Artificial neural networks (ANNs)

SUMMARY

Supervised leaning

- **Predictive** modelling
    - prediction
    - detection
    - forecasting

1. Artificial neural networks (ANNs)

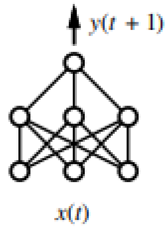
- Biological inspirations
    - Properties of the brain
        - it can **learn**, reorganize itself from experience
        - it **adapts** to changing conditions
        - it is **robust** and fault tolerant
- **Robustness** in ML?
    - the degree that a model's performance changes when using new data
        - noise
    - ideally, performance should not deviate significantly
    - how to test it?
        - CV, CIs

- **Two types of learning in NNs**
    - **supervised**
        - FFNNs, RBFNs, RNNs, DNNs, CNNs, …
    - **unsupervised**
        - self-organizing maps (SOM)
        - Hebbian learning
        - **autoencoders**
            - self-supervised learning
            - **encoding** part

- **Characteristics** of supervised NN learning models
    - represent (complex) non-linear functions
    - **eager** inductive learning models
    - appropriate for **offline** and **online** learning
    - used for **classification** and **regression**
    - black-box models
        - human readability is unimportant
    - are robust to noisy data
    - NNs are used as statistical tools
        - adjust nonlinear functions to fulfill a task
        - need of multiple and representative examples
    - NNs enable to model complex **static** phenomena (Feed-forward neural networks – FFNNs) as well as **dynamic** ones (Recurrent neural networks – RNNs)
        - **static** phenomena
            - time has no role
        - **dynamic** phenomena
            - temporal events
            - image and video recognition, time series, handwritten recognition, motion detection, signal processing, stock market prediction, speech recognition, aso
    - **NNs require**
        - a good representation of the data
        - training vectors must be statistically representative of the entire input space
        - the use of NNs needs a good comprehension of the problem
        - NNs require good data preprocessing (e.g. data normalization, for numerical data)
            - the range of all features should be normalized
                - comparable range for the features
                - transpose the input variables into the range of the activation function codomain (i.e. for *logistic* [0, 1], for *tanh* [-1, 1])
            - speeds up learning, faster convergence
    - Research domain: **NAS** (*Neural Architecture Search*)
        - subfield of **automated machine learning** **(AutoML)**
            - process of automating the tasks of applying ML to real-world problems
        - technique for automating the design of ANNs (both classical and deep)
            - **search space** defines the type(s) of ANN that can be designed and optimized
            - **search strategy** defines the approach used to explore the search space.
            - **performance estimation strategy** evaluates the performance of a possible ANN from its design (without constructing and training it).
        - RL, Hill climbing, Evolutionary algorithms, PSO, Multi-objective optimization,…

2. Types of NNs for supervised learning

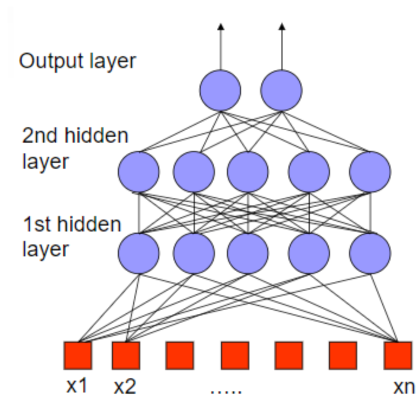
1. **Feed-forward neural networks (FFNNs)**
    - an ANN where connections between the units do not form a directed cycle
    - the first and simplest form of ANN
    - the information moves in only one direction, forward, from the input nodes through the hidden nodes and the output nodes
    - there are no cycles or loops in the network (time has no role)



