FoML

24 Backpropagation

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Recap

- Gradient of a scalar valued function $f(\mathbf{x})$: $\mathbf{x} \to \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_D}\right)$

Recap

- Gradient of a scalar valued function $f(\mathbf{x})$: $\mathbf{x} \rightarrow \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_D}\right)$
- Gradient of a vector valued function $\mathbf{f}(\mathbf{x})$ is called Jacobian:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{f}}{\partial x_1} & \cdots & \frac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^{\mathrm{T}} f_1 \\ \vdots \\ \nabla^{\mathrm{T}} f_m \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

MLP: Some Notation

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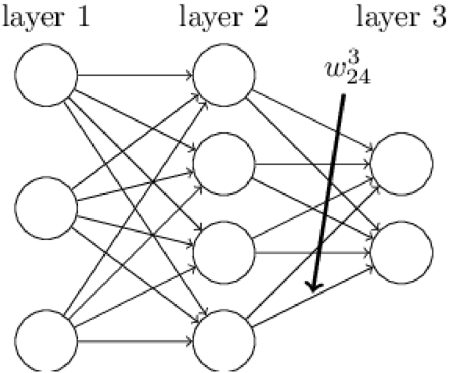

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4. Vector of activations (or, biases) at a layer l is denoted by a bold-faced $\mathbf{x}^l$ (or $\mathbf{b}^l$) and W^l is the matrix of weights into layer l

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4. σ is the activation function that applies element-wise

Gradient descent on MLP

- Loss is $\mathcal{L}(W, \mathbf{b}) = \sum_n l(f(x_n; W, \mathbf{b}), y_n) = \sum_n l(\mathbf{x}^L, y_n)$ (L is the number of layers in the MLP)

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- For applying Gradient descent, we need gradient of individual sample loss with respect to all the model parameters

$$l_n = l(f(x_n; W, \mathbf{b}), y_n)$$

$\frac{\partial l_n}{\partial W_{jk}^{(l)}}$ and $\frac{\partial l_n}{\partial \mathbf{b}_j^{(l)}}$ for all layers l

Forward pass operation

$$x^{(0)} = x \xrightarrow{W^{(1)}, \mathbf{b}^{(1)}} s^{(1)} \xrightarrow{\sigma} x^{(1)} \xrightarrow{W^{(2)}, \mathbf{b}^{(2)}} s^{(2)} \ldots x^{(L-1)} \xrightarrow{W^{(L)}, \mathbf{b}^{(L)}} s^{(L)} \xrightarrow{\sigma} x^{(L)} = f(x; W, \mathbf{b})$$

Formally, $x^{(0)} = x, f(x; W, \mathbf{b}) = x^{(L)}$

$$\forall l = 1, \ldots, L \quad \begin{cases} s^{(l)} & = W^{(l)} x^{(l-1)} + \mathbf{b}^{(l)} \\ x^{(l)} & = \sigma(s^{(l)}) \end{cases}$$

Chain rule of differential calculus

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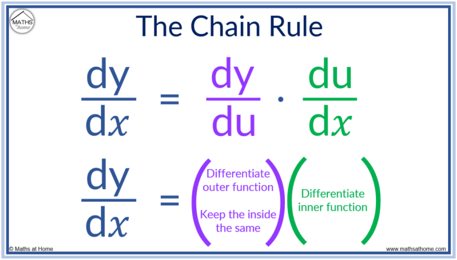
- $$(f \circ g)'(x) = f'(g(x)) \cdot g'(x)$$
- $$\frac{\partial}{\partial x} f(g(x)) = \left.\frac{\partial f(a)}{\partial a}\right|_{a=g(x)} \cdot \frac{\partial g(x)}{\partial x}$$

Chain rule of differential calculus



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- $z = g(x) \rightarrow \Delta z = \frac{dg(x)}{dx} \Delta x$

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- $y = f(z) \rightarrow \Delta y = \frac{df}{dz} \Delta z = \frac{df}{dz} \frac{dg(x)}{dx} \Delta x = \frac{df}{dg(x)} \frac{dg(x)}{dx} \Delta x$

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3. Let $g_i(x) = z_i \rightarrow y = f(z_1, z_2, \ldots, z_M)$

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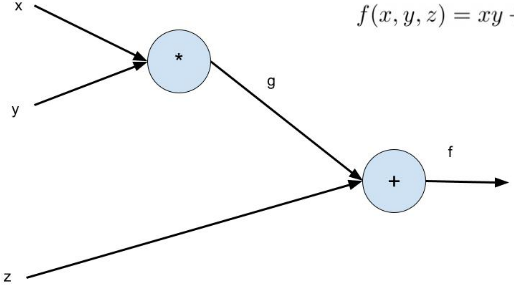
7. $\Delta y = \left(\frac{\partial f}{\partial g_1(x)} \frac{dg_1(x)}{dx} + \frac{\partial f}{\partial g_2(x)} \frac{dg_2(x)}{dx} + \ldots + \frac{\partial f}{\partial g_M(x)} \frac{dg_M(x)}{dx} \right) \Delta x$

