Applied Machine Learning

Gradient Computation & Automatic Differentiation

Siamak Ravanbakhsh

COMP 551 (winter 2020)

Learning objectives

using the chain rule to calculate the gradients

automatic differentiation

- forward mode
- reverse mode (backpropagation)

Landscape of the cost function

model two layer MLP

$$f(x; W, V) = g\big(Wh(Vx)\big)$$

image credit: https://www.offconvex.org

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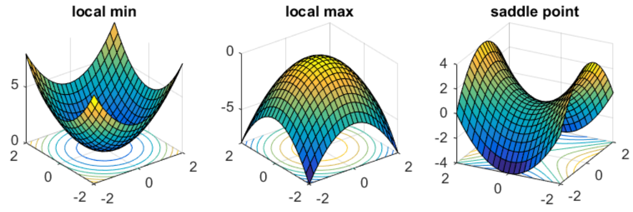

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given one global optimum we can

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- for symmetric activations: negate input/ouput of a unit
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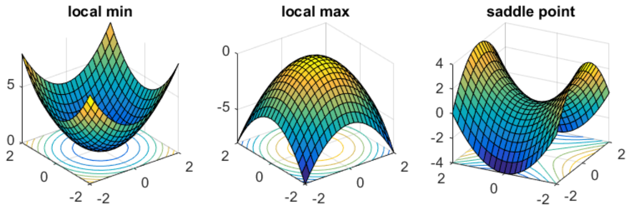

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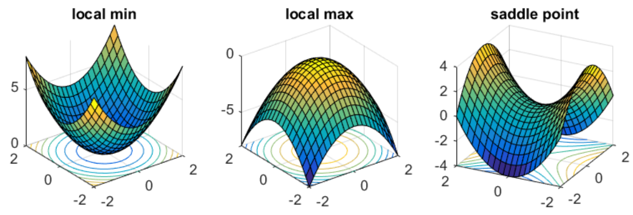

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general beliefs

supported by empirical and theoretical results in a special settings

many more saddle points than local minima

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number of local minima increases for lower costs

therefore most local optima are close to global optima

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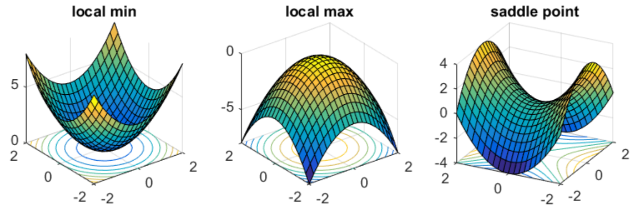

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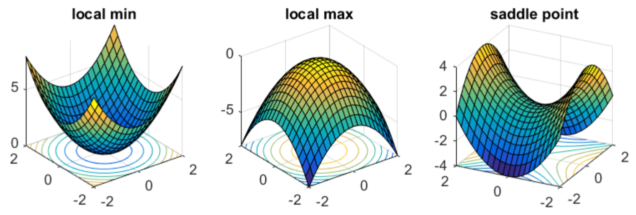

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strategy use gradient descent methods (covered earlier in the course)

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Jacobian matrix

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note that we use J also for cost function

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what if W is a matrix? we assume it is reshaped it into a vector for these calculations

Chain rule

for $f : x \mapsto z \quad \text{and} \quad h : z \mapsto y$ where $x, y, z \in \mathbb{R}$

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speed of change in z as we change x

speed of change in y as we change z

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we are looking at all the "paths" through which change in x_d *changes* y_c *and add their contribution*

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in matrix form $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial z} \frac{\partial z}{\partial x}$

C x D Jacobian

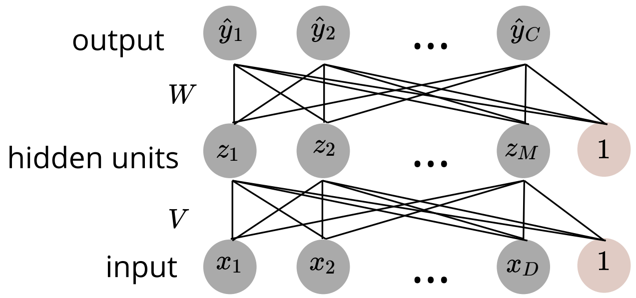
M x D Jacobian

C x M Jacobian

Training a two layer network

suppose we have

- D inputs $x_1, \ldots, x_D$
- C outputs $\hat{y}_1, \ldots, \hat{y}_C$
- M hidden *units* $z_1, \ldots, z_M$



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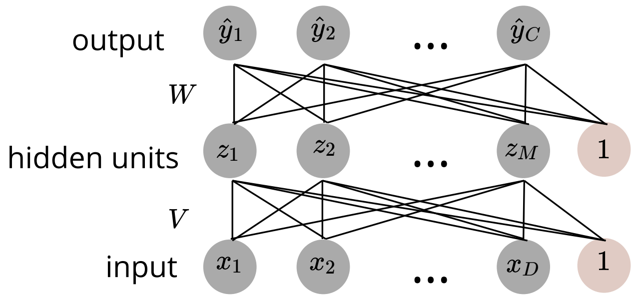

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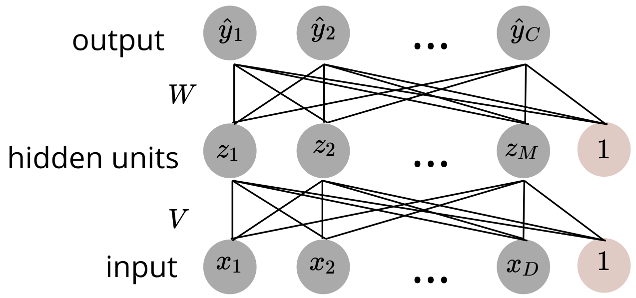

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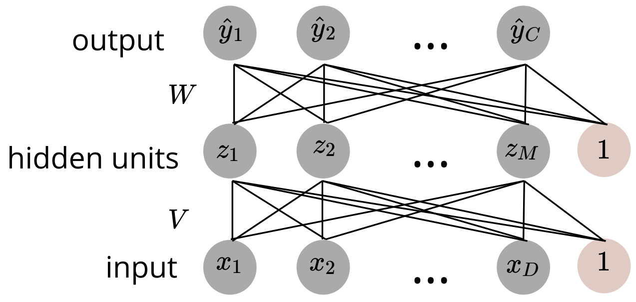

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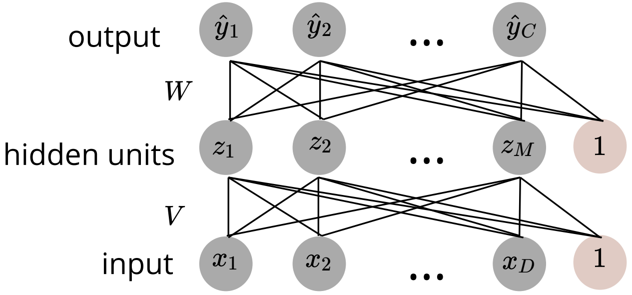
so we will calculate $\frac{\partial}{\partial W} L,\ \frac{\partial}{\partial V} L$ and recover $\frac{\partial}{\partial W} J = \sum_{n=1}^{N} \frac{\partial}{\partial W} L(y^{(n)}, \hat{y}^{(n)})$ and $\frac{\partial}{\partial V} J = \sum_{n=1}^{N} \frac{\partial}{\partial V} L(y^{(n)}, \hat{y}^{(n)})$



