5.1 Neural Networks

Machine Learning 1: Foundations

Marius Kloft *(TUK)*

Kaiserslautern, 19–26 May 2020

Recap

Previous lectures: **linear** and/or **kernel** learning methods.

- learn a linear classifier $f(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$.
- learn a kernel classifier $f(\mathbf{x}) = \text{sign}(\sum_{i=1}^{n} \alpha_i k(\mathbf{x}_i, \mathbf{x}) + b)$.

Quiz: What are the advantages of these classifiers?
What can be improved?

+ linear classifiers are easy to understand and interpret
+ linear classifiers are fast ($\rightarrow$ big data)
+ kernel learning works well even for non-linearly separable data
+ both work well in surprisingly many applications ("swiss knife")

\- **Need to have already a good feature representation**

Neural networks can **learn** a feature representation.

Contents of this Class

Example: State of the Art in Image Classification

Before 2012: two steps

1. design some hand-crafted features
2. train an SVM on these features

After 2012: train a deep convolutional neural network

- learns the **features** and the classifier together in one go
  - this means the classifier—not a human expert—guides the design of the features

Problem of Learning Good Feature Representations

- Say we are given images $\mathbf{x}_1, \ldots, \mathbf{x}_n$
- Want to learn a map ϕ that assigns any image $\mathbf{x}$ with a vector representation $\phi(\mathbf{x})$

$$\xrightarrow{\phi} \begin{pmatrix} 0.3 \\ \vdots \\ 1.4 \end{pmatrix}$$

How can we learn a good feature representation ϕ?

Core Idea to Learn a Good Feature Representation ϕ

Let the learning machine figure it out!

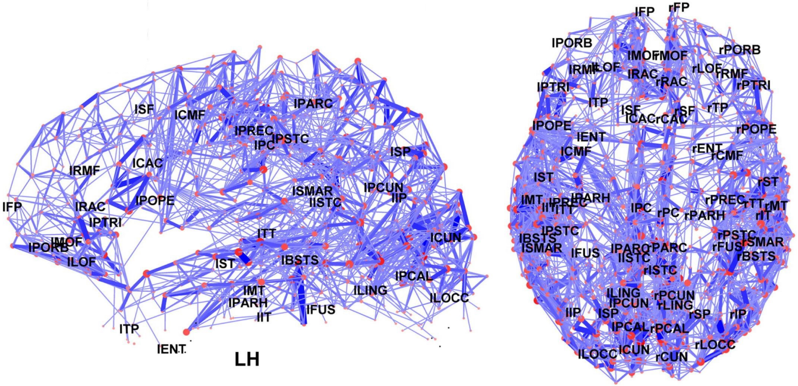
Recall logistic regression:

$$\min_{b\in\mathbb{R},\mathbf{w}\in\mathbb{R}^d,\phi} \quad \frac{1}{2}\|\mathbf{w}\|^2 \; + \; C\sum_{i=1}^{n} \ln\Big(1+\exp\Big(-y_i(\mathbf{w}^\top \phi\big(\mathbf{x}_i\big)+b)\Big)\Big)$$

- Want to learn ϕ
- Idea: Optimize also over ϕ!
- Problem: the search space of all mappings ϕ is too large... which restrictions to make?

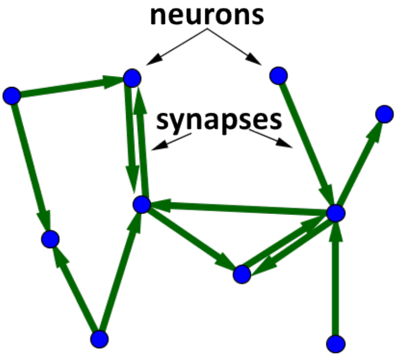
Idea: our brain also performs classification, for which it learns good feature representations ... **how does it do that?**

How Does the Brain Work?



Think of it as a graph!

