# Neural Networks for Classification

## An Introduction to Supervised ML

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06/08/26

# Outline


- Goal
- Neural Networks
- Learning: Optimising Loss
- Learning: Gradient Computation
- Learning: With Pytorch
- Example: MLP for XOR
- Learning: Variants of SGD
- Neural Networks for Classification
- Conclusion

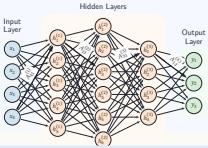
# 1
# Goal

# 1 Working Example: Build a Classifier for Images

From a set of images classified into predefined categories, we want to build: a system able to classify new images

## Input

## Output




dog

cat

hamburger

## Two-step process

1. Compute a probability for each category
2. Return the most probable category

## *Data Mining* perspective

1. Use a Neural Network (NN) to compute probabilities
2. Learn NN parameters from examples

## A small detour

Before we use NN for classification, let us see how they can model functions in general.

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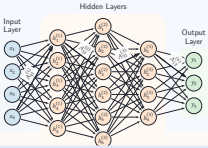


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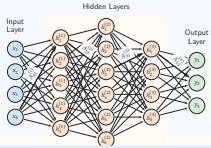


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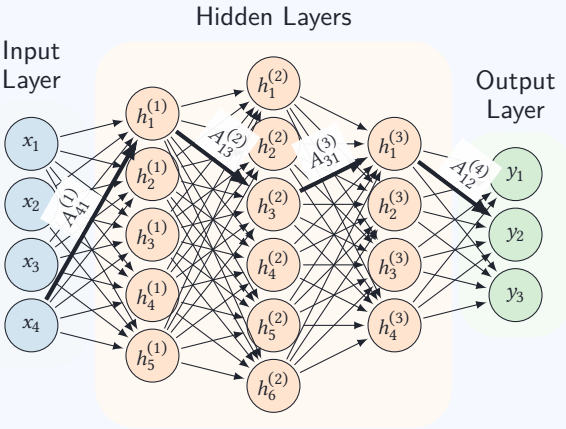
# 2
# Neural Networks

# 2 General Form (0)

## Mental Picture of a Neural Network




from https://youtu.be/MiHrd2rtCZQ?si=NUJHmjTRsaGYc4QE

## a neural network example

- implements a function $\mathbb{R}^4 \longrightarrow \mathbb{R}^3$ (i/o)
- has 3 hidden layers
- is *fully connected*
- no loop
- operations:
  1. multiply by coeff on outgoing edge
  2. sum over all incoming edges

# 2 General Form (1)

Functions transforming vectors of size $i$ to vectors of size $o$

## Linear Functions $\mathbb{R}^i \longrightarrow \mathbb{R}^o$

We write linear functions $h_{i,o} : \mathbb{R}^i \longrightarrow \mathbb{R}^o$, $h_{i,o}(x) = Ax + b$, with

- $A$ matrix in $\mathbb{R}^{o \times i}$,
- $b$ (column) vector in $\mathbb{R}^o$ called the *bias*
- $x \in \mathbb{R}^i$ the input (column) vector

This returns a (column) vector $y \in \mathbb{R}^o$ such that:

$$y = Ax + b$$

We have for each output dimension $1 \leq p \leq o$:

$$y_p = (A_p \cdot x) + b_p = (\sum_{k=1}^{i} A_{pk} \times x_k) + b_p$$

## Remarks

Yes, these are affine functions, not linear... but we call them linear anyway.

# 2 General Form (2)

## Elementary Activations

We call elementary activation the application of a function $\eta$ in $\mathbb{R} \longrightarrow \mathbb{R}$ to each element of a tensor (matrix, vector...) We note the application by $\eta$ itself.

## Example:

$\eta(x) = x^2$. then we have $\eta(\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}) = \begin{bmatrix} 1 & 4 \\ 9 & 16 \end{bmatrix}$

## Neural Network (MLP)

is a function $\mathbb{R}^i \longrightarrow \mathbb{R}^o$, constructed as follows:

$$R(x) = h^L_{o_{L-1},o} \circ \eta \circ \cdots \circ \eta \circ h^2_{o_1,o_2} \circ \eta \circ h^1_{i,o_1}(x)$$

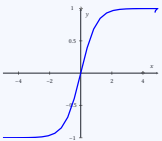
- $h^l_{i,j}$ are linear functions
- $\eta$ is the elementary application of a non-linear function
- $L$ is called *the number of layers* of the network
- $o_l$ is the *size* of layer $l$

Alias : multi-layer perceptron (hence *MLP*)

# 2 Elementary Non-linearities

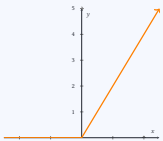
Make NN able to approximate general functions (without, only linear transformations, cf next)

## Usual Non-linear Activations



(a) $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

(b) $\sigma(x) = \frac{1}{1+e^{-x}}$



(c) ReLU$(x) = \max(0, x)$

(d) LReLU$(x) = \max(\min(0, 0.1x), x)$

Figure 1: Examples of common non-linear activations: hyperbolic tangent, sigmoid, linear rectificator, *leaky* linear rectificator

The purpose is to create threshold effects

# 2 A Universal Approximator

## Informal version

*For any function (∗) $f : \mathbb{R}^m \longrightarrow \mathbb{R}^n$ and all $\epsilon > 0$, there exists a MLP $R$ s.t. $|f(x) - R(x)| < \epsilon, \forall x$*

(∗) abuse of language, there exist functions we cannot approximate well...(discontinuous, infinite values,...)