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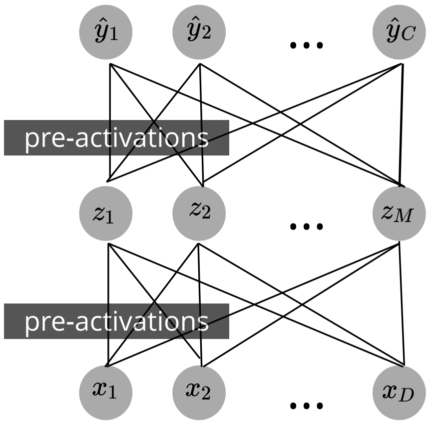
Gradient calculation



Gradient calculation

$$L(y, \hat{y})$$

$$\uparrow$$

$$\hat{y}_c = g(u_c)$$

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$$u_c = \sum_{m=1}^{M} W_{c,m} z_m$$

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$$z_m = h(q_m)$$

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$$q_m = \sum_{d=1}^{D} V_{m,d} x_d$$

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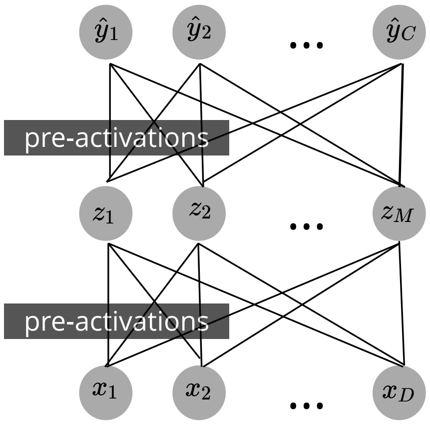
$$x_d$$



Gradient calculation

using the chain rule

$$\frac{\partial}{\partial W_{c,m}} L = \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial W_{c,m}}$$

depends on the loss function

depends on the activation function

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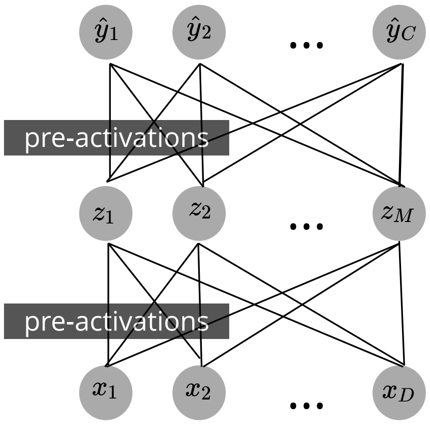

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similarly for V

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial z_m} \frac{\partial z_m}{\partial q_m} \frac{\partial q_m}{\partial V_{m,d}}$$

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$W_{c,m}$

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depends on the activation function

depends on the middle layer activation

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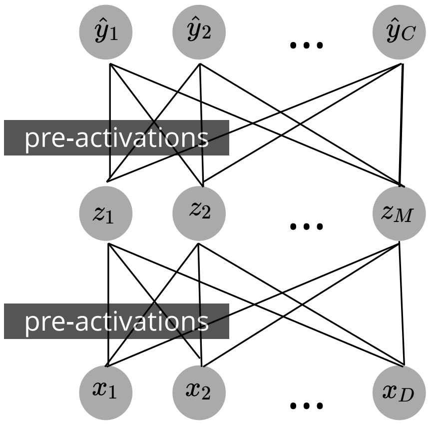

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regression

$$\begin{cases} \hat{y} = g(u) = u = Wz \\ L(y, \hat{y}) = \frac{1}{2}||y - \hat{y}||_2^2 \end{cases}$$

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taking derivative

$$\frac{\partial}{\partial W_{c,m}} L = (\hat{y}_c - y_c) z_m$$

we have seen this in linear regression lecture

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binary classification

scalar output C=1

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substituting and simplifying (see logistic regression lecture)

$$L(y, u) = y \log(1 + e^{-u}) + (1-y) \log(1 + e^{u})$$

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$$x_d$$

binary classification

scalar output C=1

$$\begin{cases} \hat{y} = g(u) = \left(1 + e^{-u}\right)^{-1} \\ L(y, \hat{y}) = y \log \hat{y} + (1 - y) \log(1 - \hat{y}) \end{cases}$$

substituting and simplifying (see logistic regression lecture)

$$\begin{cases} L(y, u) = y \log(1 + e^{-u}) + (1 - y) \log(1 + e^{u}) \\ u = \sum_m W_m z_m \end{cases}$$

substituting u in L and taking derivative $\frac{\partial}{\partial W_m} L = (\hat{y} - y) z_m$

Gradient calculation

using the chain rule

$$\frac{\partial}{\partial W_{c,m}} L = \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial W_{c,m}}$$

depends on the loss function

depends on the activation function

z_m

multiclass classification

C is the number of classes

$$\begin{cases} y = g(u) = \mathrm{softmax}(u) \\ L(y, \hat{y}) = \sum_k y_k \log \hat{y}_k \end{cases}$$

$L(y, \hat{y})$

$\hat{y}_c = g(u_c)$

$u_c = \sum_{m=1}^{M} W_{c,m} z_m$

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$$L(y, \hat{y})$$

$$\uparrow$$

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Gradient calculation

gradient wrt V:

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_m} \underbrace{\frac{\partial u_m}{\partial z_m}}_{W_{k,m}} \frac{\partial z_m}{\partial q_m} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{x_d}$$

depends on the middle layer activation

$$L(y, \hat{y})$$

$$\hat{y}_c = g(u_c)$$

$$u_c = \sum_{m=1}^{M} W_{c,m} z_m$$

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Gradient calculation

gradient wrt V:

we already did this part

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \boxed{\frac{\partial L}{\partial \hat{y}_c}\frac{\partial \hat{y}_c}{\partial u_m}} \underbrace{\frac{\partial u_m}{\partial z_m}}_{W_{k,m}} \frac{\partial z_m}{\partial q_m} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{x_d}$$

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$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \overbrace{\frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_m}}^{\text{we already did this part}} \underbrace{\frac{\partial u_m}{\partial z_m}}_{W_{k,m}} \underbrace{\frac{\partial z_m}{\partial q_m}}_{\text{depends on the middle layer activation}} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{x_d}$$

logistic function	$\sigma(q_m)(1-\sigma(q_m))$
hyperbolic tan.	$1-\tanh(q_m)^2$
ReLU	$\begin{cases} 0 & q_m \leq 0 \\ 1 & q_m > 0 \end{cases}$

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x_d

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gradient wrt V:

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$$x_d$$

example logistic sigmoid

$$\frac{\partial}{\partial V_{m,d}} J = \sum_n \sum_c (\hat{y}_c^{(n)} - y_c^{(n)}) W_{c,m} \sigma(q_m^{(n)})(1-\sigma(q_m^{(n)})) x_d^{(n)}$$

Gradient calculation

gradient wrt V:

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \overbrace{\boxed{\frac{\partial L}{\partial \hat{y}_c}\frac{\partial \hat{y}_c}{\partial u_m}}}^{\text{we already did this part}} \underbrace{\frac{\partial u_m}{\partial z_m}}_{W_{k,m}} \underbrace{\frac{\partial z_m}{\partial q_m}}_{\text{depends on the middle layer activation}} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{x_d}$$

