How to compute a derivative

Computing derivatives of complicated functions

- How do you compute the derivatives in an LSTM or GRU cell?
- How do you compute derivatives of complicated functions in general
- In these slides we will give you some hints
- In the slides we will assume vector functions and vector activations.
- But we will also give you scalar versions of the equations to provide intuition
- The two sets will be almost identical, except that when we deal with vector functions
 - The notation becomes uglier and less intuitive
 - We must ensure that the dimensions come out right
- Please compare vector versions of equations to their scalar counterparts for better intuition, if needed

First: Some notation and conventions

- We will refer to the derivative of scalar L with respect to x as $\nabla_{\!x} L$
 - Regardless of whether the derivative is a scalar, vector, matrix or tensor
- The derivative of a scalar L w.r.t an $N \times 1$ column vector x is a $1 \times N$ row vector $\nabla_x L$
- The derivative of a scalar L w.r.t an $N \times M$ matrix X is an $M \times N$ matrix $\nabla_X L$
 - Remember our gradient update rule : $W = W \eta \nabla_W L^T$
- The derivative of an $N \times 1$ vector Y w.r.t an $M \times 1$ vector X is an $N \times M$ matrix $J_X(Y)$
 - The Jacobian

Rules: 1 (scalar)

$$z = Wx$$

- All terms are scalars
- $\frac{\partial L}{\partial z}$ is known

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} W$$

$$\frac{\partial L}{\partial W} = x \frac{\partial L}{\partial z}$$

Rules: 1 (vector)

$$z = Wx$$

- z is an $N \times 1$ vector
- x is an $M \times 1$ vector
- W is an $N \times M$ matrix
- L is a function of z
- $\nabla_z L$ is known (and is a $1 \times N$ vector)

$$\nabla_{\mathcal{X}}L = (\nabla_{\mathcal{Z}}L)W$$

$$\nabla_W L = \chi(\nabla_Z L)$$

Please verify that the dimensions match!

Rules: 2 (vector, schur multiply)

$$z = x \circ y$$

- x, y and z are all $N \times 1$ vectors
- "o" represents component-wise multiplication
- $\nabla_z L$ is known (and is a $1 \times N$ vector)

$$\nabla_{x}L = (\nabla_{z}L) \circ y^{T}$$

$$\nabla_{\mathcal{V}} L = (\nabla_{\mathcal{Z}} L) \circ \mathcal{X}^T$$

Please verify that the dimensions match!

Rules: 3 (scalar)

$$z = x + y$$

- All terms are scalars
- $\frac{\partial L}{\partial z}$ is known

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}$$

$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}$$

Rules: 3 (vector)

$$z = x + y$$

- x, y and z are all $N \times 1$ vectors
- $\nabla_z L$ is known (and is a $1 \times N$ vector)

$$\nabla_{\mathcal{X}}L = \nabla_{\mathcal{Z}}L$$

$$\nabla_{\mathcal{V}}L = \nabla_{\mathcal{Z}}L$$

Please verify that the dimensions match!

Rules: 4 (scalar)

$$z = g(x)$$

- x and z are scalars
- $\frac{\partial L}{\partial z}$ is known

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} g'(x)$$

Rules: 4 (vector)

$$z = g(x)$$

- x and z are $N \times 1$ vectors
- $\nabla_z L$ is known (and is a $1 \times N$ vector)
- $J_x g$ is the Jacobian of g(x) with respect to x
 - May be a diagonal matrix

$$\nabla_{x}L = \nabla_{z}L J_{x}g$$

Please verify that the dimensions match!

Rules: 4b (vector) component-wise multiply notation

$$z = g(x)$$

- x and z are $N \times 1$ vectors
- $\nabla_z L$ is known (and is a $1 \times N$ vector)
- g(x) is actually a vector of *component-wise* functions
 - i.e. $z_i = g(x_i)$
- g'(x) is a column vector consisting of the derivatives of the individual components of g(x) w.r.t individual components of x

$$\nabla_{x}L = \nabla_{z}L \circ g'(x)^{T}$$
 Please verify that the dimensions match!