Chain rule of differential calculus

1. $f(x) = e^{sin(x^2)}$, let's find $\frac{\partial f}{\partial x}$

Chain rule of differential calculus

$$g = xy$$
$$f = g + z$$
$$f(x, y, z) = xy + z$$



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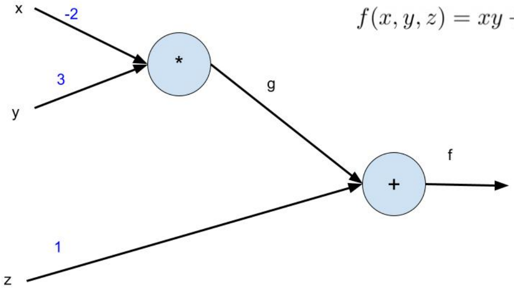

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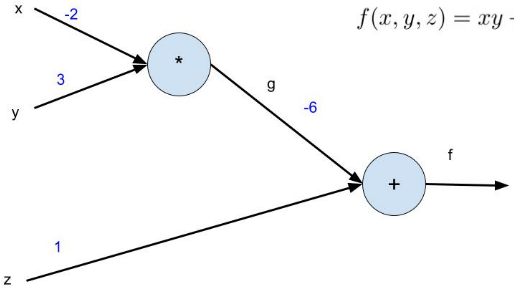

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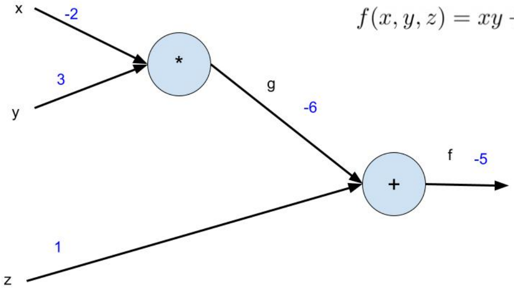

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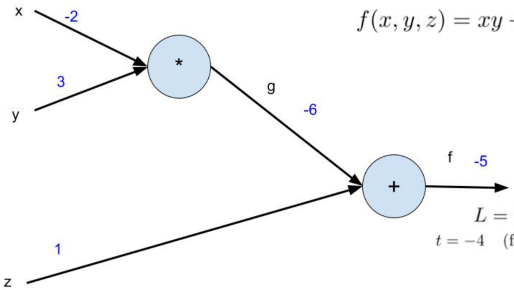

$$L = (f - t)^2$$

$t = -4$ (for this input)

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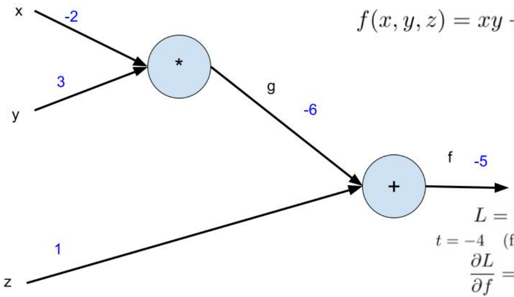

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$$\frac{\partial L}{\partial f} = 2(f - t)$$

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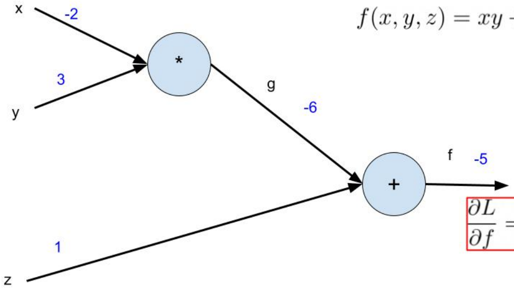

$$\boxed{\frac{\partial L}{\partial f} = -2}$$

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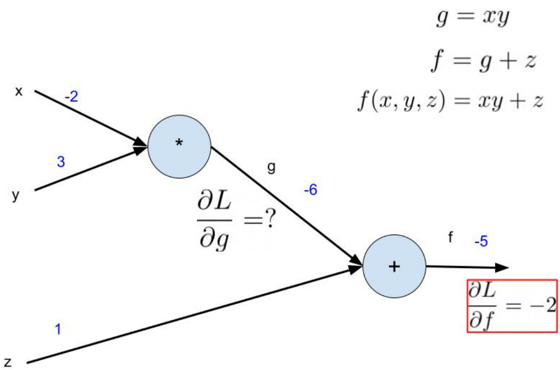