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$$= \sum_n \sum_c (\hat{y}_c^{(n)} - y_c^{(n)}) W_{c,m} z_m^{(n)} (1 - z_m^{(n)}) x_d^{(n)}$$

Gradient calculation

gradient wrt V:

we already did this part

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \boxed{\frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_m}} \underbrace{\frac{\partial u_m}{\partial z_m}}_{W_{k,m}} \frac{\partial z_m}{\partial q_m} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{x_d}$$

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$$= \sum_n \sum_c (\hat{y}_c^{(n)} - y_c^{(n)}) W_{c,m} z_m^{(n)} (1 - z_m^{(n)}) x_d^{(n)}$$

for biases we simply assume the input is 1. $x_0^{(n)} = 1$

Gradient calculation

a common pattern

$$\frac{\partial}{\partial W_{c,m}} L = \underbrace{\frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c}}_{\text{error from above } \frac{\partial L}{\partial u_c}} \underbrace{\frac{\partial u_c}{\partial W_{c,m}}}_{\text{input from below } z_m}$$

$$\frac{\partial}{\partial V_{m,d}} L = \underbrace{\sum_c \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial z_m} \frac{\partial z_m}{\partial q_m}}_{\text{error from above } \frac{\partial L}{\partial q_m}} \underbrace{\frac{\partial q_m}{\partial V_{m,d}}}_{\text{input from below } x_d}$$

Gradient calculation

a common pattern

$$\frac{\partial}{\partial W_{c,m}} L = \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial W_{c,m}}$$

error from above $\frac{\partial L}{\partial u_c}$ input from below z_m

$$\frac{\partial}{\partial V_{m,d}} L = \sum_c \frac{\partial L}{\partial \hat{y}_c} \frac{\partial \hat{y}_c}{\partial u_c} \frac{\partial u_c}{\partial z_m} \frac{\partial z_m}{\partial q_m} \frac{\partial q_m}{\partial V_{m,d}}$$

error from above $\frac{\partial L}{\partial q_m}$ input from below x_d

$L(y, \hat{y})$

$\uparrow$

$\hat{y}_c = g(u_c)$

$\uparrow$

$u_c = \sum_{m=1}^{M} W_{c,m} z_m$

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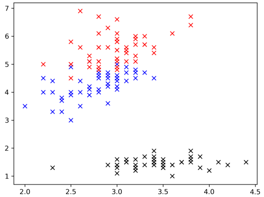
x_d

Example: classification



Iris dataset (D=2 features + 1 bias)

M = 16 hidden units

C=3 classes

$$L(y, \hat{y})$$

$$\hat{y} = \text{softmax}(u)$$

$$u_c = \sum_{m=1}^{M} W_{c,m} z_m$$

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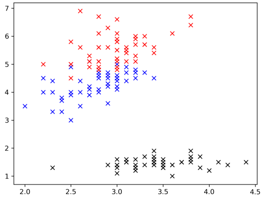

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cost is softmax-cross-entropy

```python
def cost(X, #N x D
         Y, #N x C
         W, #M x C
         V, #D x M
        ):
    Q = np.dot(X, V) #N x M
    Z = logistic(Q) #N x M
    U = np.dot(Z, W) #N x K
    Yh = softmax(U)
    nll = - np.mean(np.sum(U*Y, 1) - logsumexp(U))
    return nll
```

helper functions

```python
def logsumexp(
    Z,# NxC
):
    Zmax = np.max(Z,axis=1)[:, None]
    lse = Zmax + np.log(np.sum(np.exp(Z - Zmax), axis=1))[:, None]
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  def softmax(
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    u_exp = np.exp(u - np.max(u, 1)[:, None])
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```

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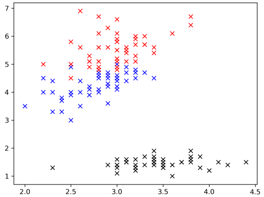

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$$J = -\sum_{n=1}^{N} y^{(n)\top} u^{(n)} + \log \sum_c e^{u_c^{(n)}}$$

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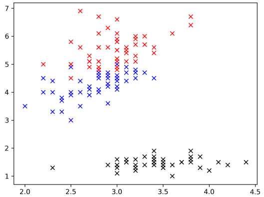

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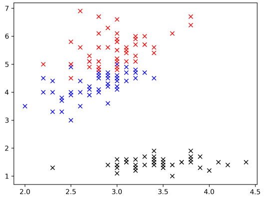

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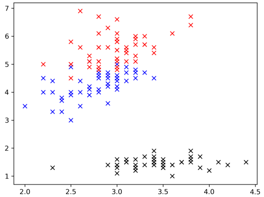

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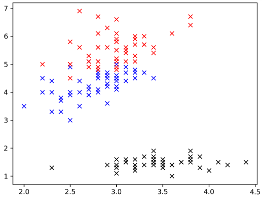

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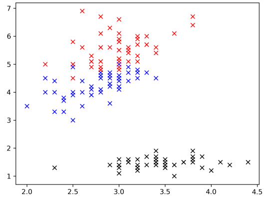

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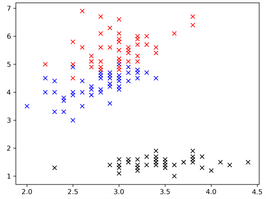

Iris dataset (D=2 features + 1 bias)

M = 16 hidden units

C=3 classes

```
def gradients(X,#N x D
              Y,#N x K
              W,#M x K
              V,#D x M
             ):
    Z = logistic(np.dot(X, V))#N x M
    N,D = X.shape
    Yh = softmax(np.dot(Z, W))#N x K
    dY = Yh - Y #N x K
    dW= np.dot(Z.T, dY)/N #M x K
    dZ = np.dot(dY, W.T) #N x M
    dV = np.dot(X.T, dZ * Z * (1 - Z))/N #D x M
    return dW, dV
```

$$\frac{\partial}{\partial W_m} L = (\hat{y} - y) z_m$$

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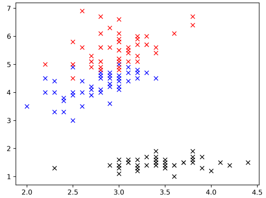
Example: classification



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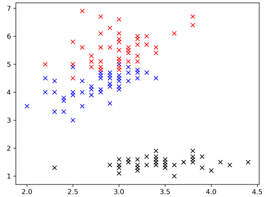

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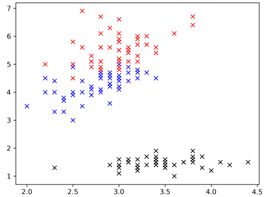

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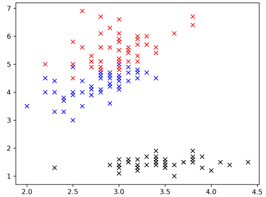

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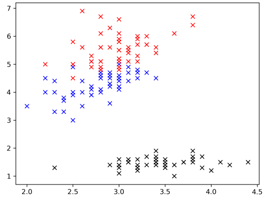

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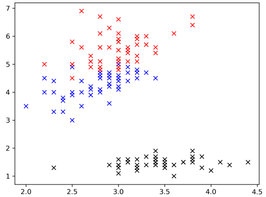

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using GD for optimization