- Actually, several theorems depending on $f$, $R$ and norm
- In these theorems $R$ has either:
  1. a possibly infinite number of layers,
  2. 2 layers : $R(x) = h^2_{t,o} \circ \eta \circ h^1_{i,t}(x)$ but layer size $t$ can be arbitrary large.

## Idea of the proof

Divide the output space in intervals, return average value on interval.

- approximation quality increase with number of intervals
- see contruction on neuralnetworksanddeeplearning.com

## Remarks

1. Above result theoretical
   - in practice number of parameters is limited
2. Still, MLP used to approximate (with error)

## In practice

*Depth matters more than width*

Why Depth Wins

- Hierarchy Early layers spot basic shapes, deeper combine into objects.
- Efficiency Adding layers splits input space exponentially faster than widening
- Savings Deep networks approximate functions with a linear or polynomial scale, whereas wide networks need exponential neuron counts.

# 3
# Learning: Optimising Loss

# *Learning* Parameters: Approximate a function $f$

Hyperparameters being fixed, we search the parameters for which the difference between the two systems ($f$ and the network) is zero.

## Error Approximation Function [cf. IMRL/Robotics INFO2]

To measure the quality of approximation we define an error function. An example of such error function is MSE:

$$E_{f,R}(x) = \frac{1}{n}\sum_{k=1}^{n}\frac{1}{2}(f(x)[k] - R(x)[k])^2$$

## Remark

- $E : \mathbb{R}^m \longrightarrow \mathbb{R}^+$ the result is a positive (or zero) scalar
- This is an example, other Error functions are possible (and better sometimes)

## Good Approximation

If $E_{f,R}(x) < \varepsilon$ for all input $x$ we have effectively managed to approximate $f$ with $R$ (with positive error $\varepsilon$ that we want close to zero).

# 3 *Learning* Parameters: Approximate *unknown* $f$

In general, we want to approximate a function that we do not know analytically, but for which we only a subset of its graph $T = \{(x_i, y_i = f(x_i))\}_i$ (*i.e.* instances of input/output $f$).

## Loss Function

We will assign parameters to approximate these examples. We define a new function, a *loss function* which averages errors made on these instances:

$$L = \frac{1}{|T|} \sum_{(x_i,y_i)\in T} E_{y_i,R}(x_i) = \frac{1}{|T|} \sum_{(x_i,y_i)\in T} \frac{1}{n} \sum_{k=1}^{n} \frac{1}{2}(y_i[k] - R(x_i)[k])^2$$

- If $L$ is close to zero, $R$ approximates $f$ on instances.

## Supervised Learning vs. Reinforcement Learning

- here we have $x$ and $y$, input and correct output ($\neq$ IMRL/Robotics INFO2)
- gradient methods are exact

# 3 Example: Computing MSE Loss

```
# T: set of examples (x,y)
# x vector in R^2, y scalar (in R)
# beware: not efficient (we will fix that later)
local_losses = [ torch.mean(torch.square(y - net(x))/2) for (x,y) in T]

# transform list to tensor and 'averaging'
loss = torch.mean(torch.stack(local_losses))
```

# 3 Learning Parameters: Generalisation vs. Overfitting

While we learn on given training set, we are interested in applying our model on new data. How good is it?

## Overfitting

Can we expect a model to be accurate if training set loss is low (0)?

- No, with enough parameters, an MLP can learn the training set by heart, and still be unable to predict from new data.
- We need to evaluate on a disjoint set, mimickin new data, called the the test set.

## Generalisation

We want to select the model that performs best on unseen data:

- We use a validation set, disjoint from both training set and test set, to choose when to stop gradient descent.

We will write $R$ with additional arguments in order to make parameters explicit, *i.e.* $R(x;\theta)$ with $\theta$ the concatenation of all parameters (elements of vectors/matrices)

**Parametrised Error Function**

$$E_{y,R}(x;\theta) = \frac{1}{n}\sum_{k=1}^{n}(y[k] - R(x;\theta)[k])^2$$

**Parametrised Loss Function**

$$L(\theta) = \frac{1}{|T|}\sum_{i} E_{y_i,R}(x_i;\theta)$$

# 3 Learning and Optimisation

Since function $L$ is positive or null (if no error), learning parameters for $R$ can be cast as the following problem:

## Learning Objective

$$\theta^* = \underset{\theta}{\operatorname{argmin}}\, L(\theta) = \underset{\theta}{\operatorname{argmin}}\, \frac{1}{|T|} \sum_{(x_i, y_i) \in T} E_{y_i, R}(x_i; \theta)$$

We search parameters which minimize $L$ ($\longrightarrow$ which zero $L$)

## Remarks

1. If differentiable elem. non-linearities (wrt $\theta$), $R$ differentiable too;
2. gradient of function $f$: vector of partial derivatives wrt a vector of variables. For $L(\theta)$, we note its gradient wrt to $\theta$ as $\nabla_\theta L(\theta)$ or simply $\nabla L(\theta)$;
3. Solution to above problem is among solutions of $\nabla L(\theta) = \mathbf{0}$
4. $L$ is not convex in general: several solutions.
5. Not important (What!!???): local minima will be good enough.
6. Problem: $\nabla L(\theta) = \mathbf{0}$ too difficult to solve analytically

# 3 Learning by gradient descent (1/5)

We will solve our problem (find a local minimum of $L(\theta)$) by an iterative method:

## Gradient Descent Algorithm

- Initialize $\theta^0$ randomly
- $t = 0$
- While $\|\nabla L(\theta^t)\|_2 \geq \epsilon$
  - Determine the size of step $\alpha^t > 0$ (more on that later)
  - $\theta^{t+1} = \theta^t - \alpha^t \nabla L(\theta^t)$
  - t = t+1
- return final $\theta$

Simple, provided we can compute gradient $\nabla L(\theta^t)$, does this work?