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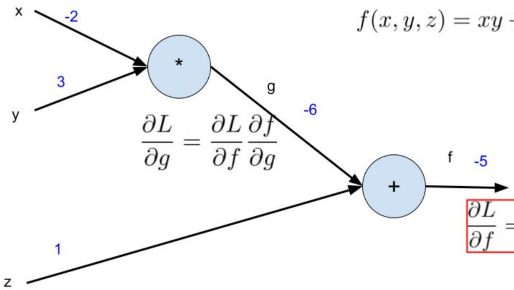

$$\frac{\partial L}{\partial g} = \frac{\partial L}{\partial f}\frac{\partial f}{\partial g}$$

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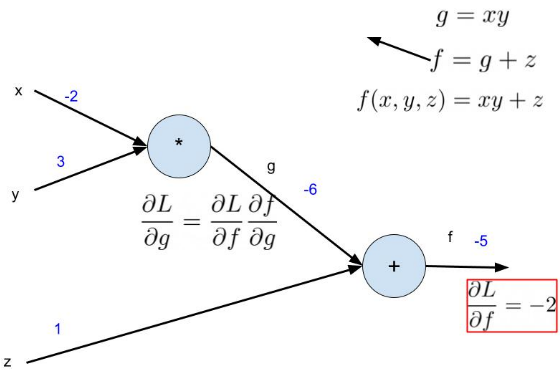

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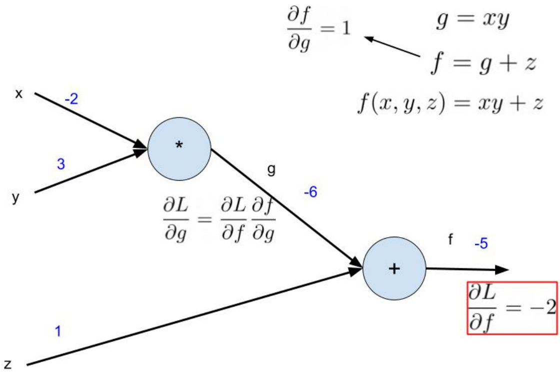

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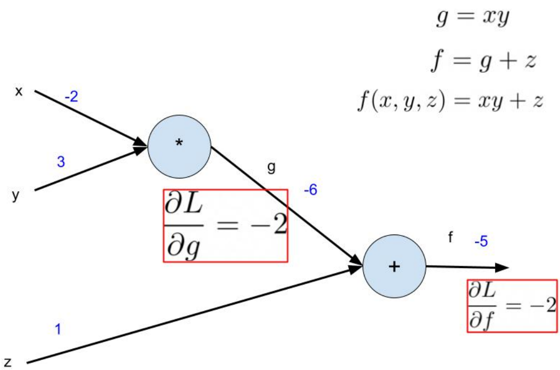

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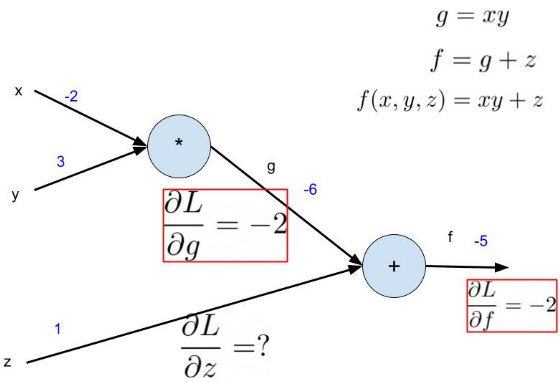

Chain rule of differential calculus

భారతీయ సాంకేతిక విజ్ఞాన సంస్థ హైదరాబాద్
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
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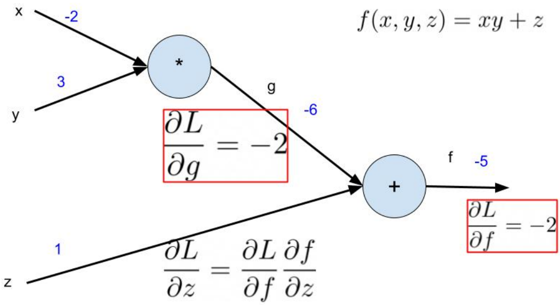

$$\boxed{\frac{\partial L}{\partial g} = -2}$$

$$\boxed{\frac{\partial L}{\partial f} = -2}$$

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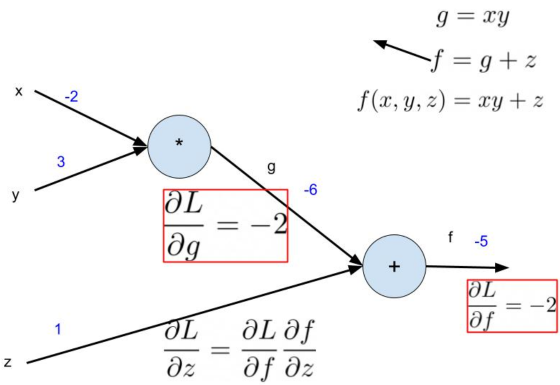
Chain rule of differential calculus