```
def GD(X, Y, M, lr=.1, eps=1e-9, max_iters=100000):
    N, D = X.shape
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    W = np.random.randn(M, K)*.01
    V = np.random.randn(D, M)*.01
    dW = np.inf*np.ones_like(W)
    t = 0
    while np.linalg.norm(dW) > eps and t < max_iters:
        dW, dV = gradients(X, Y, W, V)
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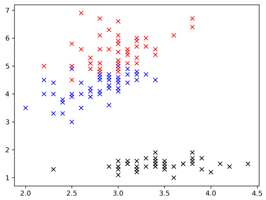

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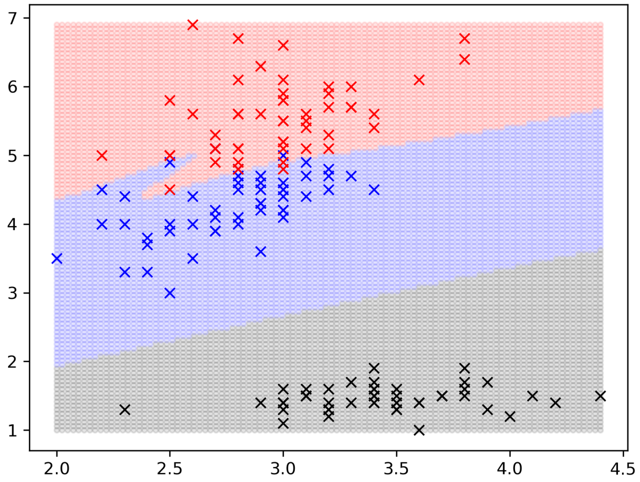
the resulting decision boundaries



Automating gradient computation

gradient computation is tedious and mechanical.

can we automate it?

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- approximates partial derivatives using finite difference $\frac{\partial f}{\partial w} \approx \frac{f(w+\epsilon)-f(w)}{\epsilon}$
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automatic / algorithmic differentiation is what we want

write code that calculates various functions, *e.g., the cost function*

automatically produce (partial) derivatives *e.g., gradients used in learning*

Automatic differentiation

idea

use the chain rule + derivative of simple operations $*, \sin, \frac{1}{x} \ldots$

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step 1 — break down to atomic operations

$$L = \frac{1}{2}(y - wx)^2 \rightarrow$$

$$\begin{aligned}
a_1 &= w \\
a_2 &= x \\
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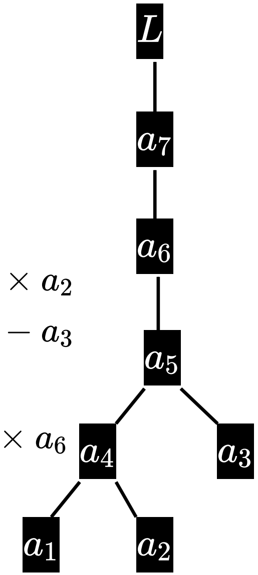

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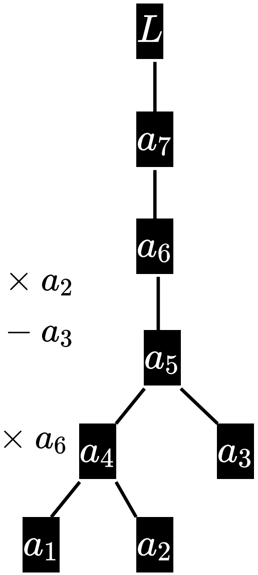

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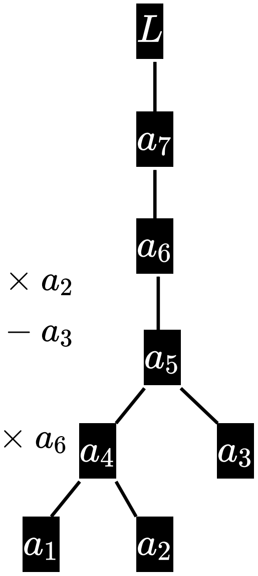

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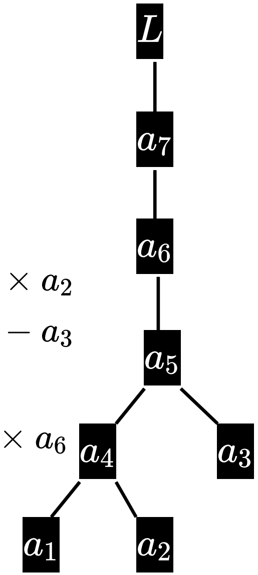

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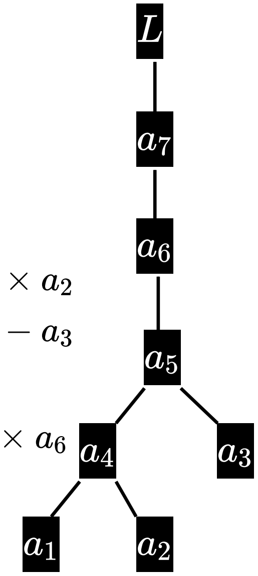

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this second procedure is called **backpropagation** when applied to neuran networks

Forward mode

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 &= \sin(w_1 x + w_0) \\ y_2 &= \cos(w_1 x + w_0) \end{cases}$

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	$a_2 = w_1$	$\dot{a}_2 = 1$	this means $\dot{\square} = \frac{\partial \square}{\partial w_1}$
	$a_3 = x$	$\dot{a}_3 = 0$	
$w_1 x$	$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$	x
$w_1 x + w_0$	$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$	x
$y_1 = \sin(w_1 x + w_0)$	$a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$	$x \cos(w_1 x + w_0) = \frac{\partial y_1}{\partial w_1}$
$y_2 = \cos(w_1 x + w_0)$	$a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \sin(a_5)$	$-x \sin(w_1 x + w_0) = \frac{\partial y_2}{\partial w_1}$

Forward mode

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can calculate both y_1, y_2 and derivatives $\frac{\partial y_1}{\partial w_1}$ $\frac{\partial y_2}{\partial w_1}$ in a single forward pass

	evaluation	**partial derivatives**	
	$a_1 = w_0$	$\dot{a}_1 = 0$	we initialize these to identify which derivative we want
	$a_2 = w_1$	$\dot{a}_2 = 1$	this means $\dot{\square} = \frac{\partial \square}{\partial w_1}$
	$a_3 = x$	$\dot{a}_3 = 0$	
$w_1 x$	$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$	x
$w_1 x + w_0$	$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$	x
$y_1 = \sin(w_1 x + w_0)$	$a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$	$x \cos(w_1 x + w_0) = \frac{\partial y_1}{\partial w_1}$
$y_2 = \cos(w_1 x + w_0)$	$a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \sin(a_5)$	$-x \sin(w_1 x + w_0) = \frac{\partial y_2}{\partial w_1}$

note that we get all partial derivatives $\frac{\partial \square}{\partial w_1}$ in one forward pass

Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

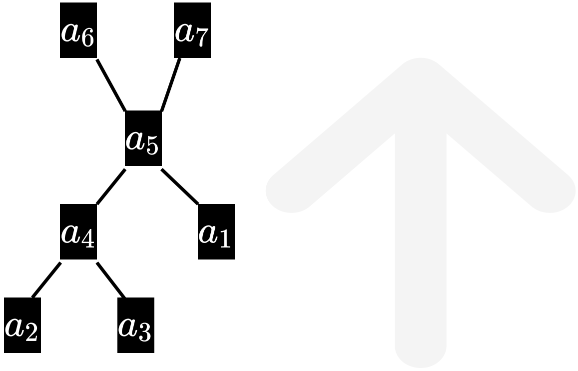
evaluation	partial derivatives
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	**partial derivatives**
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

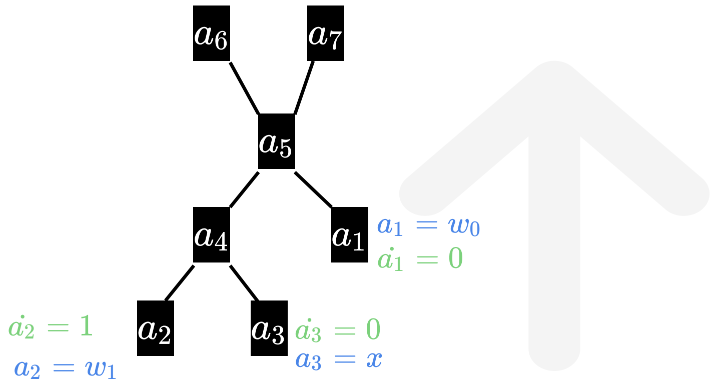


Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	partial derivatives
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

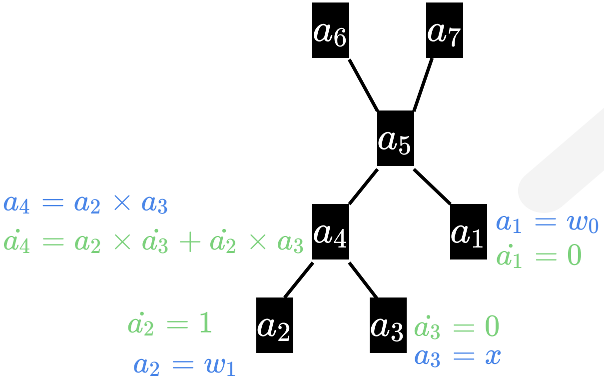


Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	**partial derivatives**
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

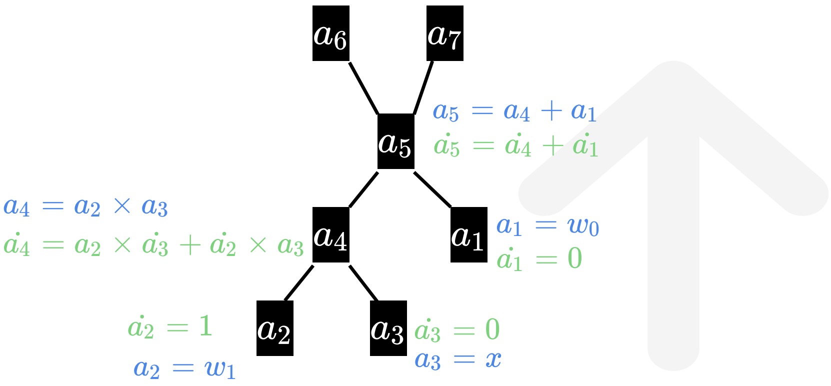


Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	partial derivatives
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

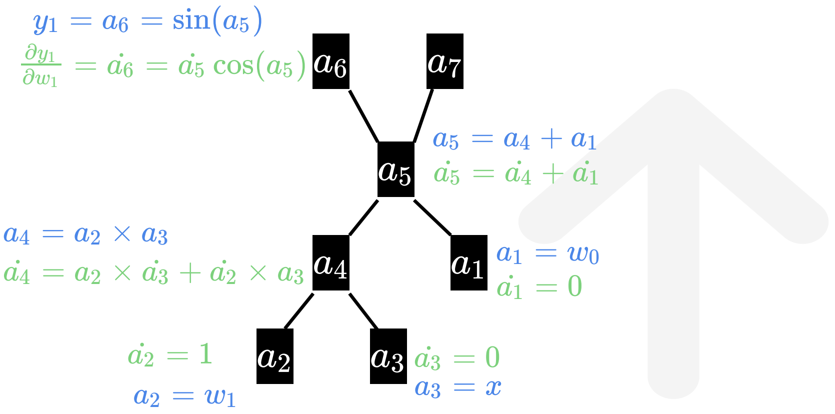


Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	**partial derivatives**
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$

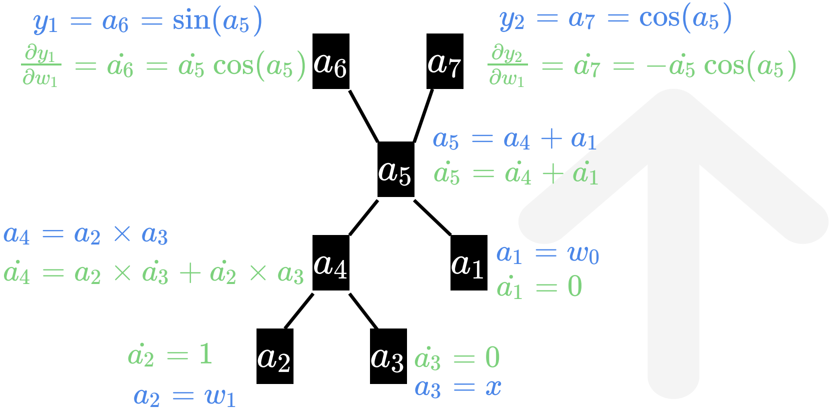


Forward mode: computational graph

suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

evaluation	partial derivatives
$a_1 = w_0$	$\dot{a}_1 = 0$
$a_2 = w_1$	$\dot{a}_2 = 1$
$a_3 = x$	$\dot{a}_3 = 0$
$a_4 = a_2 \times a_3$	$\dot{a}_4 = a_2 \times \dot{a}_3 + \dot{a}_2 \times a_3$
$a_5 = a_4 + a_1$	$\dot{a}_5 = \dot{a}_4 + \dot{a}_1$
$y_1 = a_6 = \sin(a_5)$	$\dot{a}_6 = \dot{a}_5 \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a}_7 = -\dot{a}_5 \cos(a_5)$



Forward mode: computational graph

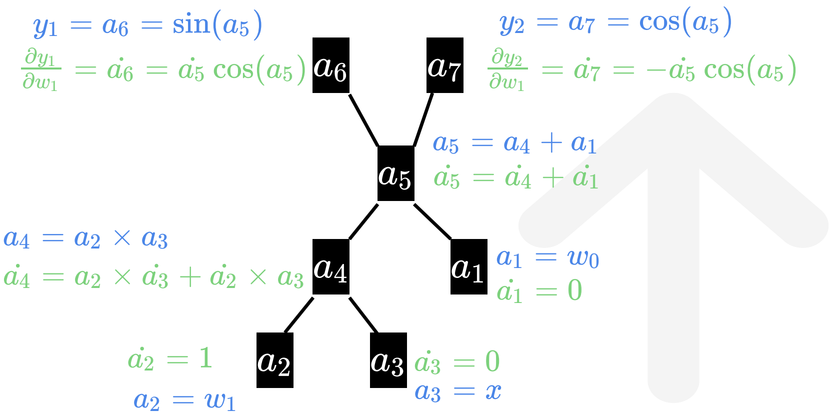
suppose we want the derivative $\frac{\partial y_1}{\partial w_1}$ where $\begin{cases} y_1 = \sin(w_1 x + w_0) \\ y_2 = \cos(w_1 x + w_0) \end{cases}$

we can represent this computation using a graph

once the nodes up stream calculate their values and derivatives we may discard a node

