{Div} \odot (f_{t+1} + C_t \odot \sigma'(.)W_{Cf} + \tilde{C}_{t+1} \odot \sigma'(.)W_{Ci} \ldots)
\]

\[
\nabla_{h_t} \text{Div} = \nabla_{z_t} \text{Div} \nabla_{h_t} z_t + \nabla_{C_{t+1}} \text{Div} \odot C_t \odot \sigma'(.)W_{hf}
\]
Backpropagation rules: Backward

\[
\nabla_{C_t} D_i v = \nabla_{h_t} D_i v \circ (o_t \circ \tanh'(.) + \tanh(.) \circ \sigma'(.)W_{CO}) + \\
\nabla_{C_{t+1}} D_i v \circ (f_{t+1} + C_t \circ \sigma'(.)W_{CF} + \tilde{C}_{t+1} \circ \sigma'(.)W_{CI} ...)
\]

\[
\nabla_{h_t} D_i v = \nabla_{z_t} D_i v \nabla_{h_t} z_t + \nabla_{C_{t+1}} D_i v \circ (C_t \circ \sigma'(.)W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{hi})
\]
Backpropagation rules: Backward

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

$$\nabla_{h_t} Div = \nabla_{z_t} Div\nabla_{h_t} z_t + \nabla_{C_{t+1}} Div \circ (C_t \circ \sigma'(.)W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{hi}) + \nabla_{C_{t+1}} Div \circ i_{t+1} \circ \tanh'(.)W_{hi}$$
Backpropagation rules: Backward

\[
\nabla_{C_t} \text{Div} = \nabla_{h_t} \text{Div} \circ (o_t \circ \text{tanh}'(.) + \text{tanh}(.) \circ \sigma'(.)W_{co}) + \\
\n\nabla_{C_{t+1}} \text{Div} \circ (f_{t+1} + C_t \circ \sigma'(.)W_{cf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{ci} ...)
\]

\[
\nabla_{h_t} \text{Div} = \nabla_{z_t} \text{Div} \nabla_{h_t} z_t + \nabla_{C_{t+1}} \text{Div} \circ (C_t \circ \sigma'(.)W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.)W_{hi}) + \\
\n\nabla_{C_{t+1}} \text{Div} \circ o_{t+1} \circ \text{tanh}'(.)W_{hi} + \nabla_{h_{t+1}} \text{Div} \circ \text{tanh}(.) \circ \sigma'(.)W_{ho}
\]
Backpropagation rules: Backward

Not explicitly deriving the derivatives w.r.t weights; Left as an exercise

\[ \nabla_{C_t} Div = \nabla_{h_t} Div \circ (o_t \circ tanh'(.) + tanh(.) \circ \sigma'(.) W_{co}) + \]
\[ \nabla_{C_t+1} Div \circ (f_{t+1} + C_t \circ \sigma'(.) W_{cf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{ci} \ldots) \]

\[ \nabla_{h_t} Div = \nabla_{z_t} Div \nabla_{h_t} z_t + \nabla_{C_t+1} Div \circ (C_t \circ \sigma'(.) W_{hf} + \tilde{C}_{t+1} \circ \sigma'(.) W_{hi}) + \]
\[ \nabla_{C_t+1} Div \circ o_{t+1} \circ tanh'(.) W_{hi} + \nabla_{h_{t+1}} Div \circ tanh(.) \circ \sigma'(.) W_{ho} \]
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*
# 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, z_o, f, i, o, C_i
function [C_o, h_o] = LSTM_cell.forward(C,h,x, [W,b])
    
    z_f = W_fC + 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 o C + i o C_i # “o” 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 o tanh(C_o) # “o” is component-wise multiply

    return C_o, h_o
# Static local variables carried over from forward
static local \(z_f, z_i, z_c, z_o, f, i, o, C_i\)

function \([dC, dh, dx, d[W, b]] = \text{LSTM\_cell\_backward}(dC_o, dh_o, C, h, C_o, h_o, x, [W, b])\)

    # First invert \(h_o = o \circ \tanh(C)\)
    do = dh_o \circ \tanh(C_o)^T
    d tanhC_o = dh_o \circ o
    dC_o += dtanhC_o \circ (1-\tanh^2(C_o))^T \text{ #}(1-\tanh^2) \text{ is the derivative of } \tanh

    # Next invert \(o = \text{sigmoid}(z_o)\)
    dz_o = do \circ \text{sigmoid}(z_o)^T \circ (1-\text{sigmoid}(z_o))^T \text{ # } do \times \text{ derivative of sigmoid}(z_o)