Rule 5: Addition of derivatives

Given two variables

$$z = g(x)$$
$$y = h(x)$$

- And given $\frac{\partial L}{\partial y}$ and $\frac{\partial L}{\partial z}$
- we get

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}g'(x) + \frac{\partial L}{\partial y}h'(x)$$

The rule also extends to vector derivatives

Computing derivatives of complex functions

- We now are prepared to compute very complex derivatives
- Procedure:
 - Express the computation as a series of computations of intermediate values
 - Each computation must comprise either a unary or binary relation
 - Unary relation: RHS has one argument, e.g. y = g(x)
 - Binary relation: RHS has two arguments e.g. z = x + y or z = xy
 - Work your way backward through the derivatives of the simple relations

Example: LSTM

 Full set of LSTM equations (in the order in which they must be computed)

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

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

3  \tilde{C}_{t} = \tanh(W_{C} \cdot [h_{t-1}, x_{t}] + b_{C})

4  C_{t} = f_{t} * C_{t-1} + i_{t} * \tilde{C}_{t}

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

6  h_{t} = o_{t} * \tanh(C_{t})
```

 Its actually much cleaner to separate the individual components, so lets do that first

1.
$$f_t = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_t + b_f)$$

2.
$$i_t = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_t + b_i)$$

3.
$$\tilde{C}_t = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_t + b_C)$$

$$4. \quad C_t = f_t \circ C_{t-1} + i_t \circ \tilde{C}_t$$

5.
$$o_t = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_t + b_o)$$

6.
$$h_t = o_t \circ \tanh(C_t)$$

- This is the full set of equations in the order in which they must be computed
- Lets rewrite these in terms of unary and binary operations

1.
$$f_{t} = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_{t} + b_{f})$$
2.
$$i_{t} = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_{t} + b_{i})$$
2.
$$i_{t} = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_{t} + b_{i})$$
2.
$$i_{t} = \sigma(W_{ch}h_{t-1} + W_{cx}x_{t} + b_{c})$$

$$z_{1} = W_{fC}C_{t-1}$$

$$z_{2} = W_{fh}h_{t-1}$$

$$z_{3} = z_{1} + z_{2}$$

$$z_{4} = W_{fx}x_{t}$$

$$z_{5} = z_{3} + z_{4}$$

$$z_{6} = z_{5} + b_{f}$$

$$f_{t} = \sigma(z_{6})$$

 Lets rewrite these in terms of unary and binary operations

1.
$$z_1 = W_{fC}C_{t-1}$$

2.
$$z_2 = W_{fh} h_{t-1}$$

3.
$$z_3 = z_1 + z_2$$

4.
$$z_4 = W_{fx}x_t$$

5.
$$z_5 = z_3 + z_4$$

6.
$$z_6 = z_5 + b_f$$

7.
$$f_t = \sigma(z_6)$$

ISTM

1.
$$f_{t} = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_{t} + b_{f})$$

2. $i_{t} = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_{t} + b_{i})$
3. $\tilde{C}_{t} = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_{t} + b_{C})$
4. $C_{t} = f_{t} \circ C_{t-1} + i_{t} \circ \tilde{C}_{t}$
5. $o_{t} = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_{t} + b_{o})$
6. $h_{t} = o_{t} \circ \tanh(C_{t})$

$$z_{1} = W_{ix}C_{t-1} + z_{2} = W_{ih}h_{t-1} + z_{2} = Z_{1} + Z_{1} + Z_{1} = Z_{1} + Z_{1} = Z_{1} + Z_{1}$$

$$z_{7} = W_{iC}C_{t-1}$$

$$z_{8} = W_{ih}h_{t-1}$$

$$z_{9} = z_{7} + z_{8}$$

$$z_{10} = W_{ix}x_{t}$$

$$z_{11} = z_{9} + z_{10}$$

$$z_{12} = z_{11} + b_{i}$$

$$i_{t} = \sigma(z_{12})$$

 Lets rewrite these in terms of unary and binary operations

1.
$$z_1 = W_{fC}C_{t-1}$$

2.
$$z_2 = W_{fh} h_{t-1}$$

3.
$$z_3 = z_1 + z_2$$

4.
$$z_4 = W_{fx}x_t$$

5.
$$z_5 = z_3 + z_4$$

6.
$$z_6 = z_5 + b_f$$

7.
$$f_t = \sigma(z_6)$$

8.
$$z_7 = W_{iC}C_{t-1}$$

9.
$$z_8 = W_{ih}h_{t-1}$$

10.
$$z_9 = z_7 + z_8$$

11.
$$z_{10} = W_{ix}x_t$$

12.
$$z_{11}=z_9+z_{10}$$

13.
$$z_{12} = z_{11} + b_i$$

14.
$$i_t = \sigma(z_{12})$$

1.
$$f_t = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_t + b_f)$$