(a) Feedforward network

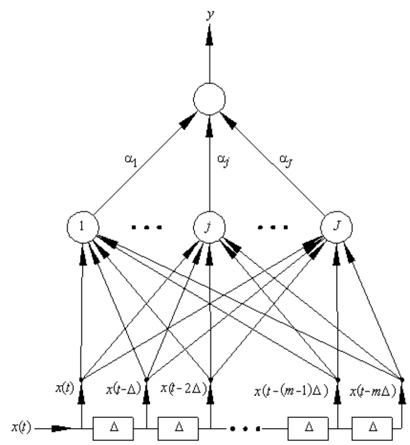
[1]

- types of FFNNs
  - **Multilayer perceptron (MLP)**
    - consists of multiple layers of nodes in a directed graph, with each layer fully connected to the next one



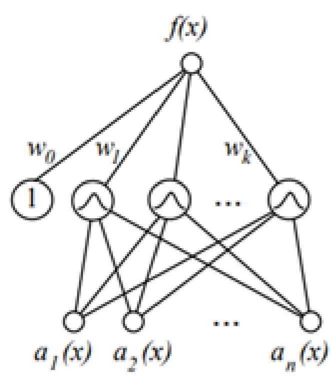
    - except for the input nodes, each node is a *neuron* (processing element) with a *nonlinear* activation function
    - utilizes a supervised learning technique called *backpropagation* for training the network
    - MLP is a modification of the standard linear perceptron and can distinguish data that are not linearly separable

  - **Time delay neural networks (TDNNs)**
    - theory
    - an alternative to a NN architecture whose purpose is to work on continuous data
    - learning a **temporal** sequence of events
    - maps a finite time sequence $\{X(t), X(t-\Delta), X(t-2\cdot\Delta) \ldots X(t-m\cdot\Delta)\}$ into a single output *y* (this can be generalized for the case when *x* and/or *y* are vectors)



- ○ [Pytorch]
- ○ helpful in many applications like:
  - time series predictions
  - online spell check
  - speech recognition (generation)
  - image analysis
  - aso
- ○ [Deep TDNN]

- **<u>Radial basis function networks (RBFNs)</u>**
  - ○ specific feed-forward architecture
  - ○ 1 hidden layer
  - ○ Gaussian activation function at the hidden layer



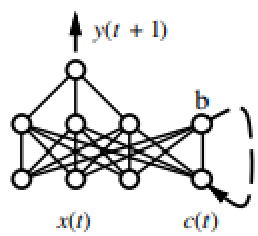
[1]

  - ○ connected to the **Instance based learning** (IBL) literature, but **eager** instead of **lazy**
    - computes a global approximation to the target function *f*, in terms of linear combination of local approximations ("**kernel**" functions)
    - is a different kind of two layer neural network
      1. the hidden units compute the values of kernel functions (local approximations)
      2. the output unit computes *f* as a linear combination of kernel functions

- applications
  - fault diagnosis
  - forecasting
  - image classification
  - image reconstruction
  - aso

2. Recurrent neural networks (RNNs)

- **sequential** or time series data
  - RNNs are a variant of the conventional FFNNs that can deal with sequential data and can be trained to hold knowledge about the past.
    - a mechanism is required to retain past or historical information to forecast future values.
- connections between units form a **directed cycle**
  - this creates an internal state of the network which allows to exhibit **dynamic temporal behavior**
  - can model systems with internal state (dynamic ones)



(b) Recurrent network [1]

- unlike FFNNs, RNNs can use their internal memory to process arbitrary sequences of inputs
- appropriate for time series data
  - learning is **sequential**
- applications:
  - handwritten recognition
  - motion detection
  - signal processing
  - text generation
  - time series prediction
  - stock market forecasting
  - aso
- the vanishing gradient problem of RNNs cause the network not to learn much → specialised versions of RNN
  - **LSTM**
  - **GRU (Gated Recurrent Unit)**

Long-Short Term Memory networks (LSTMs)

- a type of RNN
- this model is an attempt to allow the unit activations to retain important information over a much longer period of time
- applications:
  - language learning
  - robot control
  - music composition
  - speech and handwriting recognition
  - video processing
  - …