    # Next invert \(z_o = W_{oc}C_o + W_{oh}h + W_{ox}x + b_o\)
    dC_o += dz_o W_{oc} \text{ # } \text{Note - this is a regular matrix multiply}
    dh = dz_o W_{oh}
    dx = dz_o W_{ox}

    dW_{oc} = C_o dz_o \text{ # } \text{Note - this multiplies a column vector by a row vector}
    dW_{oh} = h \ dz_o
    dW_{ox} = x \ dz_o
    db_o = dz_o

    # Next invert \(C_o = f \circ C + i \circ C_i\)
    dC = dC_o \circ f
    dC_i = dC_o \circ i
    di = dC_o \circ C_i
    df = dC_o \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 $i = \text{sigmoid}(z_i)$
\[
dz_i = di \circ \text{sigmoid}(z_i)^T \circ (1-\text{sigmoid}(z_i))^T
\]

# Next invert $z_i = W_{ic}C + W_{ih}h + W_{ix}x + b_i$
\[
dC += dz_i W_{ic}
dh += dz_i W_{ih}
dx += dz_i W_{ix}
\]
\[
dW_{ic} = C \ dz_i
dW_{ih} = h \ dz_i
dW_{ix} = x \ dz_i
db_i = dz_i
\]
LSTM cell backward (continued)

# Next invert \( f = \text{sigmoid}(z_f) \)
\[ dz_f = df \circ \text{sigmoid}(z_f)^T \circ (1-\text{sigmoid}(z_f))^T \]

# Finally invert \( z_f = W_{fc}C + W_{fh}h + W_{fx}x + b_f \)
\[
\begin{align*}
\text{dC} &\leftarrow \text{dz}_f \; W_{fc} \\
\text{dh} &\leftarrow \text{dz}_f \; W_{fh} \\
\text{dx} &\leftarrow \text{dz}_f \; W_{fx} \\
\end{align*}
\]
\[
\begin{align*}
\text{d}W_{fc} &\leftarrow C \; \text{dz}_f \\
\text{d}W_{fh} &\leftarrow h \; \text{dz}_f \\
\text{d}W_{fx} &\leftarrow x \; \text{dz}_f \\
\text{d}b_f &\leftarrow \text{dz}_f \\
\end{align*}
\]

return \( \text{dC}, \; \text{dh}, \; \text{dx}, \; \text{d}[W,\; b] \)

# \( \text{d}[W,b] \) 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 l^th hidden layer
# W_o and b_o are output layer weights and biases

for t = 0:T-1  # Including both ends of the index
    h(t,0) = x(t)  # Vectors. Initialize 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) )
# 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 l-th hidden layer
# W_o and b_o are output layer weights and biases
# Y is the output of the network
# Assuming dW_o and db_o and d[W{l} b{l}] (for all l) 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) · 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: Let's simplify the LSTM

- Simplified LSTM which addresses some of your concerns of why

\[
\begin{align*}
z_t &= \sigma (W_z \cdot [h_{t-1}, x_t]) \\
r_t &= \sigma (W_r \cdot [h_{t-1}, x_t]) \\
\tilde{h}_t &= \tanh (W \cdot [r_t \cdot h_{t-1}, x_t]) \\
h_t &= (1 - z_t) \cdot h_{t-1} + z_t \cdot \tilde{h}_t
\end{align*}
\]
Gated Recurrent Units: Let's simplify the LSTM

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

\[
\begin{align*}
z_t &= \sigma (W_z \cdot [h_{t-1}, x_t]) \\
r_t &= \sigma (W_r \cdot [h_{t-1}, x_t]) \\
\tilde{h}_t &= \tanh (W \cdot [r_t \cdot h_{t-1}, x_t]) \\
h_t &= (1 - z_t) \cdot h_{t-1} + z_t \cdot \tilde{h}_t
\end{align*}
\]
Gated Recurrent Units: Let's simplify the LSTM

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

\[
\begin{align*}
    z_t &= \sigma (W_z \cdot [h_{t-1}, x_t]) \\
    r_t &= \sigma (W_r \cdot [h_{t-1}, x_t]) \\
    \tilde{h}_t &= \tanh (W \cdot [r_t \ast h_{t-1}, x_t]) \\
    h_t &= (1 - z_t) \ast h_{t-1} + z_t \ast \tilde{h}_t
\end{align*}
\]
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 $h(t)$
• 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..