2. $i_t = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_t + b_i)$
3. $\tilde{C}_t = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_t + b_C)$
4. $C_t = f_t \circ C_{t-1} + i_t \circ C_t$
5. $o_t = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_t + b_o)$
6. $h_t = o_t \circ \tanh(C_t)$

Lets rewrite these in terms of unary and binary operations

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

1.
$$f_{t} = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_{t} + b_{f})$$

2. $i_{t} = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_{t} + b_{i})$
3. $\tilde{C}_{t} = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_{t} + b_{C})$
4. $C_{t} = f_{t} \circ C_{t-1} + i_{t} \circ \tilde{C}_{t}$
5. $o_{t} = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_{t} + b_{o})$
6. $h_{t} = o_{t} \circ \tanh(C_{t})$

Lets rewrite these in terms of unary and binary operations

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

1.
$$f_t = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_t + b_f)$$

2. $i_t = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_t + b_i)$
3. $\tilde{C}_t = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_t + b_C)$
4. $C_t = f_t \circ C_{t-1} + i_t \circ \tilde{C}_t$
5. $o_t = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_t + b_o)$
6. $h_t = o_t \circ \tanh(C_t)$

$$\begin{aligned} z_{19} &= W_{oC}C_{t-1} \\ z_{20} &= W_{oh}h_{t-1} \\ z_{21} &= z_{19} + z_{20} \\ z_{22} &= W_{ox}x_t \\ z_{23} &= z_{21} + z_{22} \\ z_{24} &= z_{23} + b_o \\ o_t &= \sigma(z_{24}) \end{aligned}$$

Lets rewrite these in terms of unary and binary operations

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

1.
$$f_{t} = \sigma(W_{fC}C_{t-1} + W_{fh}h_{t-1} + W_{fx}x_{t} + b_{f})$$

2. $i_{t} = \sigma(W_{iC}C_{t-1} + W_{ih}h_{t-1} + W_{ix}x_{t} + b_{i})$
3. $\tilde{C}_{t} = \sigma(W_{Ch}h_{t-1} + W_{Cx}x_{t} + b_{C})$
4. $C_{t} = f_{t} \circ C_{t-1} + i_{t} \circ \tilde{C}_{t}$
5. $o_{t} = \sigma(W_{oC}C_{t-1} + W_{oh}h_{t-1} + W_{ox}x_{t} + b_{o})$
6. $h_{t} = o_{t} \circ \tanh(C_{t})$

$$\sum_{z=t} = \tanh(C_{t}) h_{t} = o_{t} \circ z_{25}$$

Lets rewrite these in terms of unary and binary operations

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

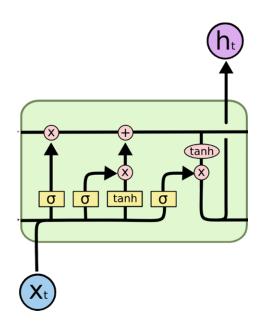
28.
$$z_{24} = z_{23} + b_0$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

LSTM forward



- The full forward computation of the LSTM can be performed by computing Equations 1-31 in sequence
- Every one of these equations is unary or binary

1.
$$z_1 = W_{fC}C_{t-1}$$

2.
$$z_2 = W_{fh} h_{t-1}$$

3.
$$z_3 = z_1 + z_2$$

4.
$$z_4 = W_{fx}x_t$$

5.
$$z_5 = z_3 + z_4$$

6.
$$z_6 = z_5 + b_f$$

7.
$$f_t = \sigma(z_6)$$

8.
$$z_7 = W_{iC}C_{t-1}$$

9.
$$z_8 = W_{ih}h_{t-1}$$

10.
$$z_9 = z_7 + z_8$$

11.
$$z_{10} = W_{ix}x_t$$

12.
$$z_{11}=z_9+z_{10}$$

13.
$$z_{12} = z_{11} + b_i$$

14.
$$i_t = \sigma(z_{12})$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

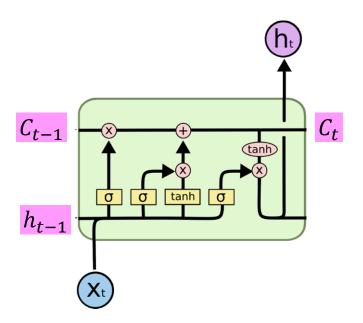
28.
$$z_{24} = z_{23} + b_0$$

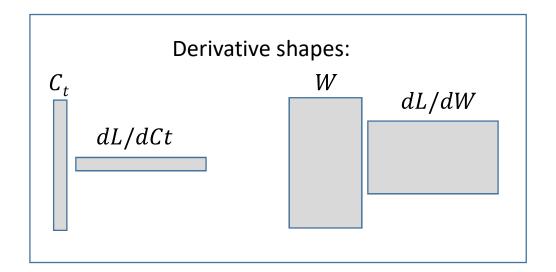
29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

Computing derivatives





- · We will now work our way backward
- We assume derivatives $\frac{dL}{dh_t}$ and $\frac{dL}{dC_t}$ of the loss w.r.t h_t and C_t are given
- We must compute $\frac{dL}{dC_{t-1}}$, $\frac{dL}{dh_{t-1}}$ and $\frac{dL}{dx_t}$
 - And also derivatives w.r.t the parameters within the cell
- Recall: the shape of the derivative for any variable will be transposed with respect to that variable

1.
$$\nabla_{o_t} L = \nabla_{h_t} L \circ z_{25}^T$$

$$2. \quad \nabla_{z_{25}} L = \nabla_{h_t} L \circ o_t^T$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_0$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