- other architectures: DeepLSTM, ConvLSTM, BiLSTM (Bidirectional LSTM), ensemble of LSTMs

3. Deep Neural Networks (DNNs)

- multiple hidden layers
- can express easier complex functions
- a layer may be viewed as a "***feature hierarchy***"
- Classes of DNNs [4]
  - DNNs for supervised learning
  - DNNs for unsupervised or generative learning
    - *generative models* – can learn and mimic any distribution of data
      - Bolzmann Machines, Restricted Boltzmann Machines, Deep Belief Networks, Deep Bolzmann Machines
      - *Generative adversarial networks* (GANs) [3]
        - two nets competing one against the other (generator/discriminator)
          - learn to generate new data
          - generating images, face, photographies
        - bidirectional GAN
        - generative adversarial exploration for reinforcement learning
    - Generative models in reinforcement learning
    - **research**: solving unsupervised learning problems with DNNs (e.g. ICA – independent component analysis, feature analysis, aso)
  - Hybrid DNNs, ensemble of DNNs, fuzzy DNNs

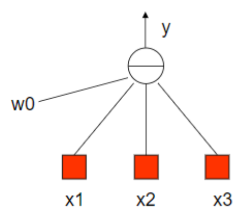
4. Convolutional Neural Networks (CNNs)

- inspired by the organization of the visual cortex (biological inspiration)
- applications:
  - computer vision [3]
  - natural language processing
    - e.g., sentence classification
  - video processing
  - object detection and recognition
- are deep FFNNs

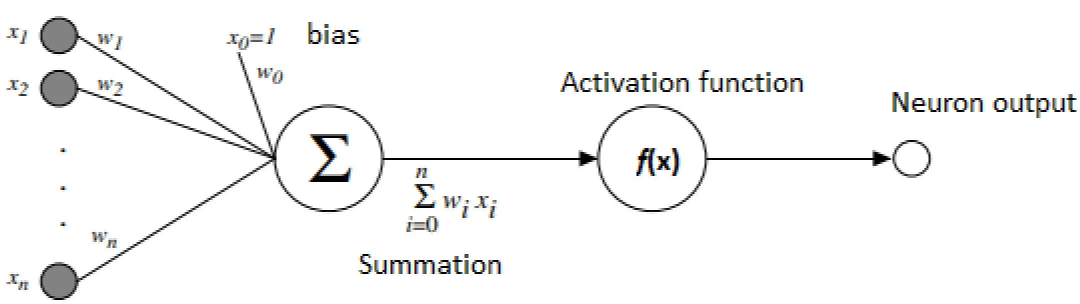
- **convolution**
  - from a dimension of an input, a filter is applied to it to take some of the interesting features from that dimension
- **GCN** - graph convolutional networks
  - graph structured data
  - handle higher dimensional (non-grid) data
  - **applications**
    - semi-supervised learning
    - supervised learning (text classification)
    - unsupervised learning
- **MobileNets** – efficient CNN architecture for mobile devices
- **low resource devices**
  - ***distillation***
    - compressing the knowledge from a large network into a smaller one
  - distilling the knowledge in a NN (Hinton, 2015), distilling knowledge from GCN
- Ensemble of CNNs

5. Classical NN architectures

- **Artificial neuron**
  - non-linear, parameterized function with restricted output range



$$y = f\left(w_0 + \sum_{i=1}^{n-1} w_i x_i\right)$$

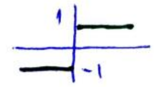


  - the output of the neuron is obtained by applying an (non-linear) **activation function *f*** on the linear combination of the neuron inputs

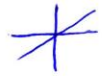
  - **Activation functions**
    - *Signum* – output range: -1, +1
      - does not have a derivative, undifferentiable in 0
      - perceptron

- *Identity* – output range: (-∞, +∞)
- *Hyperbolic* – output range: (-1, +1)
  - smooth approximation for the perceptron function
  - learning smoother than the perceptron
- *Sigmoid* (*logistic*) – output range: (0, +1)
  - e.g. predict a probability