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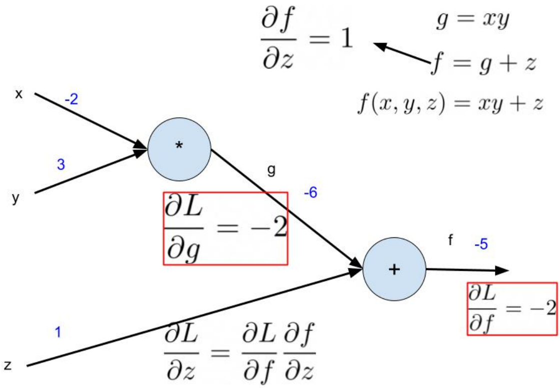

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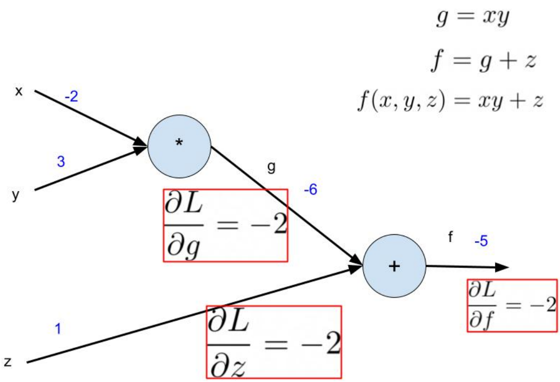

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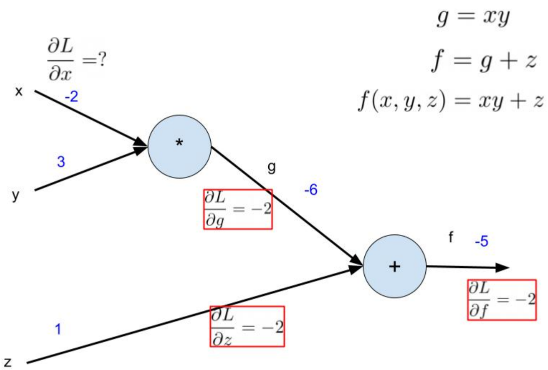

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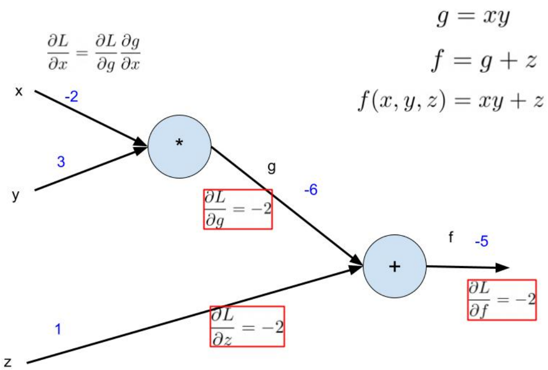

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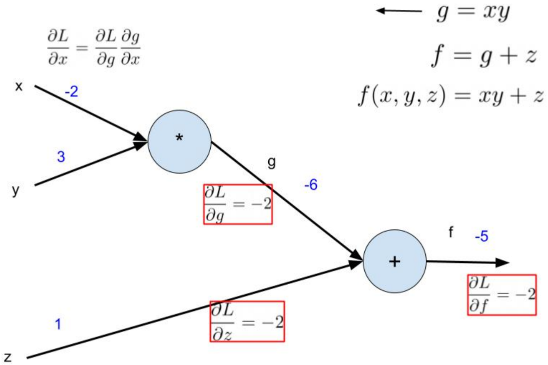

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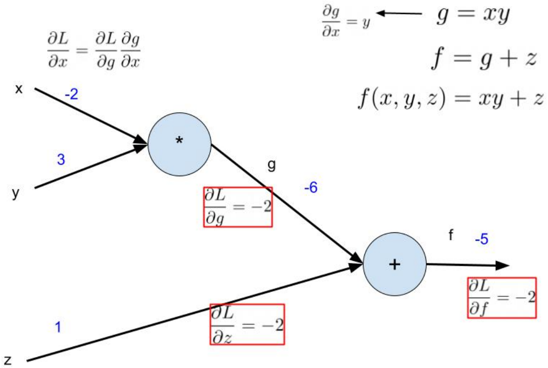

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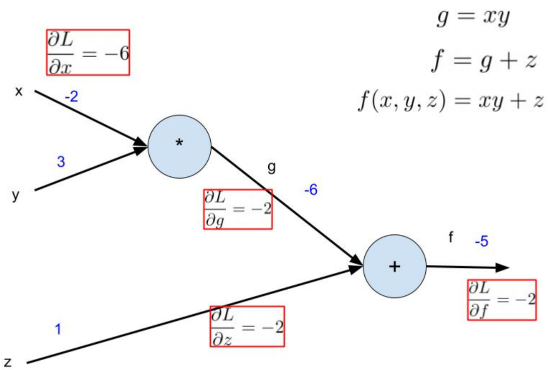