1.
$$\nabla_{o_t} L = \nabla_{h_t} L \circ z_{25}^T$$

$$2. \quad \nabla_{z_{25}} L = \nabla_{h_t} L \circ o_t^T$$

3.
$$\nabla_{C_t} L = \nabla_{Z_{25}} L \circ (1 - \tanh^2(C_t))^T$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21} = z_{19} + z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25}$$
=tanh(C_t)

31.
$$h_t = o_t \circ z_{25}$$

1.
$$\nabla_{o_t} L = \nabla_{h_t} L \circ z_{25}^T$$

$$2. \quad \nabla_{z_{25}} L = \nabla_{h_t} L \circ o_t^T$$

3.
$$\nabla_{C_t} L = \nabla_{Z_{25}} L \circ (1 - \tanh^2(C_t))^T$$

4.
$$\nabla_{z_{24}} L = \nabla_{o_t} L \circ \sigma(z_{24})^T \circ (1 - \sigma(z_{24}))^T$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

1.
$$\nabla_{o_t} L = \nabla_{h_t} L \circ z_{25}^T$$

$$2. \quad \nabla_{z_{25}} L = \nabla_{h_t} L \circ o_t^T$$

3.
$$\nabla_{C_t} L = \nabla_{Z_{25}} L \circ (1 - \tanh^2(C_t))^T$$

4.
$$\nabla_{z_{24}} L = \nabla_{o_t} L \circ \sigma(z_{24})^T \circ (1 - \sigma(z_{24}))^T$$

5.
$$\nabla_{z_{23}}L = \nabla_{z_{24}}L$$

$$6. \quad \nabla_{b_o} L = \nabla_{z_{24}} L$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23} = z_{21} + z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

Equations highlighted in yellow show derivatives w.r.t. parameters

7.
$$\nabla_{z_{22}}L = \nabla_{z_{23}}L$$

8.
$$\nabla_{z_{21}} L = \nabla_{z_{23}} L$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{0x}x_t$$

$$z_{7}$$
. $z_{23}=z_{21}+z_{22}$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

7.
$$\nabla_{z_{22}}L = \nabla_{z_{23}}L$$

8.
$$\nabla_{z_{21}} L = \nabla_{z_{23}} L$$

$$9. \quad \nabla_{W_{ox}} L = x_t \nabla_{z_{22}} L$$

10.
$$\nabla_{x_t} L = \nabla_{z_{22}} L W_{ox}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21}=z_{19}+z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23} = z_{21} + z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

7.
$$\nabla_{z_{22}}L = \nabla_{z_{23}}L$$

8.
$$\nabla_{z_{21}} L = \nabla_{z_{23}} L$$

$$9. \quad \nabla_{W_{ox}} L = x_t \nabla_{Z_{22}} L$$

10.
$$\nabla_{x_t} L = \nabla_{z_{22}} L W_{ox}$$

11.
$$\nabla_{z_{20}} L = \nabla_{z_{21}} L$$

12.
$$\nabla_{z_{19}}L = \nabla_{z_{21}}L$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21} = z_{19} + z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

7.
$$\nabla_{z_{22}}L = \nabla_{z_{23}}L$$

8.
$$\nabla_{z_{21}} L = \nabla_{z_{23}} L$$

9.
$$\nabla_{W_{ox}}L = x_t \nabla_{z_{22}}L$$

10.
$$\nabla_{x_t} L = \nabla_{z_{22}} L W_{ox}$$

11.
$$\nabla_{z_{20}} L = \nabla_{z_{21}} L$$

12.
$$\nabla_{z_{19}}L = \nabla_{z_{21}}L$$

13.
$$\nabla_{W_{oh}} L = h_{t-1} \nabla_{Z_{20}} L$$

14.
$$\nabla_{h_{t-1}} L = \nabla_{z_{20}} L W_{oh}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh} h_{t-1}$$

25.
$$z_{21} = z_{19} + z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_0$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

7.
$$\nabla_{z_{22}}L = \nabla_{z_{23}}L$$

8.
$$\nabla_{z_{21}} L = \nabla_{z_{23}} L$$

9.
$$\nabla_{W_{ox}} L = x_t \nabla_{Z_{22}} L$$

10.
$$\nabla_{x_t} L = \nabla_{z_{22}} L W_{ox}$$

11.
$$\nabla_{z_{20}} L = \nabla_{z_{21}} L$$

12.
$$\nabla_{z_{19}} L = \nabla_{z_{21}} L$$

13.
$$\nabla_{W_{oh}} L = h_{t-1} \nabla_{Z_{20}} L$$

14.
$$\nabla_{h_{t-1}} L = \nabla_{z_{20}} L W_{oh}$$

15.
$$\nabla_{W_{oC}} L = C_{t-1} \nabla_{Z_{19}} L$$

16.
$$\nabla_{C_{t-1}} L = \nabla_{Z_{19}} L W_{oC}$$

23.
$$z_{19} = W_{oC}C_{t-1}$$

24.
$$z_{20} = W_{oh}h_{t-1}$$

25.
$$z_{21} = z_{19} + z_{20}$$

26.
$$z_{22} = W_{ox}x_t$$

27.
$$z_{23}=z_{21}+z_{22}$$

28.
$$z_{24} = z_{23} + b_0$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18}=i_t\circ \tilde{C}_t$$

22.
$$C_t = Z_{17} + Z_{18}$$

7.
$$\nabla_{z_{18}}L = \nabla_{C_t}L$$

8.
$$\nabla_{z_{17}}L = \nabla_{C_t}L$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