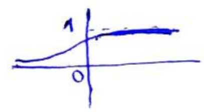
Sigmum $f(x) = \begin{cases} +1 & x > 0 \\ -1 & \text{otherwise} \end{cases}$



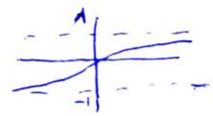
Identity $f(x) = x$



Sigmoid $f(x) = \dfrac{1}{1+e^{-x}}$ $(\sigma(x))$



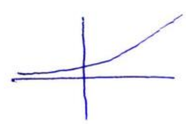
Hyperbolic $f(x) = \dfrac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$



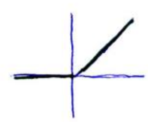
- *Gaussian* – output range: (0, 1)
- *ReLU* (Rectified Linear Unit) – output range: (0, ∞)
  - undifferentiable in 0
  - deep architectures
- *Soft plus* – output range: (0, ∞)

Gaussian $f(x) = \dfrac{1}{\sigma\sqrt{2\pi}} \cdot e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

Soft plus $f(x) = \ln(1 + e^{x})$



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



- *eLU* (Exponential Linear Unit) – output range: (0, ∞)
  - common in CNNs
  - can produce negative values
- *PReLU* (Parametric Rectified Linear Unit) – output range: (-∞, ∞)
  - undifferentiable in 0
  - deep learning
  - solves the problem with activation functions like sigmoid, where gradients would often vanish.

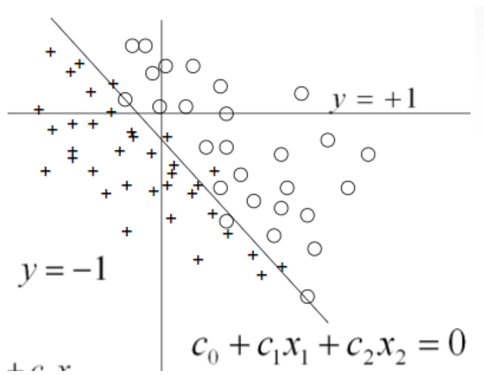
ELU

$$f(x) = \begin{cases} \alpha(e^{x}-1) & x<0 \\ x & x\geq 0 \end{cases}$$

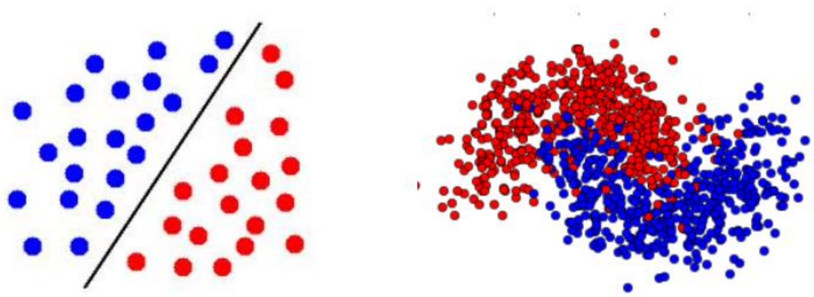
PReLU

$$f(x) = \begin{cases} \alpha \cdot x & x<0 \\ x & x\geq 0 \end{cases}$$

- **Perceptron**
  - represents a hyperplane decision surface in the high dimensional space of instances



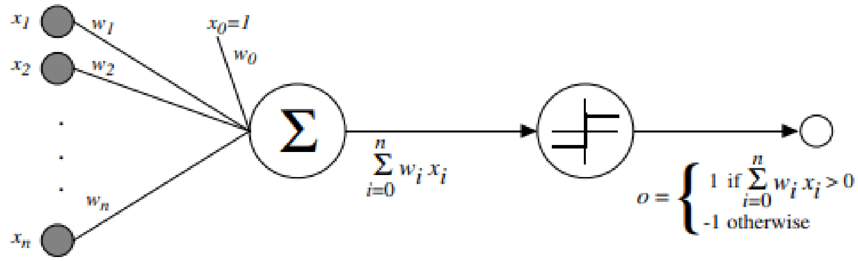
  - binary classification (outputs: -1, +1)



