Introduction to Deep Learning

Tools and deep learning of NNet

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MILES Machine Intelligence and Learning Systems

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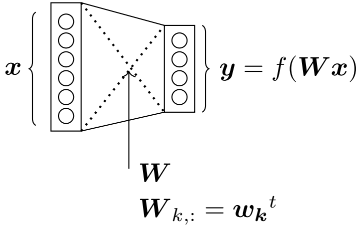
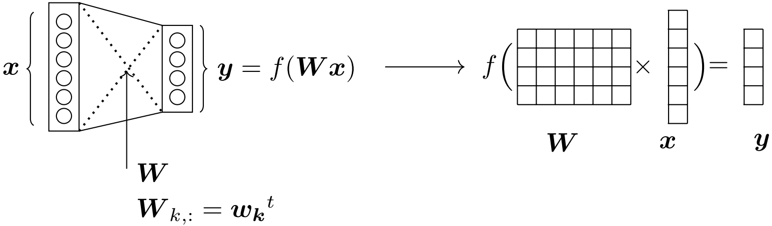
Outline

Outline

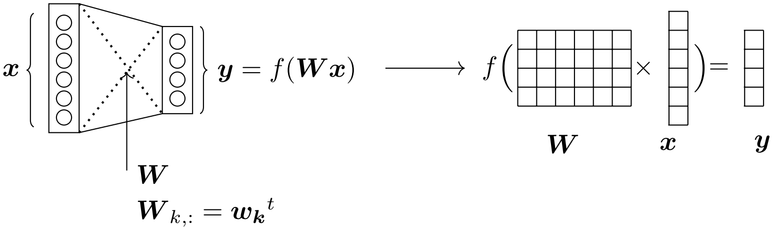
Two layers fully connected: a linear separation



Two layers fully connected: a linear separation



Two layers fully connected: a linear separation



Activation f:

- f is usually a non-linear function
- f is a component wise function
- tanh, sigmoid, relu, ...

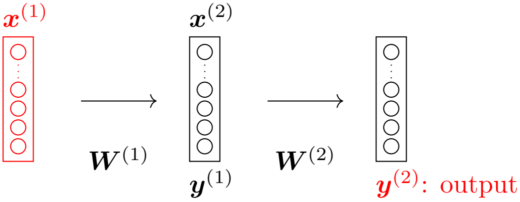
e.g the softmax function:

Dimensions:

- $\boldsymbol{x} : D \times 1$
- $\boldsymbol{W} : C \times D$
- $\boldsymbol{y} : (C \times \cancel{D) \times (D} \times 1) = C \times 1$

$$y_k = P(c = k|\boldsymbol{x}) = \frac{e^{\boldsymbol{w_k}^t \boldsymbol{x}}}{\sum_{k'} e^{\boldsymbol{w_{k'}}^t \boldsymbol{x}}} = \frac{e^{\boldsymbol{W}_{k,:}\boldsymbol{x}}}{\sum_{k'} e^{\boldsymbol{W}_{k',:}\boldsymbol{x}}}$$

From linear to non-linear case



$$\boldsymbol{\theta} = (\boldsymbol{W}^{(1)}, \boldsymbol{W}^{(2)})$$

Trained by back-propagation of the gradient

Universal approximation theorem

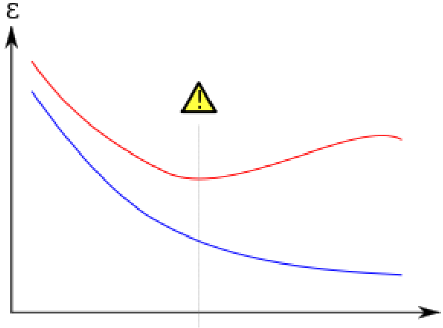
> *a feed-forward network with a single hidden layer containing a finite number of neurons can approximate continuous functions on compact subsets of* $\mathbb{R}^n$*, under mild assumptions on the activation function. (...)*