## Intuition

*We move the current estimate by moving it (a tiny bit) in the direction that reduces the loss most steeply*

# 3 Learning by Gradient Descent (2/5)

Easy part,each iteration improves the solution (less errors on examples). We start from the Taylor Expansion of $L$ around $\theta^t$:

$$\begin{aligned} L(\theta^{t+1}) = L(\theta^t - \alpha^t \nabla L(\theta^t)) &= L(\theta^t) + \langle \nabla L(\theta^t), (\theta^t - \alpha^t \nabla L(\theta^t)) - \theta^t \rangle + o(|\alpha^t \nabla L(\theta^t)|) \\ &= L(\theta^t) + \langle \nabla L(\theta^t), -\alpha^t \nabla L(\theta^t) \rangle + o(|\alpha^t \nabla L(\theta^t)|) \\ &= L(\theta^t) - \alpha^t \|\nabla L(\theta^t)\|^2 + o(|\alpha^t \nabla L(\theta^t)|) \\ &\approx L(\theta^t) - \alpha^t \|\nabla L(\theta^t)\|^2 \text{ for small enough } \alpha^t \\ &\leq L(\theta^t) \end{aligned}$$

**Technical problems (for math people)**

1. What does *small enough* $\alpha^t$ means?
2. What if $L(\theta^{t+1}) = L(\theta^t)$ (if $\alpha^t = 0$), does it work?

To prove (rate of) convergence we would need stronger assumptions on $L$ (smoothness, strong convexity, blabla...)

# 3 Learning by Gradient Descent (3/5)

**Technical problem for non-math people: too slow**

$$\nabla L(\theta) = \nabla \frac{1}{|T|} \sum_{(x,y)\in T} E(y, R(x;\theta))$$

- hidden nested loop: iterate through all examples to compute the average gradient!
- too slow, and impossible to use with *big-data* (millions of examples)

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## Approximate (near-)infinte Average ? We saw that last year...

Computing average ≡ expectation

$$\nabla L(\theta) = \nabla \frac{1}{|T|} \sum_{(x,y)\in T} E(y, R(x;\theta)) = \sum_{(x,y)\in T} \frac{1}{|T|} \nabla E(y, R(x;\theta)) = \mathbb{E}_{(x,y)\sim p(x,y)}[\nabla E(y, R(x;\theta))]$$

with uniform distribution from $T$: $\forall (x,y) \in T, p(x,y) = \frac{1}{|T|}$.

- We can approximate the expectation with MC sampling (cf. INFO2)
- (we could prove this is an unbiased estimator, so everything will be fine...)

# 3 Learning by Gradient Descent (4/5)

## *Stochastic* Gradient Descent: update after each example

- Initialize $\theta^0$ randomly; $t = 0$
- While $\theta^t$ *is different from* $\theta^{t+1}$
  - pick up an example $(x, y)$ randomly in $T$
  - Determine step size $\alpha^t > 0$
  - Update: $\theta^{t+1} = \theta^t - \alpha^t \nabla E(y, R(x; \theta^t))$ and $t = t + 1$

## Intuition and Remarks

- Numerous small updates give useful parameters very early in training
- But: we do not have $L(\theta^{i+1}) < L(\theta^i)$ (reasoning *in expectation*)
- Solution: hybrid the 2 methods and perform updates on $k << |T|$ examples (gradient descent on *batches*).

# 3 Learning by Stochastic Gradient Descent (5/5)

WLOG, we assume that $R$ approximates $f$ a function in $\mathbb{R}^m \longrightarrow \mathbb{R}$

## How to compute a gradient ?

For our approximation error $E$ (MSE):

$$\begin{aligned} \nabla E_{y,R}(x;\theta) &= \nabla \frac{1}{2}(y - R(x;\theta))^2 \\ &= -y\nabla R(x;\theta) + R(x;\theta)\nabla R(x;\theta) \\ &= (R(x;\theta) - y)\nabla R(x;\theta) \end{aligned}$$

Of course, this must be adapted if we use a different error function.

## But... how to compute $\nabla R(x;\theta)$?

- $R$ is a composition of functions
- use the chain rule (remember $f(g(x))' = f'(g(x)) \cdot g'(x)$)
- can be done automatically, computable in $O(n)$ where $n$ is the number of parameters : this is called *backpropagation*
- no need to compute gradient by hand 🤯

# 4
# Learning: Gradient Computation

# 4 Gradient Computation: How Does this Work?

## NN toolkit implement efficient gradient computation

gradient of the loss function wrt NN parameters $\theta$. Based on:

- the chain rule $(f(g(x)))' = f'(g(x)) \times g'(x)$
- the *Computation Graph* a graph describing the computation: parameters are leaf nodes

## Example Computation (from the pytorch website)

```
x1, x2 = 0.5, 0.75
z = log(x1 * x2) * sin(x2)
```

We decompose as:

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y3  = x1 * x2
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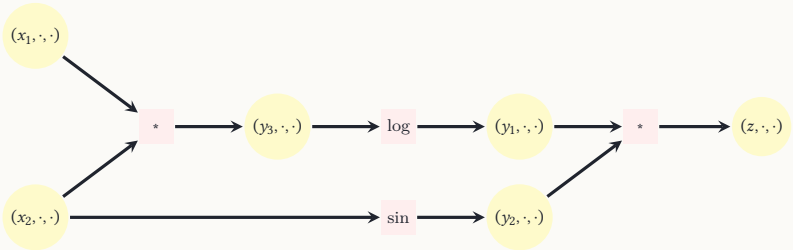


We know how to compute values i.e the *forward pass*: from input to output, apply operator semantics when incoming nodes are ready, and propagate.