(a) (b)

(a) **linearly separable** data set (i..e, data set can be separated by a straight line)
(b) the classes are **not** linearly separable

  - linear classifier
  - appropriate for online learning



[1]

$$o(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Learning task

- **training examples** $D = \{(x_d, t_d)\}_{d=1,s}$ $x_d = (x_{1d}, x_{2d}, \ldots x_{nd}) \in \Re^n$, $t_d \in \{-1,+1\}$
- **goal**
  - learn the separating hyperplane
  - hypothesis: $w=(w_0, w_1, \ldots w_n) \in \Re^{n+1}$
- **error function**
  - **online learning**
    $$E_d(\vec{w}) = t_d - o_d$$
  - **offline learning**
    $$E(\vec{w}) = \frac{\sum_{d=1}^{s} |t_d - o_d|}{s}$$

- weights initialization
  - small random values (or 0)

- **Training rule**

$$w_i \leftarrow w_i + \Delta w_i$$

where

$$\Delta w_i = \eta(t - o)x_i$$

Where:

- $t = c(\vec{x})$ is target value
- o is perceptron output
- η is small constant (e.g., .1) called *learning rate* [1]

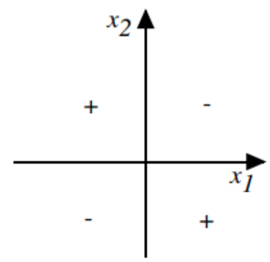
- **Linear classifier**

$$o(\vec{x}) = \begin{cases} 1 & \text{if } \vec{w} \cdot \vec{x} > 0 \\ -1 & \text{otherwise.} \end{cases}$$

- Example - perceptron

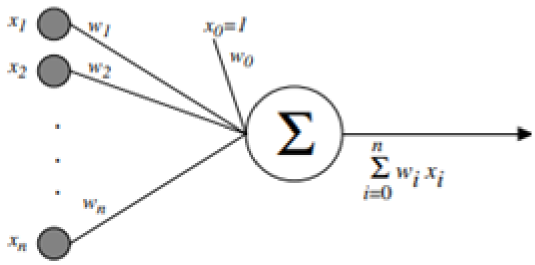
- The perceptron is able represent some useful boolean function: AND, OR, ˥AND, ˥OR

- converges only if training data is linearly separable and the learning rate is sufficiently small (e.g., 0.1)
  - Perceptron convergence theorem Rosenblatt
    - for a finite set of linearly separable labeled examples, after a finite number of iterations, the algorithm yields a vector *w* that classifies perfectly all the examples.
  - XOR function is not representable using a perceptron ⇒ we need multilayered networks



XOR function

- **Linear unit**
  - consider a *linear unit*, whose output *o* is $o = w_0 + w_1 x_1 + \cdots + w_n x_n$