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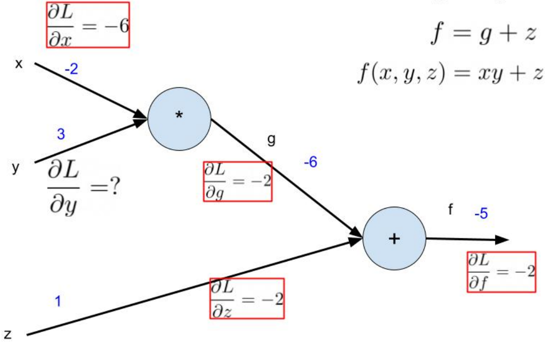

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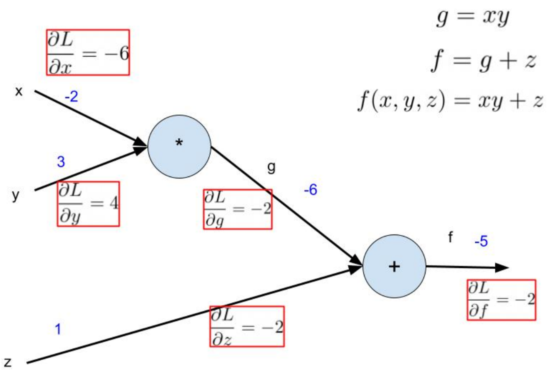
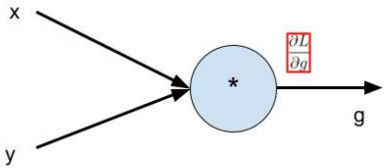


Gradient Flow



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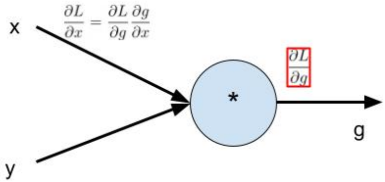

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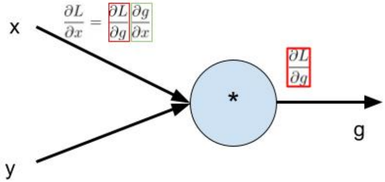

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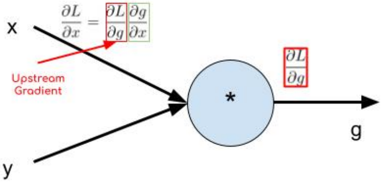

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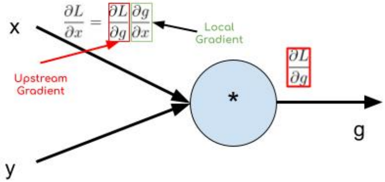

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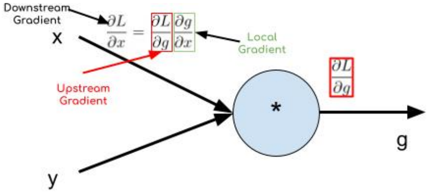

Chain rule of differential calculus for an MLP

- $$J_{f_N \circ f_{N-1} \circ \ldots f_1(x)} = J_{f_N(f_{N-1}(\ldots f_1(x)))} \cdot J_{f_{N-1}(f_{N-2}(\ldots f_1(x)))} \cdots J_{f_2(f_1(x))} \cdot J_{f_1(x)}$$

  $J_{f(x)}$ is Jacobian of f computed at x.

Consider a specific Layer

- $x^{(l-1)} \xrightarrow{W^{(l)},\mathbf{b}^{(l)}} s^{(l)} \xrightarrow{\sigma} x^{(l)}$

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- $x^{(l-1)} \xrightarrow{W^{(l)},\mathbf{b}^{(l)}} s^{(l)} \xrightarrow{\sigma} x^{(l)}$
- $x_i^{(l)} = \sigma(s_i^{(l)})$
- Since $s^{(l)}$ influences loss $\mathcal{L}$ through only $x^{(l)}$,

$$\frac{\partial \ell}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \sigma'(s_i^{(l)})$$

Consider a specific Layer

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$$\frac{\partial \ell}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \frac{\partial x_i^{(l)}}{\partial s_i^{(l)}} = \frac{\partial \ell}{\partial x_i^{(l)}} \sigma'(s_i^{(l)})$$

- $$s_i^{(l)} = \Sigma_j W_{i,j}^{(l)} x_j^{(l-1)} + b_i^{(l)}$$

Consider a specific Layer

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भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