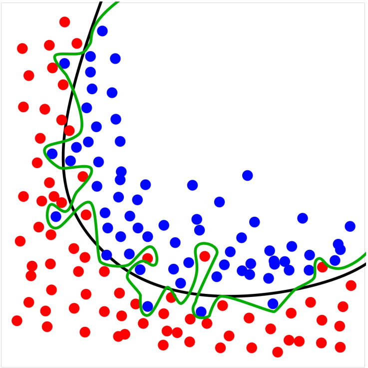
(Cybenko1989)

However, it does not touch upon the algorithmic learnability of those parameters.

Overfitting

The danger of the over-parametrization

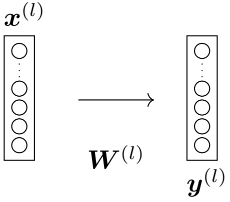




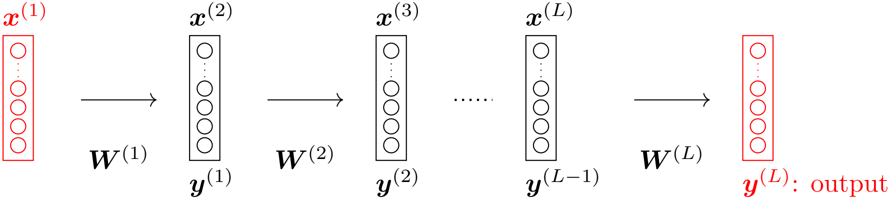
Source: Wikipedia

Multi-layer neural network (feed-forward)

One layer, indexed by l



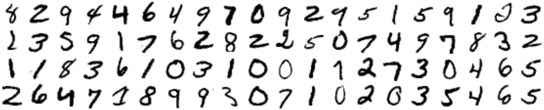
- $\boldsymbol{x}^{(l)}$: input of the layer l
- $\boldsymbol{y}^{(l)} = f^{(l)}(\boldsymbol{W}^{(l)}\ \boldsymbol{x}^{(l)})$
- stacking layers: $\boldsymbol{y}^{(l)} = \boldsymbol{x}^{(l+1)}$
- $\boldsymbol{x}^{(1)}$ = a data example



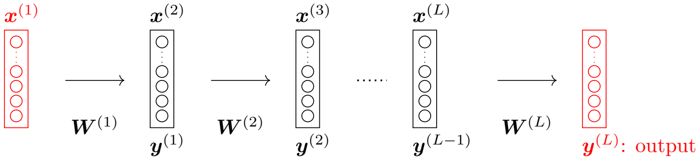
Outline

Experimental observations (MNIST task) - 1

The MNIST database



Comparison of different depth for feed-forward architecture



- Hidden layers have a sigmoid activation function.
- The output layer is a softmax.

Experimental observations (MNIST task) - 2

Varying the depth

- Without hidden layer: $\approx 88\%$ accuracy
- 1 hidden layer (30): $\approx 96.5\%$ accuracy
- 2 hidden layers (30): $\approx 96.9\%$ accuracy
- 3 hidden layers (30): $\approx 96.5\%$ accuracy
- 4 hidden layers (30): $\approx 96.5\%$ accuracy

Experimental observations (MNIST task) - 2

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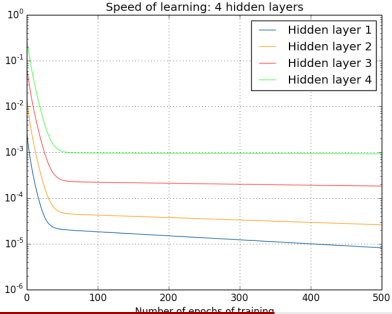
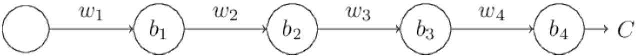
- 4 hidden layers (30): $\approx 96.5\%$ accuracy



(From `http://neuralnetworksanddeeplearning.com/chap5.html`)

Intuitive explanation

Let consider the simplest deep neural network, with just a single neuron in each layer.



w_i, b_i are resp. the weight and bias of neuron i and C some cost function.