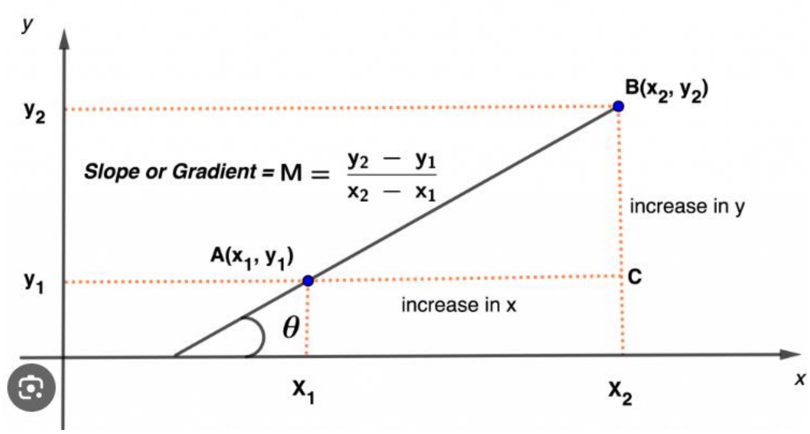
<u>Learning task</u>

- **training examples** $D = \{(x_d, t_d)\}$ $x_d = (x_{1d}, x_{2d}, \ldots x_{nd}) \in \Re^n$, $t_d \in \Re$
  - t_d represents the output of the neuron for the input instance *d*
- **goal**
  - learn the weights that minimize the squared error (e.g., using the *gradient descent optimization algorithm*)
    - **batch mode gradient descent**
      - over the training samples *D* $E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2$
    - **incremental (stochastic) gradient descent**
      - for each training sample $d \in D$ $E_d(\vec{w}) = \frac{1}{2}(t_d - o_d)^2$

- **Gradient descent**
  - the gradient of a function is a vector of *first derivatives* taken with respect to its constituent variables

$$\nabla f(p) = \begin{bmatrix} \frac{\partial f}{\partial x_1}(p) \\ \vdots \\ \frac{\partial f}{\partial x_n}(p) \end{bmatrix}$$

  - the gradient specifies the direction that produces the steepest increase in E
    - - $\nabla E[\vec{w}]$ - the direction of steepest descent
  - e.g., the **gradient** (*slope*) of a line shows how steep it is



Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

$$\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i} \frac{1}{2} \sum_d (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d \frac{\partial}{\partial w_i} (t_d - o_d)^2 \\
&= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d) \\
&= \sum_d (t_d - o_d) \frac{\partial}{\partial w_i} (t_d - \vec{w} \cdot \vec{x_d}) \\
\frac{\partial E}{\partial w_i} &= \sum_d (t_d - o_d)(-x_{i,d})
\end{aligned}$$

[1]

  - Training rule for
    - **batch mode gradient descent**

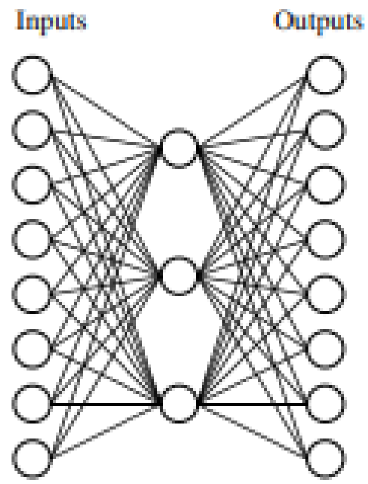
$$\Delta w_i = \eta \cdot \sum_{d \in D} (t_d - o_d) \cdot x_{i,d}$$

    - **stochastic gradient descent** (Delta rule)

$$\Delta w_i = \eta \cdot (t_d - o_d) \cdot x_{i,d}$$

- linear unit training rule using gradient descent is guaranteed to converge
  - to hypothesis H with minimum squared error
  - given a small learning rate
  - even when training data contains noise
  - even when training data not separable by H

- **Multilayer network**
  - also known as Multilayer perceptron (MLP [3])
  - can express a rich variety of non-linear decision surfaces



[1]

  - NN learning
    - learning model – ***network***
    - ***hypothesis*** – the vector of weights
  - Example of two 2-layer perceptron network for representing the XOR function
  - *Gradient descent* (GD) training rule over a multilayer network is the ***backpropagation*** training algorithm
    - **idea**
      - For each training example
        - propagate the input forward through the network
        - propagate the errors backward through the network
      - derive gradient descent rules for training
        - one network unit (e.g. *sigmoid*)
        - *multilayer network* of units → ***backpropagation*** [1]
    - batch mode GD
      - The learning rule is applied after all training instances are provided
    - stochastic GD
      - The learning rule is applied incrementally, after each training instance
  - Optimization algorithms [3] used in NN learning
    - GD
    - stochastic GD
      - extension: **Adam** (Adaptive moment estimation)
        - a learning rate is maintained for each network weight (parameter) and separately adapted