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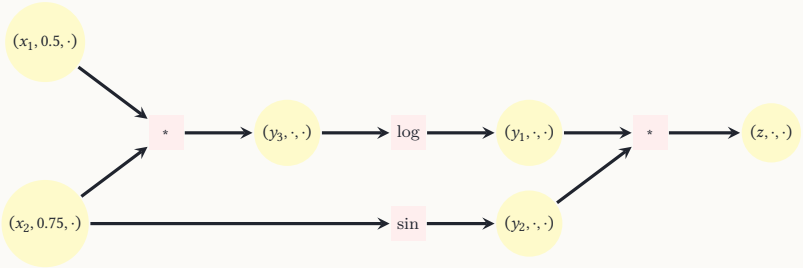


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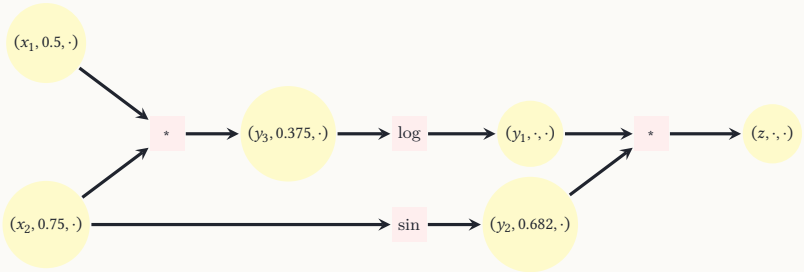


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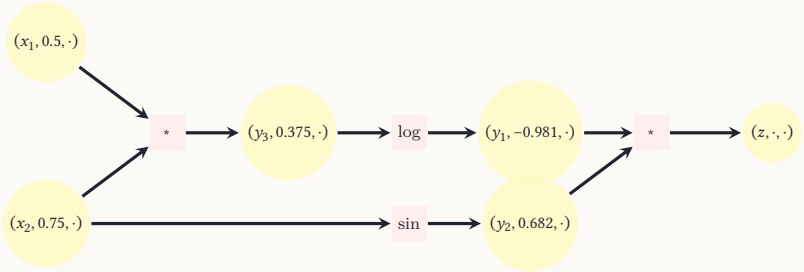


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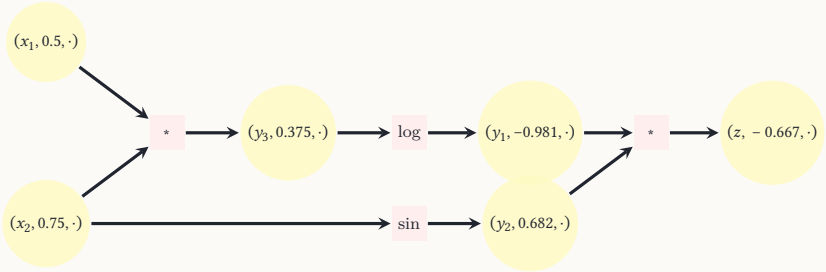


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# 4 Computing derivatives by hand: the chain rule

We want to derive $z = g_1(\log(g_2(x1, x2)), sin(x2))$ where $g_1(x, y) = g_2(x, y) = xy$

We note: $y_1 = \log\left(g_2(x1, x2)\right)$ $y_2 = \sin(x2)$ $y_3 = g_2(x1, x2)$

$$\frac{\partial z}{\partial x1} = \frac{\partial y_1}{\partial x_1}\frac{\partial g_1(y_1, y_2)}{\partial y_1} + \frac{\partial y_2}{\partial x_1}\frac{\partial g_1(y_1, y_2)}{\partial y_2} = \frac{\partial y_1}{\partial x_1}y_2 + \frac{\partial y_2}{\partial x_1}y_1 = 0.682\frac{\partial y_1}{\partial x_1} - 0.981\frac{\partial y_2}{\partial x_1} \quad (1)$$

$$\frac{\partial y_1}{\partial x1} = \frac{\partial y_3}{\partial x_1}\frac{\partial \log y_3}{\partial y_3} = \frac{\partial y_3}{\partial x_1}\frac{1}{y_3} = \frac{\partial y_3}{\partial x_1}\frac{1}{x_1 x_2} = \frac{1}{0.375}\frac{\partial y_3}{\partial x_1} \quad (2)$$

$$\frac{\partial y_2}{\partial x1} = \frac{\partial x_2}{\partial x_1}\frac{\partial \sin x_2}{\partial x_2} = 0\cos x_2 = 0 \quad (3)$$

$$\frac{\partial y_3}{\partial x1} = \frac{\partial g(x_1, x_2)}{\partial x_1} = x_2 = 0.75 \quad (4)$$

Putting it all together: $\frac{\partial z}{\partial x_1} = x_2\frac{1}{x_1 x_2}\sin(x_2) + 0\log(g_2(x1, x2)) = \frac{sin(x_2)}{x_1} = \frac{0.682}{0.5} = 1.36$

The same thing applies to $\frac{\partial z}{\partial x_2}$, we could do them in parallel by computing the vector of derivatives at each time