- *e.g.*, once $a_5, \dot{a_5}$ are obtained we can discard the values and partial derivatives for $a_4, \dot{a_4}, a_1, \dot{a_1}$

evaluation	partial derivatives
$a_1 = w_0$	$\dot{a_1} = 0$
$a_2 = w_1$	$\dot{a_2} = 1$
$a_3 = x$	$\dot{a_3} = 0$
$a_4 = a_2 \times a_3$	$\dot{a_4} = a_2 \times \dot{a_3} + \dot{a_2} \times a_3$
$a_5 = a_4 + a_1$	$\dot{a_5} = \dot{a_4} + \dot{a_1}$
$y_1 = a_6 = \sin(a_5)$	$\dot{a_6} = \dot{a_5} \cos(a_5)$
$y_2 = a_7 = \cos(a_5)$	$\dot{a_7} = -\dot{a_5} \cos(a_5)$



Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$

$$a_2 = w_1$$

$$a_3 = x$$

$w_1 x$ $$a_4 = a_2 \times a_3$$

$w_1 x + w_0$ $$a_5 = a_4 + a_1$$

$y_1 = \sin(w_1 x + w_0)$ $$y_1 = a_6 = \sin(a_5)$$

$y_2 = \cos(w_1 x + w_0)$ $$y_2 = a_7 = \cos(a_5)$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

then use these values to calculate partial derivatives in a backward pass

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$

$w_1 x$ $\quad a_4 = a_2 \times a_3$

$w_1 x + w_0$ $\quad a_5 = a_4 + a_1$

$y_1 = \sin(w_1 x + w_0)$ $\quad y_1 = a_6 = \sin(a_5)$

$y_2 = \cos(w_1 x + w_0)$ $\quad y_2 = a_7 = \cos(a_5)$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$
$$w_1 x \qquad a_4 = a_2 \times a_3$$
$$w_1 x + w_0 \qquad a_5 = a_4 + a_1$$
$$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$$
$$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$$\left.\begin{array}{l}\bar{a}_7 = 1 \\ \bar{a}_6 = 0\end{array}\right\} \text{this means } \bar{\square} = \frac{\partial y_2}{\partial \square}$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$
$$w_1 x \qquad a_4 = a_2 \times a_3$$
$$w_1 x + w_0 \qquad a_5 = a_4 + a_1$$
$$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$$
$$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$$\frac{\partial y_2}{\partial y_2} = 1 \qquad \bar{a_7} = 1$$
$$\frac{\partial y_2}{\partial y_1} = 0 \qquad \bar{a_6} = 0$$

this means $\bar{\square} = \frac{\partial y_2}{\partial \square}$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$
$$w_1 x \qquad a_4 = a_2 \times a_3$$
$$w_1 x + w_0 \qquad a_5 = a_4 + a_1$$
$$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$$
$$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$$\frac{\partial y_2}{\partial y_2} = 1$$
$$\frac{\partial y_2}{\partial y_1} = 0$$
$$\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} = -\sin(w_1 x + w_0)$$

$$\left.\begin{aligned}\bar{a}_7 &= 1\\ \bar{a}_6 &= 0\end{aligned}\right\}$$ this means $\bar{\square} = \frac{\partial y_2}{\partial \square}$

$$\bar{a}_5 = \bar{a}_6 \cos(a_5) - \bar{a}_7 \sin(a_5)$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$
$$w_1 x \qquad a_4 = a_2 \times a_3$$
$$w_1 x + w_0 \qquad a_5 = a_4 + a_1$$
$$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$$
$$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$$

then use these values to calculate partial derivatives in a backward pass

$$\frac{\partial y_2}{\partial y_2} = 1$$
$$\frac{\partial y_2}{\partial y_1} = 0$$
$$\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} = -\sin(w_1 x + w_0)$$
$$\frac{\partial y_2}{\partial a_4} = -\sin(w_1 x + w_0)$$

2) partial derivatives

$$\left.\begin{aligned}\bar{a_7} &= 1\\ \bar{a_6} &= 0\end{aligned}\right\} \text{this means } \bar{\square} = \frac{\partial y_2}{\partial \square}$$
$$\bar{a_5} = \bar{a_6}\cos(a_5) - \bar{a_7}\sin(a_5)$$
$$\bar{a_4} = \bar{a_5}$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$a_1 = w_0$

$a_2 = w_1$

$a_3 = x$

$w_1 x \qquad a_4 = a_2 \times a_3$

$w_1 x + w_0 \qquad a_5 = a_4 + a_1$

$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$

$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$\frac{\partial y_2}{\partial y_2} = 1 \qquad \bar{a}_7 = 1$

$\frac{\partial y_2}{\partial y_1} = 0 \qquad \bar{a}_6 = 0$

this means $\bar{\square} = \frac{\partial y_2}{\partial \square}$

$\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} = -\sin(w_1 x + w_0) \qquad \bar{a}_5 = \bar{a}_6 \cos(a_5) - \bar{a}_7 \sin(a_5)$

$\frac{\partial y_2}{\partial a_4} = -\sin(w_1 x + w_0) \qquad \bar{a}_4 = \bar{a}_5$

$\frac{\partial y_2}{\partial x} = -w_1 \sin(w_1 x + w_0) \qquad \bar{a}_3 = a_2 \bar{a}_4$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$a_1 = w_0$$
$$a_2 = w_1$$
$$a_3 = x$$
$$w_1 x \qquad a_4 = a_2 \times a_3$$
$$w_1 x + w_0 \qquad a_5 = a_4 + a_1$$
$$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$$
$$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$$

then use these values to calculate partial derivatives in a backward pass

$$\frac{\partial y_2}{\partial y_2} = 1$$
$$\frac{\partial y_2}{\partial y_1} = 0$$
$$\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} = -\sin(w_1 x + w_0)$$
$$\frac{\partial y_2}{\partial a_4} = -\sin(w_1 x + w_0)$$
$$\frac{\partial y_2}{\partial x} = -w_1 \sin(w_1 x + w_0)$$
$$\frac{\partial y_2}{\partial w_1} = -x \sin(w_1 x + w_0)$$