        - adaptive learning rates
        - deep learning
    - minibatch GD
      - performs an update for every batch with *n* training examples
    - **first order** optimization algorithms
    - **second order** optimization algorithms
      - use the second derivative (the **Hessian**)
- **characteristics of backpropagation**
    - GD over the entire network weight vector
    - training is slow (eager model)
      - using network after training is fast
    - will find a **local** error minimum (the error surface may contain many different local minima)
      - practice: run multiple times
      - weights initialization
        - Xavier initialization (using a Gaussian distribution)
    - **momentum**
        - speed up the convergence of the network
        - avoid convergence to a local minimum
- **optimize** the NN architecture
    - number of hidden layers, number of hidden neurons/layer, learning rate, momentum, etc
    - **genetic algorithms**
- **Problems** with gradient-based learning methods and backpropagation (the weights receive an update proportional to the partial derivative of the error function with respect to the weight)
    - **vanishing gradient**
      - in some cases, the gradient will be vanishingly small $\Rightarrow$ preventing the weights in changing their values
        - classical activation functions such as **sigmoid** or **hyperbolic tangent** have gradients in (0,1)
      - solutions to prevent the vanishing gradient problem
        - use other activations functions (whose derivative has a larger domain): ReLU, eLU, PReLU
        - use residual networks (ResNet)
        - use batch normalization layers, normalize the input
    - **exploding gradient**
      - the gradient is too large
      - the model became **unstable** and unable to learn from the training data
      - solutions to prevent the exploding gradient problem
        - fewer layers in the network
        - *clipping*
          - thresholding the value of the gradient
          - before performing the GD, assign a clip value if the gradient exceeds a threshold
        - weight regularization (L1, L2)
- ***loss functions***
      - Mean Squared Error (MSE) – L2 loss

            - Sensitive to outliers
        - Mean of Absolute Errors (MAE) – L1 loss
        - Cross-entropy
            - for classification
- ***overfitting*** in ANNs
    - may be due to
        - too many neurons (complex networks)
        - insufficient training data
        - not appropriate network architecture
            - it is not close enough to the problem context
    - reducing overfitting
        - use a **validation** set during training
        - **weight decay**
            - decrease weights with a small factor during each iteration
        - **regularization** techniques (L1, L2)
            - penalize large weights
            - add to the error function a regularization term
        - **dropout**
            - randomly drop up neurons (with their connections) during training
            - deep networks
- ***underfitting*** in ANNs
    - the model is too simple, it cannot capture the essence of the data
    - insufficient training, simplicity of the model, insufficient neurons

- Expressive capabilities of classical/traditional ANNs

Boolean functions:

- Every boolean function can be represented by network with single hidden layer
- but might require exponential (in number of inputs) hidden units

Continuous functions:

- Every bounded continuous function can be approximated with arbitrarily small error, by network with one hidden layer [Cybenko 1989; Hornik et al. 1989]
- Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].

[1]

6. Other ANNs related research topics

- Boosted ANNs
    - using a boosting algorithm for improving the performance of ANNs
- Ensemble of ANNs (LSTMs, Deep LSTMs)
- Fuzzy ANNs, Fuzzy Deep Neural Networks

- Lazy ANNs
- Hybrid models
    - ANN + DT
    - ANN + SVM (Support Vector Machines)
    - ANN for function approximation in Reinforcement Learning (RL)
- Parallel/Distributed ANNs
- Deep Residual Networks (ResNets), Progressive Neural Networks, Attention mechanism [3]
- GANs
- ….

[SLIDES]

- Artificial neural networks (T. Mitchell) [1]

[READING]

- Artificial neural networks (T. Mitchell) [1]
- Modern practical Deep networks (Goodfellow et al.) [2]
- CNNs and CNN architectures (Zhang et al.) [3]
- RNNs and Moderns RNNs (Zhang et al.) [3]

Bibliography

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