- $x^{(l-1)} \xrightarrow{W^{(l)}, \mathbf{b}^{(l)}} s^{(l)} \xrightarrow{\sigma} x^{(l)}$
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- $$\frac{\partial \ell}{\partial W_{i,j}^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} \frac{\partial s_i^{(l)}}{\partial W_{i,j}^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} x_j^{(l-1)} \tag{1}$$
- $$\frac{\partial \ell}{\partial b_i^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} \frac{\partial s_i^{(l)}}{\partial b_i^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} \tag{2}$$

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- Then wrt the parameters

$$\frac{\partial \ell}{\partial w_{i,j}^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}} x_j^{(l-1)} \text{ and } \frac{\partial \ell}{\partial b_i^{(l)}} = \frac{\partial \ell}{\partial s_i^{(l)}}$$

Jocobian in Tensorial form

- $\psi : \mathcal{R}^N \rightarrow \mathcal{R}^M$ then $\left[\frac{\partial \psi}{\partial x}\right] = \begin{bmatrix} \frac{\partial \psi_1}{\partial x_1} & \cdots & \frac{\partial \psi_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi_M}{\partial x_1} & \cdots & \frac{\partial \psi_M}{\partial x_N} \end{bmatrix}$

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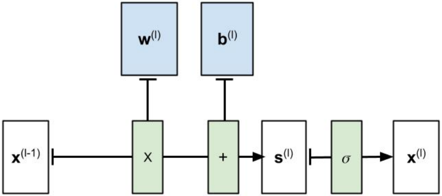
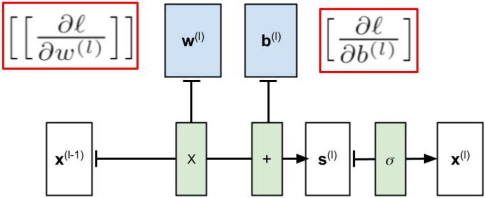
- $\psi : \mathcal{R}^{N \times M} \rightarrow \mathcal{R}$ then $\left[\left[\frac{\partial \psi}{\partial x}\right]\right] = \begin{bmatrix} \frac{\partial \psi}{\partial w_{1,1}} & \cdots & \frac{\partial \psi}{\partial w_{1,M}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \psi}{\partial w_{N,1}} & \cdots & \frac{\partial \psi}{\partial w_{N,M}} \end{bmatrix}$

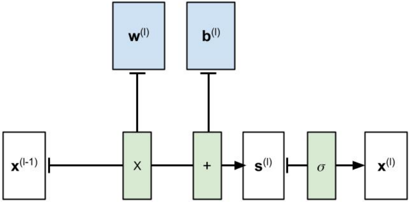
Forward Pass



Goal of Backward Pass

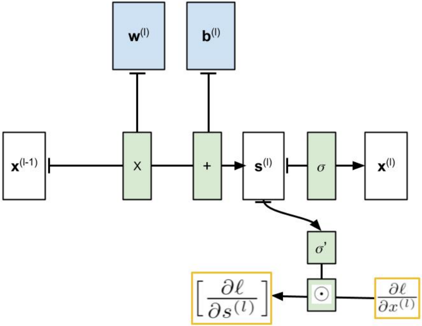


Begin from succeeding layer

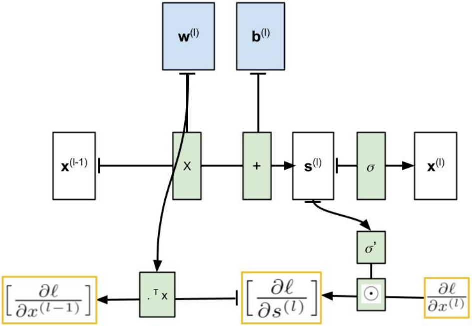


$$\boxed{\frac{\partial \ell}{\partial x^{(l)}}}$$

Begin from succeeding layer



Begin from succeeding layer



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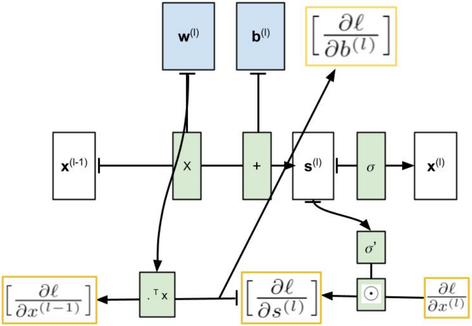

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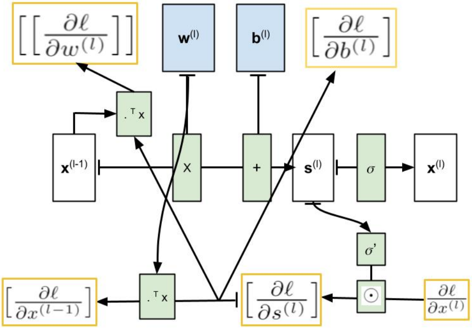