22.
$$C_t = Z_{17} + Z_{18}$$

7.
$$\nabla_{z_{18}}L = \nabla_{C_t}L$$

8.
$$\nabla_{z_{17}}L = \nabla_{C_t}L$$

9.
$$\nabla_{i_t} L = \nabla_{z_{18}} L \circ \tilde{C}_t^T$$

10.
$$\nabla_{\tilde{C}_t} L = \nabla_{Z_{18}} L \circ i_t^T$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18}=i_t\circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

7.
$$\nabla_{z_{18}}L = \nabla_{C_t}L$$

8.
$$\nabla_{z_{17}}L = \nabla_{C_t}L$$

9.
$$\nabla_{i_t} L = \nabla_{z_{18}} L \circ \tilde{C}_t^T$$

10.
$$\nabla_{\tilde{C}_t} L = \nabla_{Z_{18}} L \circ i_t^T$$

11.
$$\nabla_{C_{t-1}} L += \nabla_{Z_{17}} L \circ f_t^T$$

12.
$$\nabla_{f_t} L = \nabla_{z_{17}} L \circ C_{t-1}^T$$

Second time we're computing a derivative for C_{t-1} , so we increment the derivative ("+=")

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

(19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18}=i_t\circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

7.
$$\nabla_{z_{18}}L = \nabla_{C_t}L$$

8.
$$\nabla_{Z_{17}}L = \nabla_{C_t}L$$

9.
$$\nabla_{i_t} L = \nabla_{z_{18}} L \circ \tilde{C}_t^T$$

10.
$$\nabla_{\tilde{C}_t} L = \nabla_{Z_{18}} L \circ i_t^T$$

11.
$$\nabla_{C_{t-1}} L += \nabla_{Z_{17}} L \circ f_t^T$$

12.
$$\nabla_{f_t} L = \nabla_{z_{17}} L \circ C_{t-1}^T$$

13.
$$\nabla_{z_{16}} L = \nabla_{\tilde{C}_t} L \circ \sigma(z_{16})^T \circ (1 - \sigma(z_{16}))^T$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

$$(18. \ z_{16} = z_{15} + b_C)$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

14.
$$\nabla_{bc}L = \nabla_{z_{16}}L$$

15.
$$\nabla_{z_{15}} L = \nabla_{z_{16}} L$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

(17.
$$z_{15} = z_{13} + z_{14}$$
)

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

14.
$$\nabla_{bc}L = \nabla_{z_{16}}L$$

15.
$$\nabla_{z_{15}} L = \nabla_{z_{16}} L$$

16.
$$\nabla_{b_C} L = \nabla_{z_{16}} L$$

17.
$$\nabla_{z_{15}}L = \nabla_{z_{16}}L$$

15.
$$z_{13} = W_{Ch} h_{t-1}$$

$$16. \ z_{14} = W_{Cx}x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

14.
$$\nabla_{b_C} L = \nabla_{z_{16}} L$$

15.
$$\nabla_{z_{15}} L = \nabla_{z_{16}} L$$

16.
$$\nabla_{b_C} L = \nabla_{z_{16}} L$$

17.
$$\nabla_{z_{15}} L = \nabla_{z_{16}} L$$

18.
$$\nabla_{W_{Cx}}L = x_t \nabla_{z_{14}}L$$

19.
$$\nabla_{x_t} L += \nabla_{z_{14}} L W_{Cx}$$

Note the "+="

15.
$$z_{13} = W_{Ch} h_{t-1}$$

16.
$$z_{14} = W_{Cx} x_t$$

17.
$$z_{15} = z_{13} + z_{14}$$

18.
$$z_{16} = z_{15} + b_C$$

19.
$$\tilde{C}_t = \sigma(z_{16})$$

20.
$$z_{17} = f_t \circ C_{t-1}$$

21.
$$z_{18} = i_t \circ \tilde{C}_t$$

22.
$$C_t = z_{17} + z_{18}$$

14.
$$\nabla_{b_c} L = \nabla_{z_{16}} L$$

15.
$$\nabla_{z_{15}}L = \nabla_{z_{16}}L$$

16.
$$\nabla_{b_C} L = \nabla_{z_{16}} L$$

17.
$$\nabla_{z_{15}}L = \nabla_{z_{16}}L$$

18.
$$\nabla_{W_{Cx}}L = x_t \nabla_{z_{14}}L$$

19.
$$\nabla_{x_t} L += \nabla_{z_{14}} L W_{Cx}$$

20.
$$\nabla_{W_{Ch}} L = h_{t-1} \nabla_{Z_{14}} L$$

21.
$$\nabla_{h_{t-1}}L += \nabla_{z_{13}}LW_{Ch}$$
Note the "+="

Continuing the computation

- Continue the backward progression until the derivatives from forward Equation 1 have been computed
- At this point all derivatives will be computed.

Overall procedure

- Express the overall computation as a sequence of unary or binary operations
 - Can be automated
- Computes derivatives incrementally, going backward over the sequence of equations!
- Since each atomic computation is simple and belongs to one of a small set of possibilities, the conversion to derivatives is trivial once the computation is serialized as above

May be easier to think of it in terms of a "derivative" routine

- Define a routine that returns derivatives for unary and binary operations
- SCALAR version (all variables are scalars)