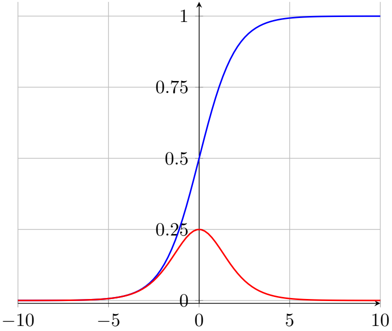
Compute the gradient of C *w.r.t* the bias b_1

$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial y_4} \times \frac{\partial y_4}{\partial a_4} \times \frac{\partial a_4}{\partial y_3} \times \frac{\partial y_3}{\partial a_3} \times \frac{\partial a_3}{\partial y_2} \times \frac{\partial y_2}{\partial a_2} \times \frac{\partial a_2}{\partial y_1} \times \frac{\partial y_1}{\partial a_1} \times \frac{\partial a_1}{\partial b_1} \tag{1}$$

$$= \frac{\partial C}{\partial y_4} \times \sigma'(a_4) \times w_4 \times \sigma'(a_3) \times w_3 \times \sigma'(a_2) \times w_2 \times \sigma'(a_1) \tag{2}$$

Intuitive explanation - 2

The derivative of the activation function: σ'



$$\sigma'(x) = \sigma(x)(1 - \sigma(x))$$

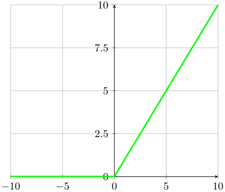
But weights are initialize around 0.

The different layers in our deep network are learning at vastly different speeds:

- when later layers in the network are learning well,
- early layers often get stuck during training, learning almost nothing at all.

A first Solution

Change the activation function (Rectified Linear Unit or ReLU)



- Avoid the vanishing gradient
- Some units can "die"

See (Glorot et al.2011) for more details

Variants

- Leaky ReLU (Maas et al.2013)
- Soft-plus $log(1 + e^x)$

And many more, see `https://pytorch.org/docs/stable/nn.html`

More details

See (Hochreiter et al.2001; Glorot and Bengio2010; LeCun et al.2012)

A question

Why adding a layer can lower the performance ?

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- Overfitting ? and what about the identity
- Vanishing gradient ? and with the *Relu* ?

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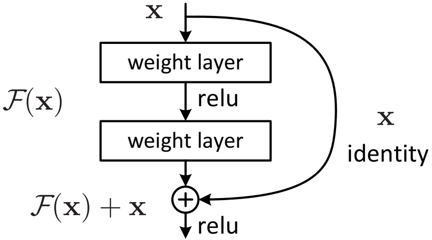
Residual block

From (He et al.2015)

- Add a skip connection
- The model learn the "residual"

$$\boldsymbol{y} = \mathcal{F}(\boldsymbol{x}) = \boldsymbol{x} + \mathcal{R}(\boldsymbol{x})$$



A simple version of highway networks (Srivastava et al.2015)

Residual block

Forward

$$\begin{aligned} \boldsymbol{y} &= \mathcal{F}(\boldsymbol{x}) = \boldsymbol{x} + \mathcal{R}(\boldsymbol{x}), \text{ or} \\ \boldsymbol{y} &= \boldsymbol{W}_s\boldsymbol{x} + \mathcal{R}(\boldsymbol{x}), \text{ to adapt the dimension} \end{aligned}$$

Backward

Assume a residual block for the layer l in the network. Training requires:

- $\frac{\partial l}{\partial \boldsymbol{W}^{(l)}}$ for the update of the layer
- $\frac{\partial l}{\partial \boldsymbol{x}^{(l)}}$ for the backpropagation

$$\begin{aligned} \frac{\partial l}{\partial \boldsymbol{x}^{(l)}} &= \frac{\partial l}{\partial \boldsymbol{y}^{(l)}} \times \frac{\partial \boldsymbol{y}^{(l)}}{\partial \boldsymbol{x}^{(l)}} \\ &= \frac{\partial l}{\partial \boldsymbol{y}^{(l)}} \times (1 + \frac{\partial \mathcal{R}(\boldsymbol{x}^{(l)})}{\partial \boldsymbol{x}^{(l)}}) \end{aligned}$$

Outline

Regularization l^2 or gaussian prior or weight decay

The basic way:

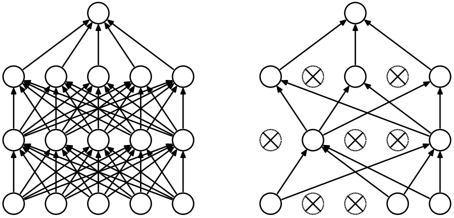
$$\mathcal{L}(\boldsymbol{\theta}; \mathcal{D}) = \sum_{i=1}^{N} l(\boldsymbol{\theta}, \boldsymbol{x}_{(i)}, c_{(i)}) + \frac{\lambda}{2} ||\boldsymbol{\theta}||^2$$

- The second term is the regularization term.
- Each parameter has a gaussian prior : $\mathcal{N}(0, 1/\lambda)$.
- λ is a hyperparameter.
- The update has the form:

$$\boldsymbol{\theta} = (1 + \eta_t \lambda)\boldsymbol{\theta} - \eta_t \nabla_{\boldsymbol{\theta}}$$

Dropout

A new regularization scheme (Srivastava and Salakhutdinov2014)



(a) Standard Neural Net

(b) After applying dropout.

- For each training example: randomly turn-off the neurons of hidden units (with $p = 0.5$)
- At test time, use each neuron scaled down by p

- Dropout serves to separate effects from strongly correlated features and
- prevents co-adaptation between units
- It can be seen as averaging different models that share parameters.
- It acts as a powerful regularization scheme.

Dropout - implementation

The layer should keep:

- $\boldsymbol{W}^{(l)}$: the parameters
- $f^{(l)}$: its activation function
- $\boldsymbol{x}^{(l)}$: its input
- $\boldsymbol{a}^{(l)}$: its pre-activation associated to the input
- $\boldsymbol{\delta}^{(l)}$: for the update and the back-propagation to the layer $l-1$
- $\boldsymbol{m}^{(l)}$: the dropout mask, to be applied on $\boldsymbol{x}^{(l)}$

Forward pass

For $l = 1$ to $(L-1)$

- Compute $\boldsymbol{y}^{(l)} = f^{(l)}(\boldsymbol{W}^{(l)}\boldsymbol{x}^{(l)})$
- $\boldsymbol{x}^{(l+1)} = \boldsymbol{y}^{(l)} = \boldsymbol{y}^{(l)} \circ \boldsymbol{m}^{(l)}$

$\boldsymbol{y}^{(L)} = f^{(L)}(\boldsymbol{W}^{(L)}\boldsymbol{x}^{(L)})$

Outline

Some useful libraries

Theano

Written in python by the LISA (Y. Bengio and I. Goodfellow), low-level API.

TensorFlow and Keras

The Google library with python API + high level API

pyTorch

The Facebook library with python API

And others

Caffe, MXNet, CNTK, Chainer, ...