Update the parameters

- $W^{(l)} = W^{(l)} - \eta \left[\left[\frac{\partial \ell}{\partial w^{(l)}} \right] \right]$ and $\mathbf{b}^{(l)} = \mathbf{b}^{(l)} - \eta \left[\frac{\partial \ell}{\partial b^{(l)}} \right]$

Observations

- BP is basically simple: applying chain rule iteratively

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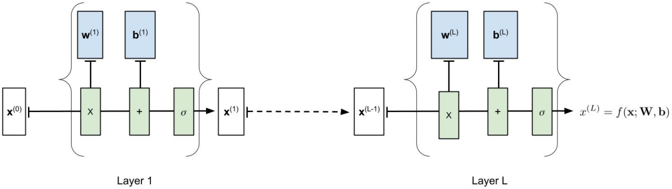
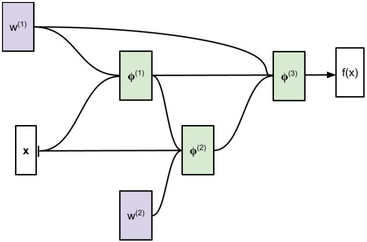
- Heavy computations are with the linear operations
- Nonlinearities go into simple element wise operations
- BP Needs all the intermediate layer results to be in memory
- Takes twice the computations of forward pass

Beyond MLP

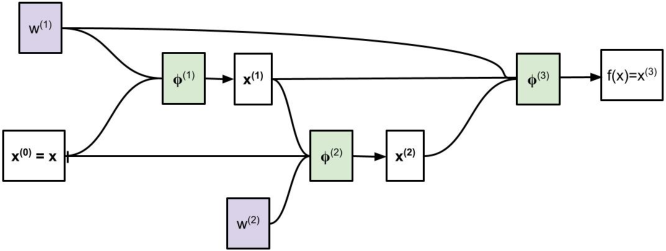
- We can generalize MLP





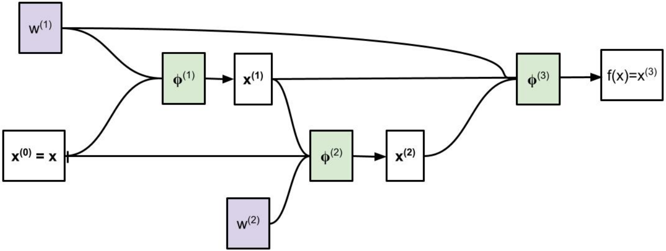
To an arbitrary Directed Acyclic Graph (DAG)

Forward pass in the computational graph



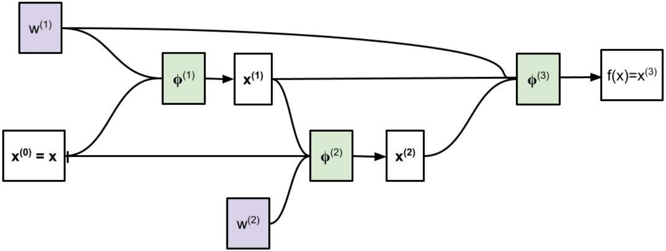
- $x^{(0)} = x$

Forward pass in the computational graph



- $x^{(0)} = x$
- $x^{(1)} = \phi^{(1)}(x^{(0)}; w^{(1)})$

Forward pass in the computational graph



- $x^{(0)} = x$
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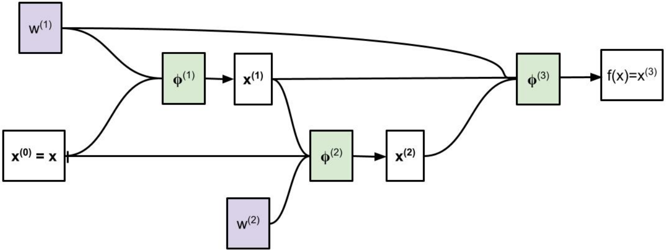
- $x^{(2)} = \phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)})$

Forward pass in the computational graph



- $x^{(0)} = x$
- $x^{(1)} = \phi^{(1)}(x^{(0)}; w^{(1)})$
- $x^{(2)} = \phi^{(2)}(x^{(0)}, x^{(1)}; w^{(2)})$
- $f(x) = x^{(3)} = \phi^{(3)}(x^{(1)}, x^{(2)}; w^{(1)})$

Notation: Jacobian of a general transformation

-
$$\text{if } (a_1 \dots a_Q) = \phi(b_1 \dots b_R) \text{ then we use the notation} \tag{3}$$
$$\left[\frac{\partial a}{\partial b}\right] = J_\phi^T = \begin{bmatrix} \frac{\partial a_1}{\partial b_1} & \cdots & \frac{\partial a_Q}{\partial b_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_1}{\partial b_R} & \cdots & \frac{\partial a_Q}{\partial b_R} \end{bmatrix} \tag{4}$$