```
function deriv(dz, x, y, operator)
  case operator:
    'none' : return dx
    '*' : return y*dz, dz*x
    '+' : return dz, dz
    '-' : return dz, -dz
    # Single argument operations
    'tanh' : return dz(1-tanh²(x))
    'sigmoid' : return dz sigmoid(x) (1-sigmoid(x))
```

Derivative routine, vector version

- Note distinction between component-wise and matrix multiplies
- Observe also that matrix and vector dimensions are correctly handled (locally)
- "o" is component-wise multiply
- "*" is matrix multiply

```
function deriv(dz, x, y, operator)
    case operator:
        'none' : return dx
       # component-wise "schur" multiply
        \circ': return dz \circ y^T, dz \circ x^T
       # Matrix multiply. X must be a matrix
        '*' : return y*dz, dz*x
        '+' : return dz, dz
        '-' : return dz, -dz
       # The following will expect a single argument
        'tanh' : return dz \circ (1-\tanh^2(x))^T
        'sigmoid' : return dz \circ sigmoid(x)^{T} \circ (1-sigmoid(x))^{T}
       # The jacobian is the full derivative matrix of the sigmoid
        'softmax' : return dz*Jacobian(sigmoid,x)
```

When to use "=" vs "+="

- In the forward computation a variable may be used multiple times to compute other intermediate variables
- During backward computations, the first time the derivative is computed for the variable, the we will use "="
- In subsequent computations we use "+="
- It may be difficult to keep track of when we first compute the derivative for a variable
 - When to use "=" vs when to use "+="
- Cheap trick:
 - Initialize all derivatives to 0 during computation
 - Always use "+="
 - You will get the correct answer (why?)