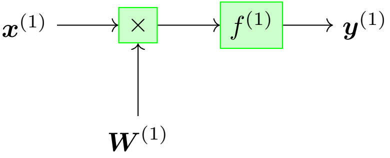
- CPU/GPU
- Automatic differentiation based on computational graph

Computation graph

A convenient way to represent a complex mathematical expressions:

- each node is an operation or a variable
- an operation has some inputs / outputs made of variables

Example 1 : A single layer network



- Setting $\boldsymbol{x}^{(1)}$ and $\boldsymbol{W}^{(1)}$
- Forward pass $\rightarrow \boldsymbol{y}^{(1)}$

$$\boldsymbol{y}^{(1)} = f^{(1)}(\boldsymbol{W}^{(1)}\boldsymbol{x}^{(1)})$$

Remark

Some toolkit refers to variable as node, and function as edge.

Building a computation graph

Variables (eq. Tensors) flow through a D.A.G

A variable is a *Tensor*

A *Tensor* stores:

- the values (as *numpy.array*);
- a link to its creator;
- (optionally) the gradient values (as a *numpy.array* of same size);

The creator is a function or tensor operation

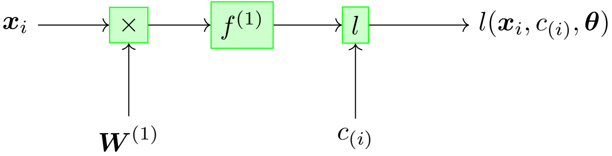
Function

A tensor operation that takes:

- several (or zero) input tensors,
- and output one new tensor as a result.

Ex: the logistic regression model

The computation graph



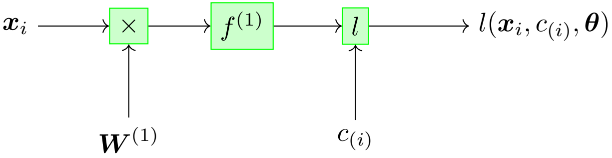
- $f^{(1)}$ is the sigmoid (σ) function
- the loss is the binary log-loss (a.k.a binary cross entropy):

$$l(\boldsymbol{x}, c, \boldsymbol{\theta} = \boldsymbol{W}) = c_{(i)} \log y + (1 - c_{(i)}) \log(1 - y),$$

- with y, a scalar, the output of $f^{(1)}$.

Ex: the logistic regression model

In numpy *vs* pytorch

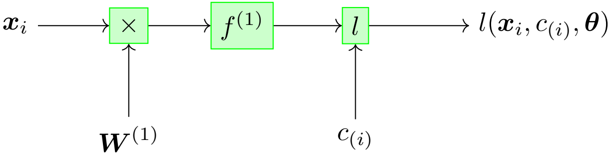



```python
import numpy as np
# explicite bias
W = np.random.randn(1,D+1)
# inference
# x the input:  np.array
a = W@x
y = 1/(1+np.exp(-a))
# a and y are np.array
# loss: c (target) np.array~~~
l = -c*np.log(y)
    - (1-c)*np.log(1-y)
```

```python
import torch as th
# explicite bias
W = th.randn(1,D+1,requires_grad=True)
# inference
# x is a th.Tensor
a = W@x # or W.matmul(x)
y = 1/(1+th.exp(-a))
# a and y are th.Tensor
# loss: c (target), a th.Tensor
l = -c*th.log(y)
    - (1-c)*th.log(1-y)
```

Ex: the logistic regression model

Compute the gradient



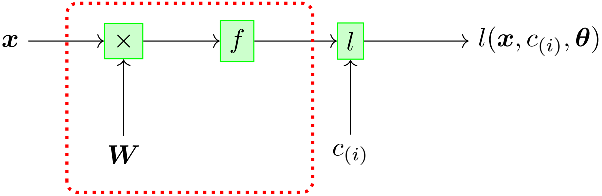
The goal :

$$\frac{\partial l}{\partial \boldsymbol{W}^{(1)}} = \frac{\partial l}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}^{(1)}}$$

Gradient computation:

$$\boxed{l} \rightarrow \frac{\partial l}{\partial \boldsymbol{y}} \rightarrow \boxed{f} \rightarrow \frac{\partial l}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{a}} \rightarrow \boxed{\times} \rightarrow \frac{\partial l}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}^{(1)}}$$