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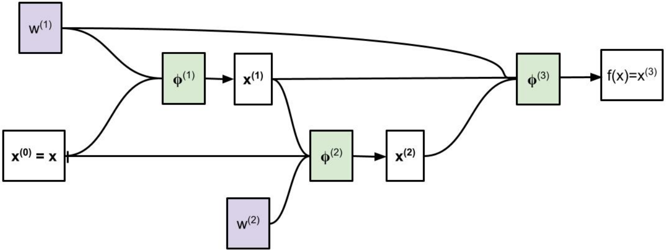
- $$\text{if } (a_1 \ldots a_Q) = \phi(b_1 \ldots b_R; c_1 \ldots c_S) \text{ then we use the notation} \tag{5}$$
  $$\left[\frac{\partial a}{\partial c}\right] = J_{\phi|c}^T = \begin{bmatrix} \frac{\partial a_1}{\partial c_1} & \cdots & \frac{\partial a_Q}{\partial c_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_1}{\partial C_S} & \cdots & \frac{\partial a_Q}{\partial c_S} \end{bmatrix} \tag{6}$$

Backward pass



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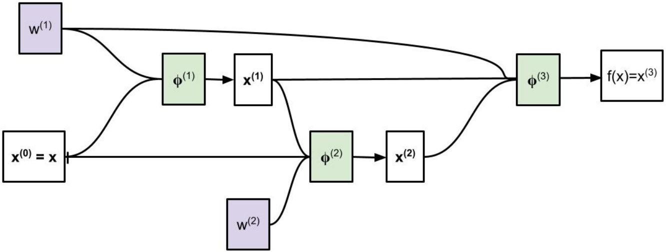
Backward pass



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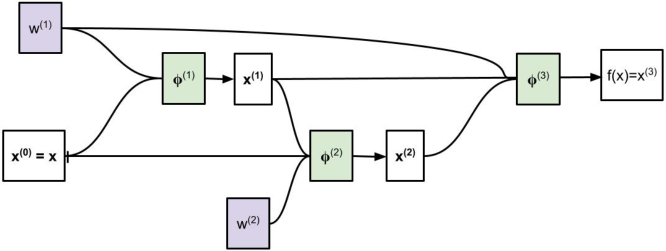
- $$\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = \left[\frac{\partial x^{(3)}}{\partial x^{(2)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] = J^T_{\phi^{(3)}|x^{(2)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right]$$

Backward pass



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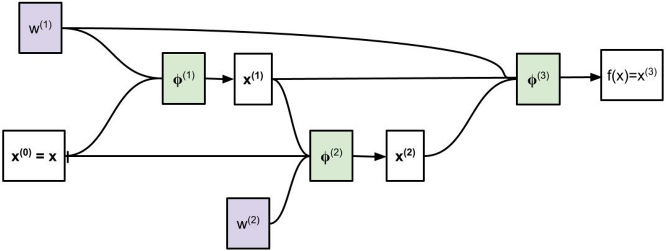
- $$\begin{aligned}\left[\frac{\partial \ell}{\partial x^{(1)}}\right] &= \left[\frac{\partial x^{(3)}}{\partial x^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] + \left[\frac{\partial x^{(2)}}{\partial x^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(2)}}\right] \\ &= J^T_{\phi^{(3)}|x^{(1)}}\left[\frac{\partial \ell}{\partial x^{(3)}}\right] + J^T_{\phi^{(2)}|x^{(1)}}\left[\frac{\partial \ell}{\partial x^{(2)}}\right]\end{aligned}$$

Backward pass



- $$\left[\frac{\partial \ell}{\partial w^{(1)}}\right] = \left[\frac{\partial x^{(3)}}{\partial w^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(3)}}\right] + \left[\frac{\partial x^{(1)}}{\partial w^{(1)}}\right]\left[\frac{\partial \ell}{\partial x^{(1)}}\right]$$
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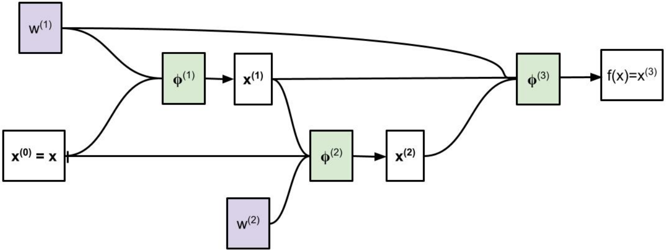
Backward pass



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- $$\left[\frac{\partial \ell}{\partial w^{(2)}}\right] = \left[\frac{\partial x^{(2)}}{\partial w^{(2)}}\right]\left[\frac{\partial \ell}{\partial x^{(2)}}\right] = J^T_{\phi^{(2)}|w^{(2)}}\left[\frac{\partial \ell}{\partial x^{(2)}}\right]$$