```
[dC_{t-1}, dx_t, dh_{t-1}, d[W,b]] = LSTM derivative(dC_t dh_t)
     initialize d(variable) = 0 (all variables)
     # Derivative of eq. 31 h_t = o_t \circ z_{25}
     [do_{+}, dz_{25}] += deriv(dh_{+}, o_{+}, z_{25}, ' \circ ')
     # Derivative of eq. 30 z_{25} = \tanh(C_t)
     [dC_+] += deriv(dz_{25}, C_+, 'tanh')
     # Derivative of eq. 29 o_t = \sigma(z_{24})
     [dz_{25}] += deriv(do_t, z_{25}, 'sigmoid')
     # Derivative of eq. 28 z_{24} = z_{23} + b_0
     [dz_{23}, db_0] += deriv(dz_{24}, z_{23}, b_0, '+')
     # Derivative of eq. 27 z_{23} = z_{21} + z_{22}
     [dz_{21}, dz_{22}] += deriv(dz_{23}, z_{21}, z_{22}, '+')
     # Derivative of eq. 26 z_{22}=W_{ox}x_t
     [dW_{ox}, dx_t] += deriv(dz_{22}, W_{ox}, x_t, '*')
     # Derivative of eq. 25 z_{21}=z_{19}+z_{20}
     [dz_{19}, dz_{20}] += deriv(dz_{21}, z_{19}, z_{20}, '+')
     # Derivative of eq. 24 z_{20}=W_{oh}h_{t-1}
     [dW_{oh}, dh_{t-1}] += deriv(dz_{20}, W_{oh}, h_{t-1}, '*')
     # Derivative of eq. 23 z_{19}=W_{oC}C_{t-1}
     [dW_{oC}, dC_{t-1}] += deriv(dz_{19}, W_{oC}, C_{t-1}, '*')
```

23.
$$z_{19} = W_{oC}C_{t-1}$$

24. $z_{20} = W_{oh}h_{t-1}$

25.
$$z_{21} = z_{19} + z_{20}$$

26.
$$z_{22} = W_{ox} x_t$$

27.
$$z_{23} = z_{21} + z_{22}$$

28.
$$z_{24} = z_{23} + b_o$$

29.
$$o_t = \sigma(z_{24})$$

30.
$$z_{25} = \tanh(C_t)$$

31.
$$h_t = o_t \circ z_{25}$$

```
... continued from previous slide
     # Derivative of eq. 22 C_t=z_{17}+z_{18}
     [dz_{17}, dz_{18}] += deriv(dC_{t}, z_{18}, z_{18}, '+')
     \# Derivative of eq. 21 z_{18}=i_t\circ 	ilde{\mathcal{C}}_t
     [di<sub>t</sub>, dtildeC<sub>t</sub>] += deriv(dz<sub>18</sub>,i<sub>t</sub>, dtildeC<sub>t</sub>,'o')
     # Derivative of eq. 20 z_{17}=f_t \circ C_{t-1}
                                                                           15. z_{13} = W_{Ch} h_{t-1}
     [df_{t}, dC_{t-1}] += deriv(dz_{17}, f_{t}, C_{t-1}, ' \circ ')
                                                                           16. z_{14} = W_{Cx} x_t
     # Derivative of eq. 19 \tilde{C}_t = \sigma(z_{16})
                                                                           17. Z_{15}=Z_{13}+Z_{14}
                                                                           18. z_{16} = z_{15} + b_C
     [dz<sub>16</sub>] += deriv(dtildeC<sub>+</sub>,'sigmoid')
                                                                           19. \tilde{C}_t = \sigma(z_{16})
     # Derivative of eq. 18 z_{16}=z_{15}+b_C
                                                                           20. z_{17} = f_t \circ C_{t-1}
     [dz_{15}, db_c] += deriv(dz_{16}, z_{15}, b_c, '+')
                                                                           21. z_{18} = i_t \circ \tilde{C}_t
     # Derivative of eq. 17 z_{15} = z_{13} + z_{14}
                                                                           22. C_t = Z_{17} + Z_{18}
     [dz_{13}, dz_{14}] += deriv(dz_{15}, z_{13}, z_{14}, '+')
     # Derivative of eq. 16 z_{14}=W_{Cx}x_t
     [dW_{Cx}, dx_t] += deriv(dz_{14}, W_{Cx}, x_t, '*')
     # Derivative of eq. 15 z_{13}=W_{Ch}h_{t-1}
     [dW_{Ch}, dh_{t-1}] += deriv(dz_{13}, W_{Ch}, h_{t-1}, '*')
```

