Deep neural networks

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Artificial neural networks

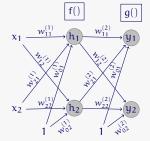
- · ANNs are networks of units (neurons) each performing basic computation: calculate the weighted sum of the inputs, apply an activation function
- · Combination of the units results in powerful learning machines
- The ANNs are inspired by biological neural networks, but they differ in quite a few ways
- The ANNs are also closely related to linear models

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Feed-forward networks: with matrix/vector notation



 $\mathbf{h} = \mathbf{f}(\mathbf{W}^{(1)}\mathbf{x})$ $\mathbf{y} = \mathbf{g}(\mathbf{W}^{(2)}\mathbf{h})$ $= g(\mathbf{W}^{(2)}f(\mathbf{W}^{(1)}\mathbf{x}))$

 f() and g() are non-linear functions, such as logistic sigmoid or tanh

Realizing that an ANN boils down to a series of matrix multiplications (linear transformations) and (non-linear) function applications is also essential for effectively using some of the libraries.

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Learning in ANNs

- ANNs implement complex functions: we need to use iterative optimization methods (e.g., gradient descent) to
- Typically error functions for ANNs are not convex, gradient descent will find a local minimum
- Optimization requires updating multiple layers of weights
- Assigning credit (or blame) the each weight during learning is not trivial
- An effective solution to the last problem is the backpropagation algorithm

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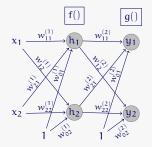
Deep learning

- During the last decade, a set of methods collectively known as deep learning became dominant
- They are (mostly) based on multi-layer neural networks
- They won many of the competitions against other ML methods (e.g., SVMs)
- The main premise is to learn useful features automatically: no need for feature engineering

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Feed-forward networks: the picture and the math



$$h_j = f\left(\sum_i w_{ij}^{(1)} x_i\right)$$

$$y_k = g\left(\sum_j w_{jk}^{(2)} h_j\right)$$

$$y_k = g\left(\sum_i w_{ik}^{(2)} f\left(\sum_i w_{ij}^{(1)} x_i\right)\right)$$

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ANNs: activation functions

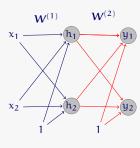
- Output layer activations depend on the problem
 - For regression, linear (e.g., identity function) I(z) = z
 - For binary classification, logistic sigmoid (called simply 'sigmoid' in the ANN literature)
 - For multi-class classification softmax $softmax_j(z) = \frac{e^{z_j}}{\sum_k e_k^z}$
- For hidden layers, *logistic* or *tanh* used to be the norm in the earlier models (but more on this later in this lecture)

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Learning in ANNs: backpropagation

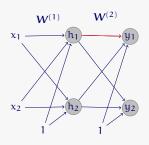


- Updating weights $W^{(2)}$ are easy: we can use gradient descent directly
- But the contribution of weights $W^{(1)}$ to the error is indirect
- Backpropagation algorithm efficiently assigns credit to weights in the earlier layers

Learning in ANNs: backpropagation

 $W^{(2)}$

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gradient descent directly • But the contribution of weights $\mathbf{W}^{(1)}$ to the error

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 Backpropagation algorithm efficiently

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Where do non-linearities come from?

(a short divergence)

In a linear model, $y = w_0 + w_1x_1 + \ldots + w_kx_k$

- The outcome is *linearly-related* to the predictors
- The effects of the inputs are additive

This is not always the case:

- · Some predictors affect the outcome in a non-linear way
 - The effect may be strong or positive only in a certain range of the variable (e.g., age)
 - Some effects are periodic (e.g., many measures of time)
- Some predictors interact 'not bad' is not 'not' + 'bad' (e.g., for sentiment analysis)

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Dealing with non-linearities (2)

assigns credit to weights in the earlier layers

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Dealing with non-linearities (1)

(a short divergence, contd.)

Non-linear transformations, kernels, feature engineering

· Note that both

$$y = w_0 + w_1 x_1 + w_2 x_1^2$$

and

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$$y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2$$

are still linear in weights.

- + The objective function is still convex, we have a global minimum
- Requires careful feature selection/engineering
- Often becomes slow to train

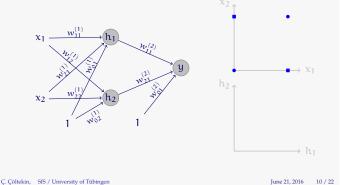
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Dealing with non-linearities (2)

(a short divergence, contd.)

Multi-layer networks (a solution to the XOR problem)

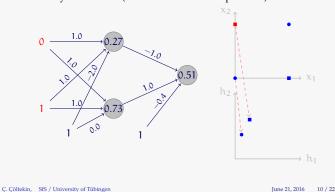


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Dealing with non-linearities (2)

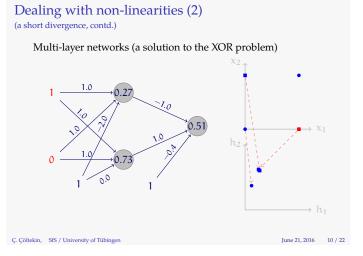
(a short divergence, contd.)