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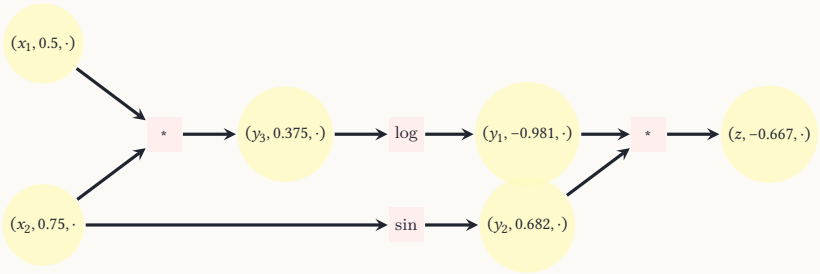


We can compute derivatives through a *backward pass*: from output to input, apply operator derivative semantics when outgoing nodes are ready, and propagate.

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We decompose as:

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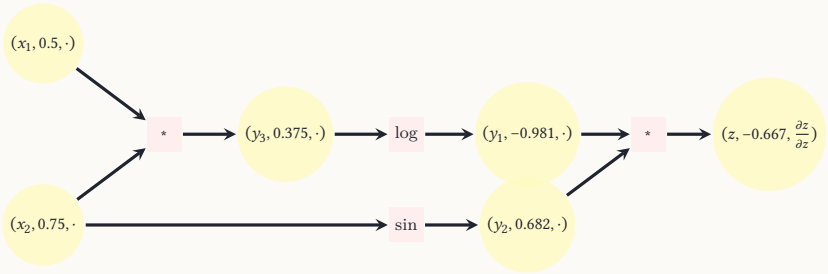
We want to compute the gradient of `z` wrt parameters `x1,x2`




We can compute derivatives through a *backward pass*: from output to input, apply operator derivative semantics when outgoing nodes are ready, and propagate.

# 4 Computing Derivatives on Computation Graph

**Example Computation (from the pytorch website)**

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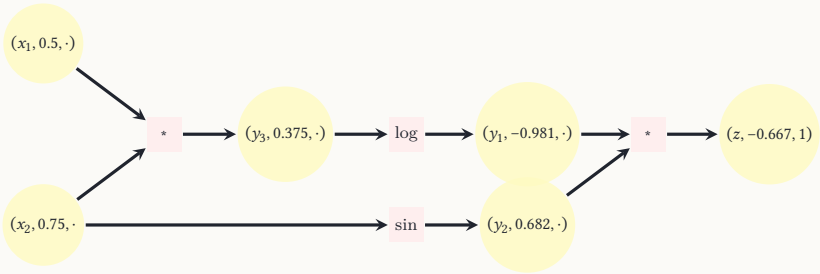


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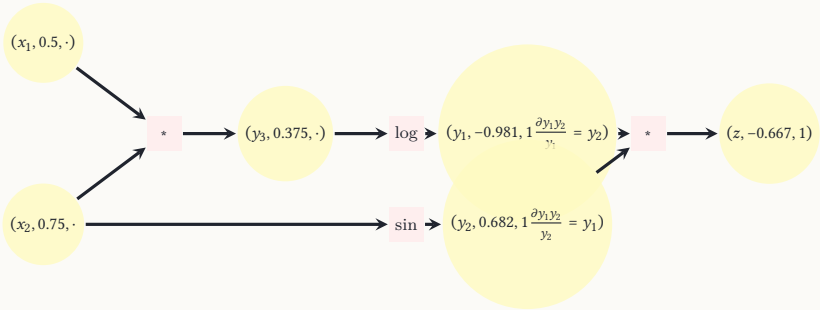


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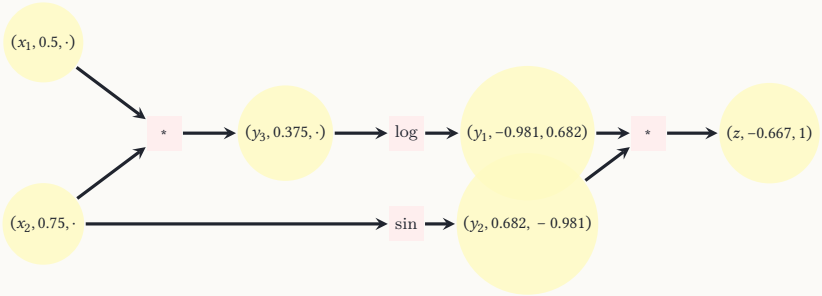


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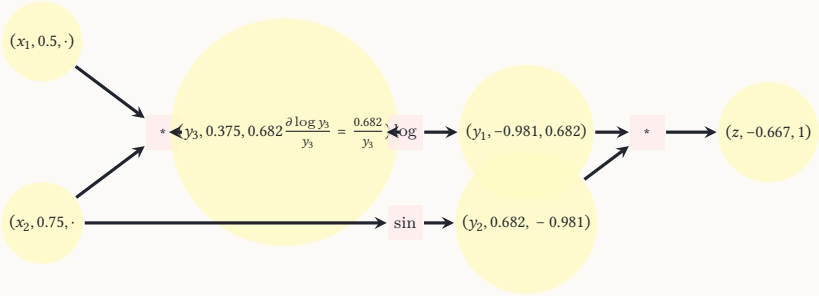