The computation graph in both directions



Forward (inference)	Backward (gradient)
$l(\boldsymbol{\theta}, \boldsymbol{x}_{(i)}, c_{(i)}) \leftarrow \boldsymbol{y}$	$\dfrac{\partial l(\boldsymbol{\theta}, \boldsymbol{x}_{(i)}, c_{(i)})}{\partial \boldsymbol{W}} = \dfrac{\partial l(\boldsymbol{\theta}, \boldsymbol{x}_{(i)}, c_{(i)})}{\partial \boldsymbol{y}}$
$\boldsymbol{y} = f(\boldsymbol{a})$	$\times \dfrac{\partial \boldsymbol{y}}{\partial \boldsymbol{a}}$
$\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x}$	$\times \dfrac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}}$

Illustration in 3 steps

Initialization (inputs of the graph)

```
import torch as th
x = th.ones(3,1)
c = th.ones(1)
W = th.randn(1,3,requires_grad=True)
  tensor([[-0.3999,  0.1500,  0.3771]], requires_grad=True)
```

Forward: build the graph

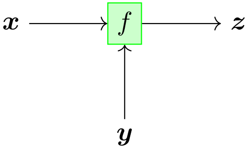
```
h = 1/(1+th.exp(-W@x))
  tensor([[0.4682]], grad_fn=<MulBackward0>)
l =  -y*th.log(h) - (1-y)*th.log(1-h)
  tensor([[0.7588]], grad_fn=<SubBackward0>)
  W.grad:  None
```

backward

```
l.backward()
  W.grad:  tensor([[0.5318, 0.5318, 0.5318]])
```

A function node

Forward pass

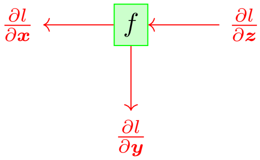


This node implements:

$$\boldsymbol{z} = f(\boldsymbol{x}, \boldsymbol{y})$$

A function node - 2

Backward pass



A function node knows :

- the "local gradients" computation

$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}, \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{y}}$$

- how to return the gradient to the inputs:

$$(\frac{\partial l}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}), (\frac{\partial l}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{y}})$$

Summary of a function node

f:

$$\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \qquad \text{\# store the values}$$

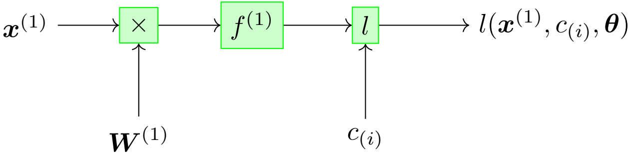
$$\boldsymbol{z} = f(\boldsymbol{x}, \boldsymbol{y}) \qquad \text{\# forward}$$

$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} \rightarrow \frac{\partial f}{\partial \boldsymbol{x}} \qquad \text{\# local gradients}$$

$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{y}} \rightarrow \frac{\partial f}{\partial \boldsymbol{y}}$$

$$(\frac{\partial l}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}}), (\frac{\partial l}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{y}}) \qquad \text{\# backward}$$

Example of a single layer network



Forward

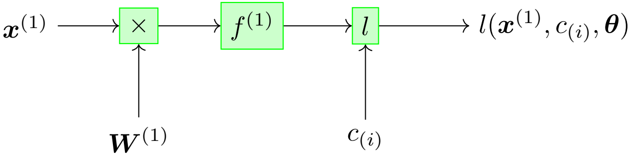
For each function node in topological order

- forward propagation

Which means:

1. $\boldsymbol{a}^{(1)} = \boldsymbol{W}^{(1)}\boldsymbol{x}^{(1)}$
2. $\boldsymbol{y}^{(1)} = f^{(1)}(\boldsymbol{a}^{(1)})$
3. $l(\boldsymbol{y}^{(1)}, c_{(i)})$