Brain As Graph



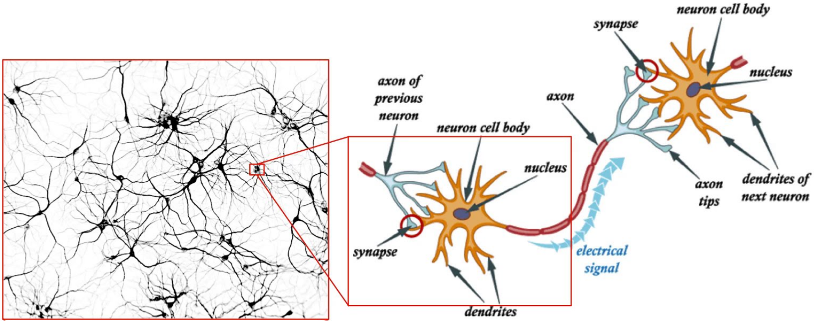
- The nodes are called **neurons**
- The edges are called **synapses**

Another word for graph is **network** and our network consists of neurons. Therefore we have a **neural network**.

Spikes and Potential

Whenever there is some action ongoing in our brain (e.g., we spotted a yummy box of chocolate)

- short pulses of electrical current (**Spikes**) shoot through our brain



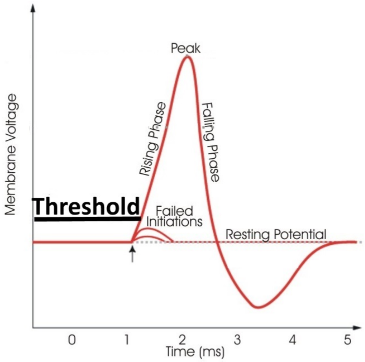
- Each neuron i receives spikes from a other neurons j
  - the stronger the synapse W_{ij}, the higher the total current (called **potential** u_i) that arrives at neuron i

Potential

Only if a neuron's potential u exceeds a threshold,

- (we say the neuron is **activated**)

it fires an impulse v (spike) to its neighbors in the neural network



Impulse can propagate from neuron to neuron through the entire brain

Artificial Neurons

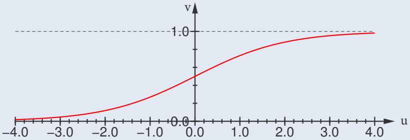
A classic neuron model is by McCulloch and Pitts (1950s):

McCulloch and Pitts model

Denote by u the neuron's potential and by v the emitted spike ("activation"). Then:

$$v = \sigma(u)$$

where σ is the **sigmoid** function: $\sigma(u) = \frac{1}{1+e^{-u}}$



Instead of the sigmoid function, today's ANNs usually use the **ReLU** activation function: $\sigma(u) := max(0, u)$

Artificial Neural Networks (ANNs)

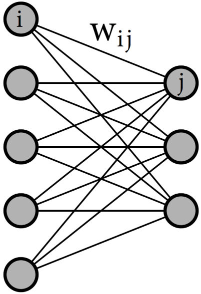
Let us propagate the activation from neuron to neuron:

- The jth neuron
  - is connected to other neurons with connection strength w_{ij}
  - thus it has potential

$$u_j = \sum_i w_{ij} v_i$$

  - and activation

$$v_j = \sigma(u_j) = \sigma\left(\sum_i w_{ij} v_i\right)$$

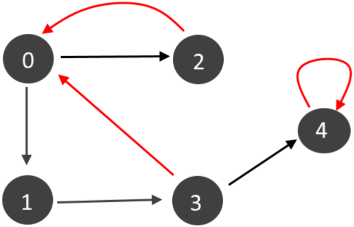


- All neurons together have
  - potential $\mathbf{u} = W^\top \mathbf{v}$
  - and activation $\mathbf{v} = \sigma(\mathbf{u}) = \sigma(W^\top \mathbf{v})$.

Problem: $\mathbf{v}$ is both on the left and right hand side of the equation (recursion) $\Rightarrow$ mathematical nightmare! :)

Notation: for a vector $\mathbf{u} = (u_1, \ldots, u_d)^\top$, we define $\sigma(\mathbf{u}) := (\sigma(u_1), \ldots, \sigma(u_d))^\top$.
The potential is also called pre-activation.

We Therefore Want to Avoid Cycles



Cycles
0->1->3->0
0->2->0
4->4

Although more difficult to deal with, there exist also cyclic ANNs, for instance, infinite impulse recurrent networks.