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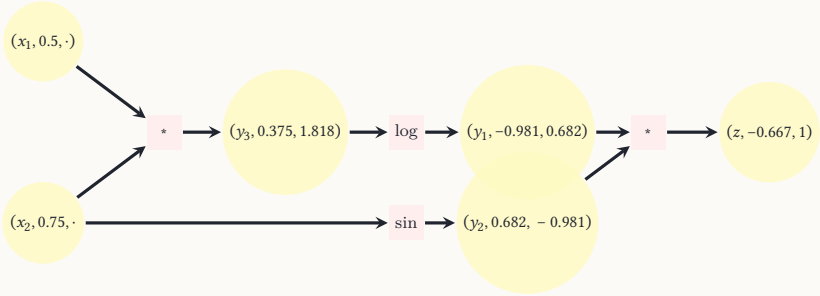


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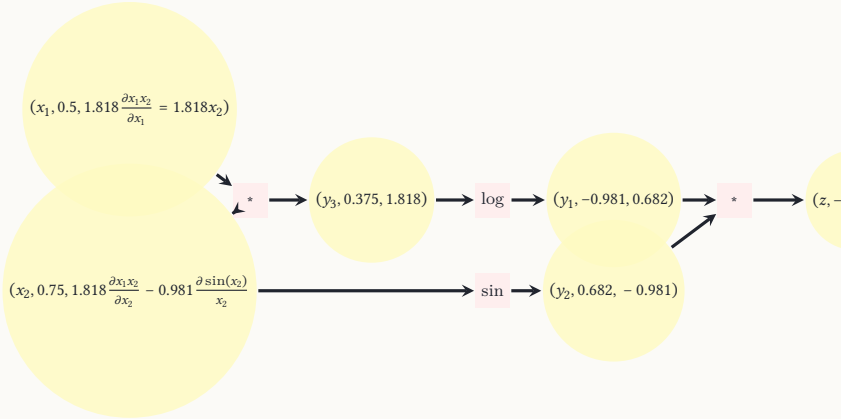


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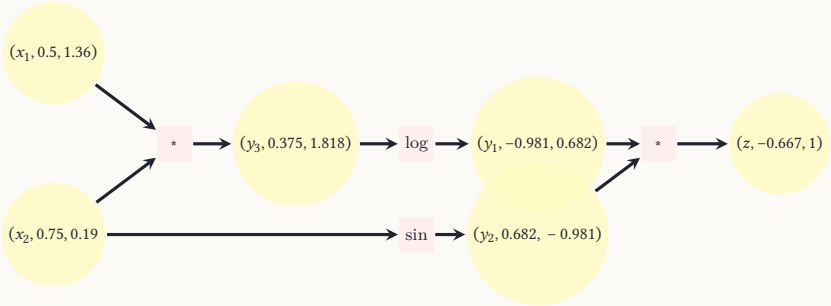


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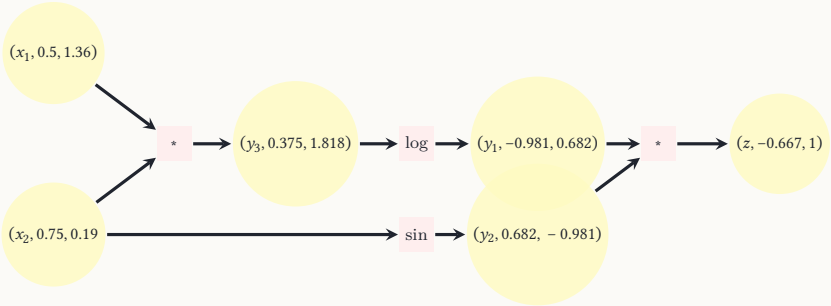



We can compute derivatives through a *backward pass*: from output to input, apply operator derivative semantics when outgoing nodes are ready, and propagate. This is backpropagation (reverse-mode automatic differentiation)

# 5
# Learning: With Pytorch

# 5 Example: Computing gradient (1/2)

```
# assume example ([2,3], 5):
local_loss = torch.square(5. - net(torch.tensor([2.,3.])))/2
print(local_loss)
#print matrix R^2 -> R^4 and its gradient
print("weight ", net.l1.weight.data)
print("grad ", net.l1.weight.grad)
```

# 5 Example: Computing gradient (2/2)

```
local_loss = torch.square(5. - net(torch.tensor([2.,3.])))/2
print(local_loss)
local_loss.backward() #compute gradient for this example
print("grad ", net.l1.weight.grad)
#update via SGD: (alpha = 0.001)
net.l1.weight.data = net.l1.weight.data - 0.001 * net.l1.weight.grad
net.l1.weight.grad=None #reset gradient
print("weight" ,net.l1.weight.data)
print(torch.square(5. - net(torch.tensor([2.,3.])))/2)
```

# 6
# Example: MLP for XOR

# 6 XOR

We want to learn function XOR (exclusive or):

| $x_1$ | $x_2$ | XOR$(x_1, x_2)$ |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

- $T = \{\big((0,0),0\big), \big((0,1),1\big), \big((1,0),1\big), \big((1,1),0\big)\}$
- we use for error *squared difference*