Example of a single layer network



Backward

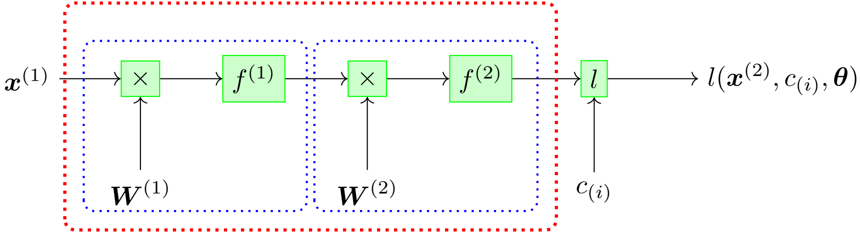
For each function node in reversed topological order

- backward propagation

Which means:

1. $\nabla_{\boldsymbol{y}^{(1)}}$
2. $\nabla_{\boldsymbol{a}^{(1)}}$
3. $\nabla_{\boldsymbol{W}^{(1)}}$

Example of a two layers network



- The algorithms remain the same,
- even for more complex architectures
- Generalization by coding your own function node or by
- Wrapping a layer in a module

Outline

pytorch in three concepts

A *Tensor* is a tensor

- Similar to numpy's *ndarrays*, but can be used on a GPU to accelerate computing.
- A node of a computation graph, holding:
  - the gradient w.r.t to it self (back-propagation)
  - a reference to its creator

Autograd

Package for building computational graphs out of Tensors, and automatically computing gradients

Module

A neural network layer, may store state or learnable Function (i.e with parameters)

An example in pytorch

```
import torch as th
# The model
D_in=2  # input size : 2
D_out=1 # output size: one value
model = th.nn.Sequential(
   th.nn.Linear(D_in, D_out),
   th.nn.Sigmoid()
   )
loss_fn = th.nn.BCELoss()
# Optimizer will update  the weights of the model.
lr0 = 1e-4
optimizer = torch.optim.SGD(model.parameters(),
                          lr=lr0)
```

An example in pytorch - 2

```
for t in  range(10):
    # Forward pass: compute predicted y by passing x.
    y_pred = model(x)
    # Compute and print loss.
    loss = loss_fn(y_pred, y)
    print(t, loss.data[0])
    # Optim in two steps
    optimizer.zero_grad()
    # Backward pass: compute gradient of the loss wrt parameters
    loss.backward()
    # Calling the step function on an Optimizer makes an update
    optimizer.step()
```

Three kinds of *Module*

Linear

- *Linear* is a *Module* for a linear transformation.
- The parameters: a *Tensor* $\boldsymbol{W}$
- Forward $\boldsymbol{x} \rightarrow \boldsymbol{W}\boldsymbol{x}$

Sigmoid

- *Sigmoid* is a *Module* for a pointwise function
- No parameters

Sequential

- *Sequential* is a container *Module*
- It contains a sequence of *Module*, i.e a feed-forward NNet

Look at the *torch.nn* doc for many examples

From CPU to GPU

```
# This vector is stored on cpu (+any operation you do on it)
a = torch.DoubleTensor([1., 2.])
# The same for GPU
a = torch.FloatTensor([1., 2.]).cuda()
a = torch.cuda.FloatTensor([1., 2.])
# it will be on the default device:
torch.cuda.current_device()
#####
# For the model:
model = model.cuda()
```

Define your module

```
class LogisticRegression(th.nn.Module):
    def __init__(self,D_in):
        super(LogisticRegression, self).__init__()
        self.lin = th.nn.Linear(D_in, 1)
        self.out = th.nn.Sigmoid()

    def forward(self, x):
        a = self.lin(x)
        return self.out(a)

mod = LogisticRegression(D_in=2)
```

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Approximation by superpositions of a sigmoidal function.
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