Multi-layer networks (a solution to the XOR problem)



(a short divergence, contd.) Multi-layer networks (a solution to the XOR problem)

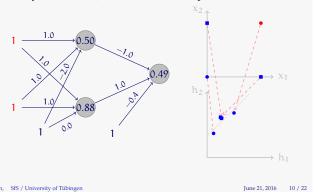
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Dealing with non-linearities (2)

(a short divergence, contd.)

Multi-layer networks (a solution to the XOR problem)



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Deep learning

- 'Deep learning' refers to a set of ML methods, mainly based on ANNs
- The major difference from what we have seen so far is the 'deep' architectures with many hidden layers
- The deep ANNs have been successful many areas of ML, since about 2006, winning competitions on most reference data sets
- The main premise is learning useful features automatically: no need for feature engineering!

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Deep networks: why do they make sense?

Another important (and practical) reason is that some problems are easier to represent using multiple layers

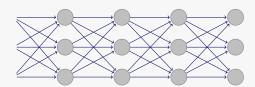
- Image processing pixels → edges → shapes → objects → ...
- $\begin{tabular}{ll} \bf Language\ processing \\ speech\ signal \rightarrow phonemes \rightarrow syllables \rightarrow words \rightarrow \dots \\ \end{tabular}$

If problem can be simplified by learning a hierarchy of features, deep networks will probably be more useful.

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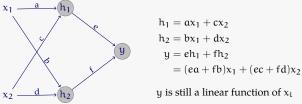
Deep networks: many hidden layers



- Deep networks are simply feed-forward networks with many layers
- The additional hidden layers bring some advantages, as well as some difficulties
- The number of (effective) layers may exceed hundreds in practice

Non-linear activation functions are necessary

Without non-linear activation functions, the ANN is eqivalent to a linar model.



Deep networks: why do we need them?

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- We noted earlier that (large) MLPs with a single hidden layer are universal approximators: they can approximate any continuous function with arbitrary precision. However,
 - theoretical results do not limit the number of units: it may require number of units exponential in the size of the data
 - being able to 'represent' does not mean being able to 'learn'
 - some families of functions can efficiently be approximated by deep networks, but require much larger networks if depth is smaller

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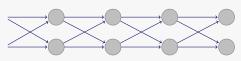
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Deep networks: why now?

- Most models/methods used in deep networks today are proposed as early as 1980's
- The reason for 'renewed' popularity/success has to do with
 - Computer hardware became faster, especially GPUs are useful for training/using ANNs
 - ANNs are more efficient (e.g., in comparison to main rival SVMs), with big amount of data
 - Some developments allowed training models that were difficult to train before

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Training deep networks: problems



- A major problem is unstable gradients, they are backpropagated to earlier layers. The gradients may
 - vanish, learning becomes too slow
 - explode, convergence becomes difficult (or impossible)
- In general, training deep networks is (still) difficult.
 Models are sensitive to initialization, many parameters, numeric stability issues, ...

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Dealing with unstable gradients

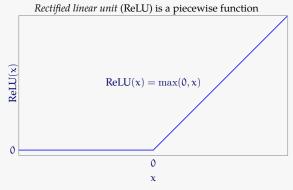
- Standard regularization methods (L1 or L2) help avoiding exploding gradients
- Another popular approach against exploding gradients is gradient clipping or or scaling
- Some activation functions are more prone to unstable gradients. For example, derivative of the logistic sigmoid is close to zero for most part of its input space
- For vanishing gradients, special regularization schemes that encourage information flow, or special architectures are suggested

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ReLU



ReLU is (currently) the most common activation function in feed-forward deep networks.

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Deep networks: interim summary

- Deep neural networks are simply ANNs with multiple hidden layers
- They have recently been successful in many ML tasks, including in NLP
- Like ANNs, they are powerful learners (but often opaque to interpretation)
- But beware of the hype: try simpler models first, often we do not need the power of a complex network
- The field is still active, many methods and tools are still experimental

Next: CNNs and RNNs

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Activation functions in deep networks

• The choice of activation function for the output units are similar to MLP

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- Linear functions for regression
- Logistic sigmoid for binary classification
- Softmax for multi-class classification
- Instead of continuous sigmoid functions, piecewise linear functions are more popular
 - + Fast computation
 - + Smaller chance for vanishing/exploding gradients
 - 'Universal approximation' is still possible
 - Not suitable with certain architectures

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Common/popular models in deep learning

- Convolutional networks: for detecting local patterns
- Recurrent neural networks: for sequence learning
- Autoencoders/decoders: unsupervised methods using (deep) neural networks
- Combining different types of networks are often possible
- We will cover these three network types next

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In-class exercise

Task: train an MLP for learning the XOR problem using keras http://keras.io/. Here is a quick reference:

```
from keras.models import Sequential from keras.layers import Dense, Activation
     import numpy as np
     # create a new model
     m = Sequential()
     # the hidden layer -- try others: 'relu', 'sigmoid', ...
     m.add(Dense(input_dim=2, output_dim=2, activation='tanh'))
     # the output layer
    m.add(Dense(output_dim=1, activation='sigmoid'))
# input and the output
    x = np.matrix('0, 0; 0, 1; 1, 0; 1, 1')
y = np.array([1, 0, 0, 1])
# fit the model and predict
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    m.compile(loss='binary_crossentropy', optimizer='sgd')
m.fit(x, y, nb_epoch=10000)
     m.predict(x)
```

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