# 6 XOR

with linear MLP!!

```
import torch

#Input Data
Xdata = torch.tensor([[0,0],[0,1],[1,0],[1,1]], dtype=torch.float)
Ydata = torch.tensor([0,1,1,0], dtype=torch.float)

# A linear function
class MLP1(torch.nn.Module):
  def __init__(self):
    super(MLP1, self).__init__()
    self.l1 = torch.nn.Linear(2,1) # linear transform from R^2 to R^1

  #definition of the computation
  def forward(self, x):
    return self.l1(x)
```

```
def train(network, nb_exp=1000, frq_eval=10, alpha=0.1):
  mean_error_score = 0
  for m in range(nb_exp):
    # example selection: 1 sample   0 <=s < nb examples
    i = torch.randint(0, Xdata.size(0),(1,))
    # error computation
    # we do not divide by 2 and the number of examples
    # the learning rate alpha will be adapted
    error = torch.square(Ydata[i] - network(Xdata[i]))

    mean_error_score += error.item()

    # gradient computation
    error.backward()

    #gradient descent for all parameters
    for param in network.parameters():
      param.data.copy_(param.data - alpha * param.grad)
      param.grad = None #reset gradient

    #displayinformation
    if ((m+1) % frq_eval) == 0:
      print(m+1, mean_error_score/(m+1))
```

# 6 What is going on? (1/2)

```
net1 = MLP1()

train(net1, nb_exp=100000,frq_eval=10000)
```

```
10000 0.3166704567254973
20000 0.31482294204291567
30000 0.3154012085853026
40000 0.3151980722819008
50000 0.31485916941647885
60000 0.314789082526171
70000 0.3146943392594383
80000 0.3145794869730803
90000 0.314728939228619
100000 0.3151644724246957
```

Loss not really decreasing...

# 6 What is going on? (2/2)

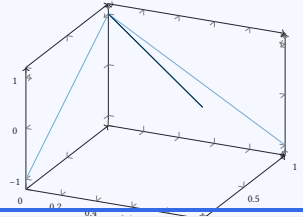
## Tests

```
print(net1(torch.tensor([0.,0.])))
print(net1(torch.tensor([0.,1.])))
print(net1(torch.tensor([1.,0.])))
print(net1(torch.tensor([1.,1.])))
```

```
tensor([0.8819], grad_fn=<ViewBackward0>)
tensor([0.5641], grad_fn=<ViewBackward0>)
tensor([0.8478], grad_fn=<ViewBackward0>)
tensor([0.5299], grad_fn=<ViewBackward0>)
```

## Linear MLP could not find useful parameters !!

Expected, impossible to find a linear function to approximate XOR (draw picture)



# 6 With Non-Linear Function (1/2)

```
net2 = MLP2()
train(net2, nb_exp=100000,frq_eval=10000)
```

# 6 With Non-Linear Function (2/2)

## Tests

```
print(net2(torch.tensor([0.,0.])))
print(net2(torch.tensor([0.,1.])))
print(net2(torch.tensor([1.,0.])))
print(net2(torch.tensor([1.,1.])))
```

## MLP2 found good parameters!

# 7
# Learning: Variants of SGD

# 7 Gradient Descent

Different variants of SGD. Implemented as subclasses of `torch.optim.optimizer`

- `SGD` vanilla stochastic gradient descent
- `AdaGrad`, `Adam`, `AmsGrad` maintain average of previous gradients to adjust $\alpha$ steps for each parameter individually
- `LBFGS` uses 2nd-order derivatives to compute optimal $\alpha$

# 7 Parameter Update with `Optimizer` (1/3)

```
def train(network, optimizer, nb_exp=1000, frq_eval=100, alpha=0.1):
  mean_error_score = 0
  for m in range(nb_exp):
    optimizer.zero_grad() #reset gradient

    # example selection
    i = torch.randint(0, Xdata.size(0),(1,))
    #error computation
    error = torch.square(Ydata[i] - network(Xdata[i]))
    mean_error_score += error.item()

    # gradient computation
    error.backward()
    #gradient descent
    optimizer.step()

    #display some info
    if ((m+1) % frq_eval) == 0:
      print(m+1, mean_error_score/(m+1))
```

# 7 Parameter Update with `Optimizer` (2/3)

```
net2 = MLP2()
opt = torch.optim.SGD(net2.parameters(), lr=0.1)

train(net2, opt, nb_exp=100000,frq_eval=25000)

print(net2(torch.tensor([0.,0.])))
print(net2(torch.tensor([0.,1.])))
print(net2(torch.tensor([1.,0.])))
print(net2(torch.tensor([1.,1.])))
```

# 7 Parameter Update with `Optimizer` (3/3)

```
net2 = MLP2()
opt = torch.optim.Adam(net2.parameters(), lr=0.001)

print("Hello")
train(net2, opt, nb_exp=100000,frq_eval=25000)
print("World")

print(net2(torch.tensor([0.,0.])))
print(net2(torch.tensor([0.,1.])))
print(net2(torch.tensor([1.,0.])))
print(net2(torch.tensor([1.,1.])))
```

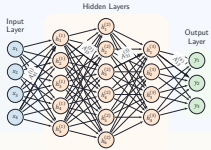
# 8 Neural Networks for Classification

# 8 Remember our Goal: Build an Image Classifier

As we said in our very first slide, from a set of images classified into predefined categories, we want to build: a system able to classify new images

## Input

## Output




dog

cat

hamburger

## Two-step process

1. Compute a probability for each category
2. Return the most probable category

## *Data Mining* perspective

1. Use a Neural Network (NN) to compute probabilities
2. Learn NN parameters from examples

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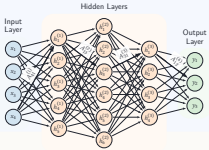


dog 0.14

cat 0.85

hamburger 0.01

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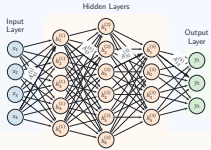


dog 0.14
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# 8 Neural Networks for Classification (1/2)

## Most tasks with NNs are classification tasks (even in the age of GenAI!)

From an input in $\mathbb{R}^d$ , assign it a class $c$ among $C$ possibilities

- given a picture predict whether it's a dog, a cat...
- given a text predict whether it's about politics, sports...