```
... continued from previous slide
    # Derivative of eq. 14 i_t = \sigma(z_{12})
    [dz<sub>12</sub>] += deriv(di<sub>t</sub>,'sigmoid')
    # Derivative of eq. 13 z_{12}=z_{11}+b_f
    [dz_{11}, db_{i}] += deriv(dz_{12}, z_{11}, b_{i}, '+')
    # Derivative of eq. 12 z_{11} = z_9 + z_{10}
    [dz_9, dz_{10}] += deriv(dz_{11}, z_9, z_{10}, '+')
    # Derivative of eq. 11 z_{10}=W_{ix}x_t
    [dW_{ix}, dx_{t}] += deriv(dz_{10}, W_{ix}, x_{t}, '+')
    # Derivative of eq. 10 z_9=z_7+z_8
    [dz_7, dz_8] += deriv(dz_9, z_7, z_8, '+')
    # Derivative of eq. 9 z_8 = W_{ih}h_{t-1}
    [dW_{ih}, dh_{t-1}] += deriv(dz_8, W_{ih}, h_{t-1}, '*')
    # Derivative of eq. 8 z_7 = W_{iC}C_{t-1}
    [dW_{ic}, dC_{t-1}] += deriv(dz_7, W_{ic}, C_{t-1}, '*')
```

8.
$$z_7 = W_{iC}C_{t-1}$$

9. $z_8 = W_{ih}h_{t-1}$
10. $z_9 = z_7 + z_8$
11. $z_{10} = W_{ix}x_t$
12. $z_{11} = z_9 + z_{10}$
13. $z_{12} = z_{11} + b_i$
14. $i_t = \sigma(z_{12})$

```
... continued from previous slide
    # Derivative of eq. 7 f_t = \sigma(z_6)
    [dz<sub>6</sub>] += deriv(df<sub>t</sub>,'sigmoid')
    # Derivative of eq. 6 z_6 = z_5 + b_f
    [dz_5, db_f] += deriv(dz_6, z_5, b_f, '+')
    # Derivative of eq. 5 z_5=z_3+z_4
    [dz_3, dz_4] += deriv(dz_5, z_3, z_4, '+')
    # Derivative of eq. 4 z_4 = W_{fx}x_t
    [dW_{fx}, dx_{+}] += deriv(dz_{4}, W_{fx}, x_{+}, '*')
    # Derivative of eq. 3 z_3=z_1+z_2
    [dz_1, dz_2] += deriv(dz_3, z_1, z_2, '+')
    # Derivative of eq. 2 z_2 = W_{fh}h_{t-1}
    [dW_{fh}, dh_{t-1}] += deriv(dz_2, W_{fh}, h_{t-1}, '*')
    # Derivative of eq. 1 z_1 = W_{fC}C_{t-1}
    [dW_{fC}, dC_{t-1}] += deriv(dz_7, W_{fC}, C_{t-1}, '*')
    return dC_{t-1}, dh_{t-1}, dx_t, d[W,b]
```

1.
$$z_1 = W_{fC}C_{t-1}$$

2. $z_2 = W_{fh}h_{t-1}$
3. $z_3 = z_1 + z_2$
4. $z_4 = W_{fx}x_t$
5. $z_5 = z_3 + z_4$
6. $z_6 = z_5 + b_f$
7. $f_t = \sigma(z_6)$

Caveats

- The deriv() routine given is missing several operators
 - Operations involving constants (z = 2y, z = 1-y, z = 3+y)
 - Division and inversion (e.g z = x/y, z = 1/y, $z = A^{-1}$)
 - You may have to extend it to deal with these, or rewrite your equations to eliminate such operations if possible
- In practice many of the operations will be grouped together for computational efficiency
 - And to take advantage of parallel processing capabilities
- But the basic principle applies to *any* computation that can be expressed as a serial operation of unary and binary relations
 - If you can do it on a computer, you can express it as a serial operation
- In fact the preceding logic is exactly what we use to compute derivatives in backprop
 - We saw this explicitly in the vector version of BP for MLPs.