2) partial derivatives

$$\left.\begin{array}{l} \bar{a}_7 = 1 \\ \bar{a}_6 = 0 \end{array}\right\} \text{this means } \bar{\square} = \frac{\partial y_2}{\partial \square}$$
$$\bar{a}_5 = \bar{a}_6 \cos(a_5) - \bar{a}_7 \sin(a_5)$$
$$\bar{a}_4 = \bar{a}_5$$
$$\bar{a}_3 = a_2 \bar{a}_4$$
$$\bar{a}_2 = a_3 \bar{a}_4$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$$
\begin{aligned}
a_1 &= w_0 \\
a_2 &= w_1 \\
a_3 &= x \\
w_1 x \qquad\qquad & a_4 = a_2 \times a_3 \\
w_1 x + w_0 \qquad\qquad & a_5 = a_4 + a_1 \\
y_1 = \sin(w_1 x + w_0) \qquad & y_1 = a_6 = \sin(a_5) \\
y_2 = \cos(w_1 x + w_0) \qquad & y_2 = a_7 = \cos(a_5)
\end{aligned}
$$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$$
\begin{aligned}
\frac{\partial y_2}{\partial y_2} &= 1 & \bar{a}_7 &= 1 \\
\frac{\partial y_2}{\partial y_1} &= 0 & \bar{a}_6 &= 0
\end{aligned}
$$

this means $\bar{\square} = \frac{\partial y_2}{\partial \square}$

$$
\begin{aligned}
\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} &= -\sin(w_1 x + w_0) & \bar{a}_5 &= \bar{a}_6 \cos(a_5) - \bar{a}_7 \sin(a_5) \\
\frac{\partial y_2}{\partial a_4} &= -\sin(w_1 x + w_0) & \bar{a}_4 &= \bar{a}_5 \\
\frac{\partial y_2}{\partial x} &= -w_1 \sin(w_1 x + w_0) & \bar{a}_3 &= a_2 \bar{a}_4 \\
\frac{\partial y_2}{\partial w_1} &= -x \sin(w_1 x + w_0) & \bar{a}_2 &= a_3 \bar{a}_4 \\
\frac{\partial y_2}{\partial w_0} &= -\sin(w_1 x + w_0) & \bar{a}_1 &= \bar{a}_5
\end{aligned}
$$

Reverse mode

suppose we want the derivative $\frac{\partial y_2}{\partial w_1}$ where $y_2 = \cos(w_1 x + w_0)$

first do a forward pass for evaluation

1) evaluation

$a_1 = w_0$

$a_2 = w_1$

$a_3 = x$

$w_1 x \qquad a_4 = a_2 \times a_3$

$w_1 x + w_0 \qquad a_5 = a_4 + a_1$

$y_1 = \sin(w_1 x + w_0) \qquad y_1 = a_6 = \sin(a_5)$

$y_2 = \cos(w_1 x + w_0) \qquad y_2 = a_7 = \cos(a_5)$

then use these values to calculate partial derivatives in a backward pass

2) partial derivatives

$\frac{\partial y_2}{\partial y_2} = 1 \qquad \bar{a}_7 = 1$

$\frac{\partial y_2}{\partial y_1} = 0 \qquad \bar{a}_6 = 0$

this means $\bar{\square} = \frac{\partial y_2}{\partial \square}$

$\frac{\partial y_2}{\partial a_5} = \frac{\partial y_2}{\partial a_7}\frac{\partial a_7}{\partial a_5} + \frac{\partial y_2}{\partial a_6}\frac{\partial a_6}{\partial a_5} = -\sin(w_1 x + w_0) \qquad \bar{a}_5 = \bar{a}_6 \cos(a_5) - \bar{a}_7 \sin(a_5)$

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we get all partial derivatives $\frac{\partial y_2}{\partial \square}$ in one backward pass

Reverse mode: computational graph

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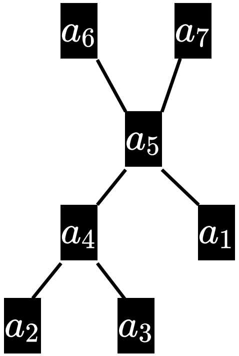

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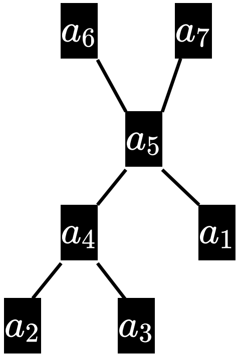

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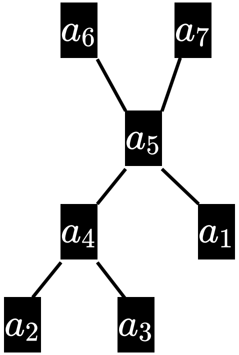

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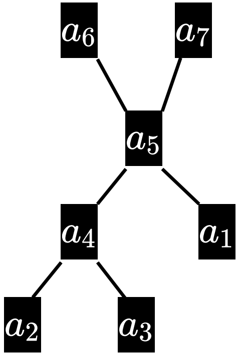

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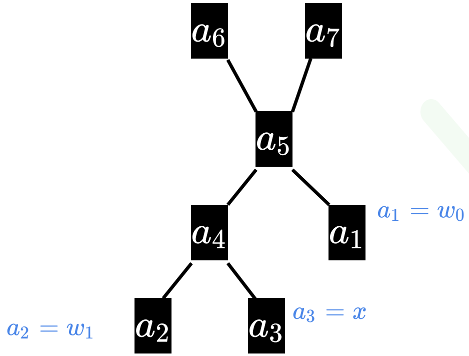

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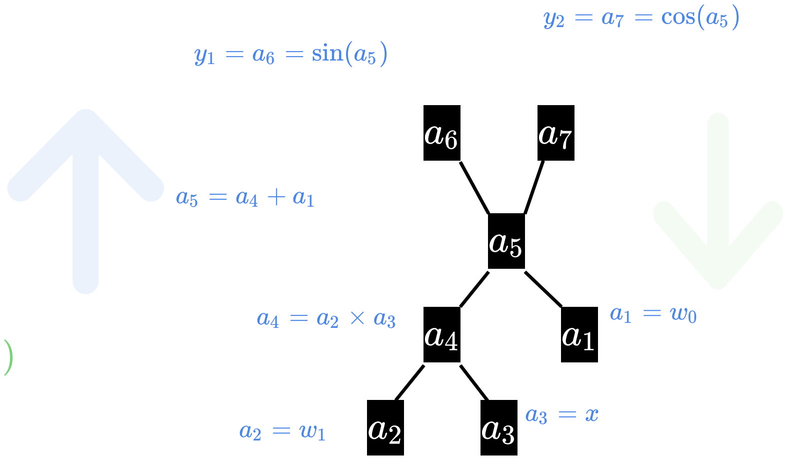

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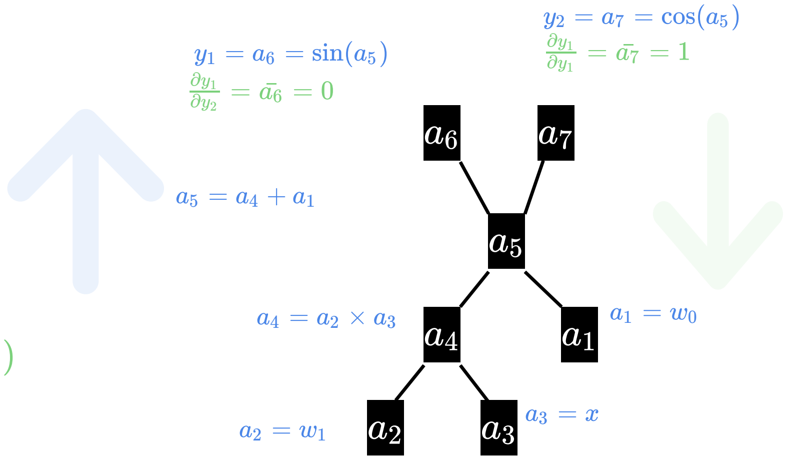