## With a MLP:

- define a MLP $R$ which approximate a function from $\mathbb{R}^d \longrightarrow \mathbb{R}^C$
- each output dimension $c$ represents the score of the $c^{\text{th}}$ class given the input
- return the dimension whose score is the highest: given $x \in \mathbb{R}^d$, return $c^* = \text{argmax}_c R(x)[c]$

## Remarks

1. We are not really interested in class scores, but how they compare to each other!!
2. The input is a picture, not a vector:
   - we flatten the pixel grid (picture as a sequence of pixels)
   - We will discuss this in more details in the next lecture

# 8 Neural Networks for Classification (2/2)

## Probabilistic loss

Learn parameters of $R$ for classification from examples

- Assume we have examples $\mathcal{T} = \{(x_i, c_i)\}_i$ (input,correct class)
- we want to train our NN to predict $c_i$ when given $x_i$, or
- we want to train our NN to predict $c_i$ the most probable class given $x_i$

## 2 Issues

1. How do we turn scores into probabilities
2. How do we formally express the learning intuition (most probable class)

## Turn scores into probabilities: the softmax function

We define the probability of class $c$ given an input $x$ as:

$$p(c|x) = \frac{\exp(R(x)[c])}{\sum_{c'} \exp(R(x)[c'])} = \text{softmax}(R(x))[c]$$

- $\exp$ to get positive values
- $\sum$ in denominator to get values between 0 and 1, which all sum to 1

This has many names (Gibb's distribution, exponential family…), and is already implemented in pytorch!

# 8 Loss function for Classification: Learning as Likelihood Estimation

**Goal**

We want examples $\mathcal{T} = \{(x_i, c_i)\}_i$ to be as probable as possible (ie. $p(c_i|x_i) \longrightarrow 1$).

**Remark**

if $\lim p(c|x) \longrightarrow 1$, it means that for $c' \neq c$ we have $\lim p(c'|x) \longrightarrow 0$

**We want to maximize the *likelihood* of $\mathcal{T}$**

$$\prod_i p(c_i|x_i)$$

This is a product... difficult to optimize (+ precision issues)

- work in the log domain $\longrightarrow$ the product becomes a sum
- multiply by -1 $\longrightarrow$ maximization becomes a minimization with optimal zero: we have a loss

**Finally the loss function to be minimized is:**

$$L(\theta) = -\sum_i \log p(c_i|x_i) = -\sum_i \log(\text{softmax}(R(x_i;\theta))[c_i]$$

# 8 Learning as Cross-Entropy (1/2)

## In Pytorch

Negative log-likelihood is called cross-entropy loss, why?

## Definition: (Conditional) Cross Entropy

between 2 distribution $q$ and $p$ for one input:

$$\texttt{CE}(q, p) = -\sum_{c} q(c|x) \log p(c|x)$$

## Equivalence

Let us compute the cross-entropy between for one input in $\mathcal{T}$

- $q$ the empirical distribution (1 for examples, 0 otherwise)
- $p$ the distribution parameterized by our MLP
- For a training example $\{x_i, c_i\}$, we can show:

$$CE(p, q) = -\log p(c_i|x_i)$$

Summing over training examples brings us back to the negative log-likelihood of the training set.

# 8 Learning as Cross-Entropy (2/2)

**Proof of the derivation**

$$\texttt{CE}(q, p) = -\sum_{c} q(c|x_i) \log p(c|x_i)$$

$$\texttt{CE}(q, p) = -q(c_i|x_i) \log p(c_i|x_i) - \sum_{c \neq c_i} q(c|x_i) \log p(c|x_i)$$

$$\texttt{CE}(q, p) = -1 \times \log p(c_i|x_i) - \sum_{c \neq c_i} 0 \times \log p(c|x_i)$$

$$\texttt{CE}(q, p) = -\log p(c_i|x_i)$$

*Summing* this for all examples gives the negative log likelihood !

# 8 Cross-Entropy in Pytorch (1/2)

```
# classifier for input of size 10, 5 classes:
net = MLP2(10,8,5)

# let us pretend the following tensor contains
# the input for 3 examples
inputs = torch.rand(3,10)

# we obtain the 5 scores for all 3 examples
preds = net(inputs)

# let us suppose that the correct classes were:
empirical = torch.tensor([0,2,1], dtype=torch.long)

loss_function = torch.nn.CrossEntropyLoss()

# note that we do not compute log softmax (inside CE)
loss = loss_function(preds, empirical)

loss.backward() # and the rest...
```

# 8 Cross-Entropy in Pytorch (2/2)

At testing time:

```
# classifier for input of size 10, 5 classes:
net = MLP2(10,8,5)

# let us pretend the following tensor contains
# the input for 3 examples
inputs = torch.rand(3,10)

# we obtain the 5 scores for all 3 examples
predictionss = net(inputs)

#apply the argmax for each line:
outputs = torch.argmax(predictionss, dim=1)
```

no cross-entropy, no softmax: why?

# 9
# Conclusion

# 9 Conclusion

## Neural Networks

- composition of linear mappings and elementary non-linear activations
- can be *learned* (parametrized) by reviewing labeled examples
- learning amounts to gradient descent of a loss function

## Classification

- Output a score for each class
- Transform into a probability with softmax
- Learn with Negative Log-Likelihood loss

## Back Propagation

- method to implement gradient descent efficiently
- works on a *computation graph* (DAG)
- share computation: linear complexity in the depth of the DAG