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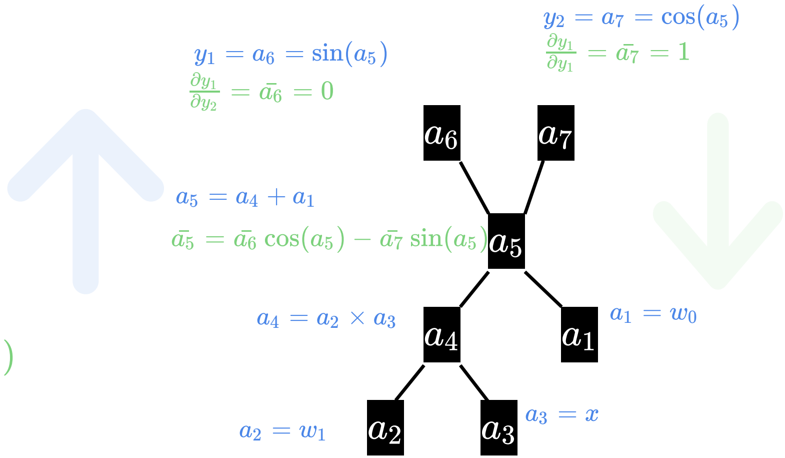

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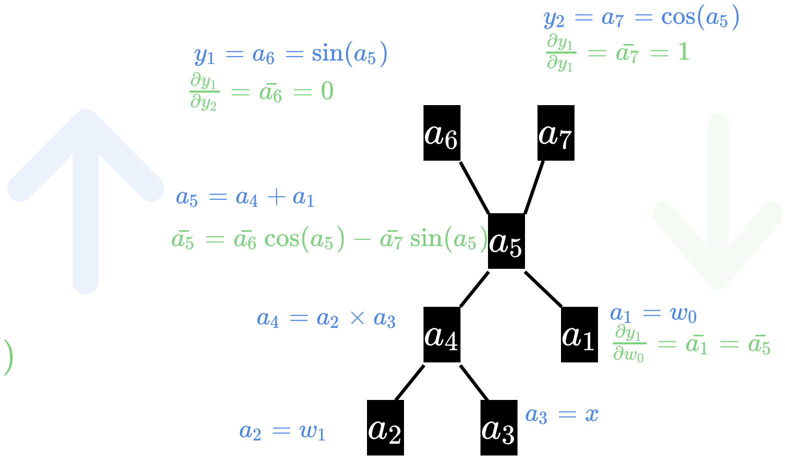

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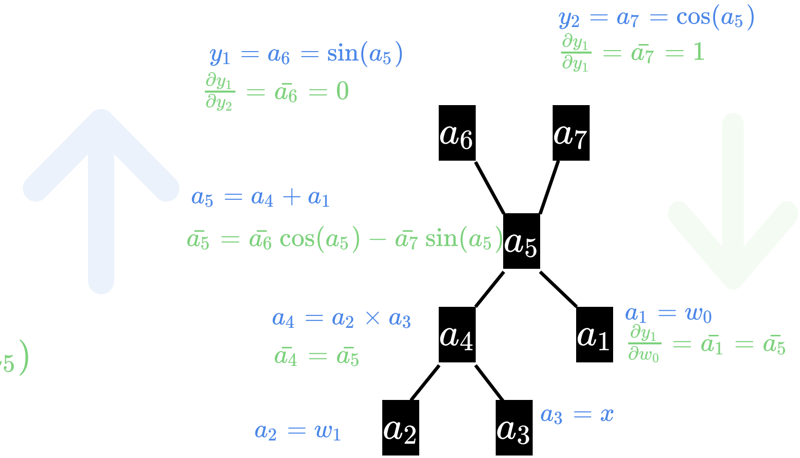

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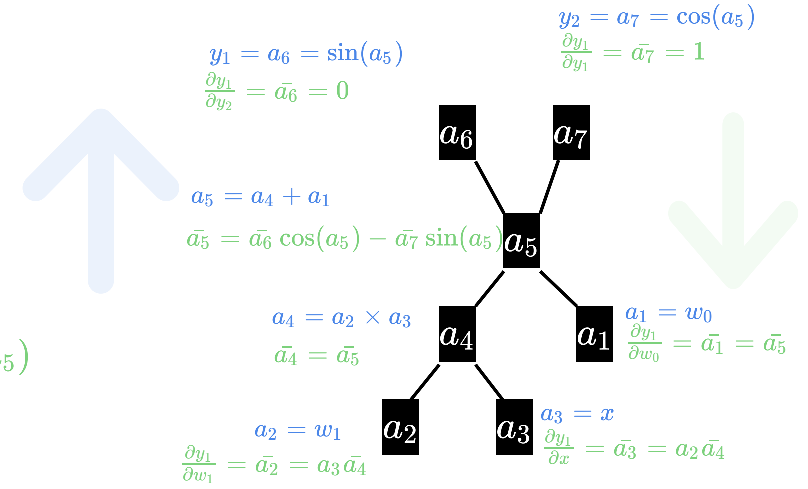

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forward mode is more natural, easier to implement and requires less memory

a single forward pass calculates $\frac{\partial y_1}{\partial w}, \ldots, \frac{\partial y_c}{\partial w}$

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many machine learning software implement autodiff:

- `autograd (extends numpy)`
- `pytorch`
- `tensorflow`

Improving optimization in deep learning

Initialization of parameters:

- random initialization (uniform or Gaussian) with small variance
- break the symmetry of hidden units

image credit: Mobahi'16

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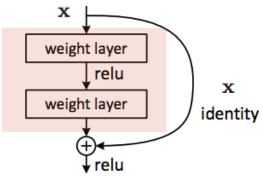

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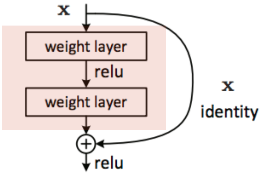

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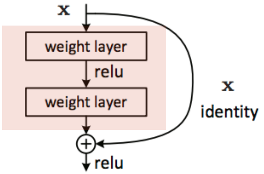

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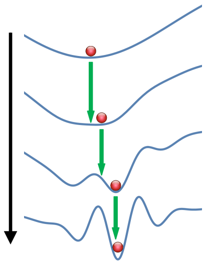

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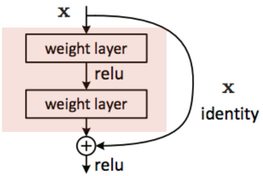

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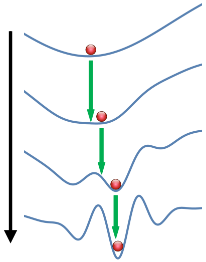

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curriculum learning (similar idea)

- increase the number of "difficult" examples over time
- similar to the way humans learn

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original motivation

- gradient descent: parameters in all layers are updated
- distribution of inputs to layer ℓ changes
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recent observations the change in distribution of activations is not a big issue empirically

BN works so well because it makes the loss function smooth

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Better optimization in deep learning:

- better initialization
- models that are easier to optimize (using skip-connection, batch-norm, ReLU)
- pre-training and curriculum learning