Feed-forward ANNs

The resulting architecture is called **feed-forward** ANN or multi-layer perceptron (MLP).

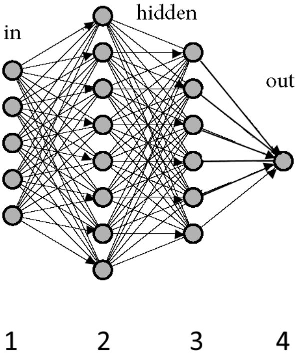
Example

Shown to the right is a network with

- an input layer (5 nodes)
- two hidden layers
  (8 and 6 neurons, respectively)
- an output layer (one node)

We index the four layers as follows:

- 1: input
- 2,3: hidden layers
- 4: output layer



Recall from Slide 15:

$$\mathbf{v} = \sigma(W^\top \mathbf{v}),$$

where:

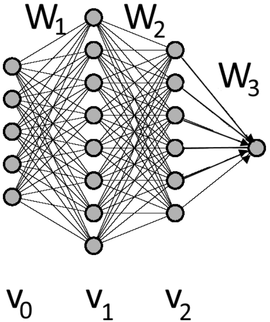
- $\mathbf{v}$ is the vector of activations of all neurons in the network
- $W = (w_{ij})$ are the weights of the connections of the neurons.

For a feed-forward ANN this simplifies:

$$\mathbf{v}_l = \sigma(\underbrace{W_l^\top \mathbf{v}_{l-1}}_{=:\mathbf{u}_l}),$$

where:

- $\mathbf{v}_l$ is the vector of activations of the neurons in the lth layer
- $W_l = (w_{lij})$ are the strengths of the connections between neurons i in the lth layer and neurons j in the $(l+1)$th layer

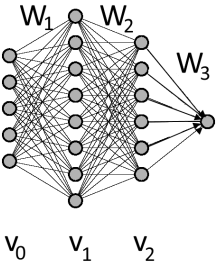


Mathematics of Feed-forward ANNs

The computation in a feed-forward ANN can be thus be summarized as a nested function:

$$f(\mathbf{x}) := \underbrace{\mathbf{w}^\top \phi_W(\mathbf{x})}_{=\mathbf{u}_{L+1}},$$

$$\phi_W(\mathbf{x}) := \underbrace{\sigma\Big(W_L^\top \sigma\big(\ldots \underbrace{\sigma(\underbrace{W_1^\top \underbrace{\mathbf{x}}_{=\mathbf{v}_0}}_{=\mathbf{u}_1})}_{=\mathbf{v}_1} \ldots\big)\Big)}_{=\mathbf{v}_L}$$



Remarks:

- We use a data point $\mathbf{v}_0 := \mathbf{x}$ as the network's initial activation.
- L denotes the number of hidden layers (example: $L = 2$).
- For a network with one output node, $\mathbf{w} := W_{L+1}$ is a vector.

Aim

In order to use f for prediction, we need to:

- find weights $\mathbf{w}, W_1, \ldots, W_L$
- such that $f(\mathbf{x}_i) \approx y_i$ on the training points.

How?

Neural Network Learning

We wrap a learning machine around the network and let it figure out good network weights!

We do so as follows:

- As learning machine we take logistic regression (LR)
- In LR, we replace all occurrences of the inputs $\mathbf{x}_i$ by $\phi_W(\mathbf{x}_i)$
- We optimize over the weights $W_1, \ldots, W_L$ of the network!

Thus We Obtain:

Feed-forward ANN

$$\min_{\mathbf{w},W} \quad \frac{1}{2}\|\mathbf{w}\|^2 + \frac{1}{2}\sum_{l=1}^{L}\|W_l\|_{\text{Fro}}^2 + C\sum_{i=1}^{n}\log(1+\exp(-y_i\mathbf{w}^\top\phi_W(\mathbf{x}_i)))$$

where

- $W := (W_1, \ldots, W_L)$
- $\phi_W(\mathbf{x}_i) := \sigma\Big(W_L^\top \sigma\big(\ldots\sigma(W_1^\top \mathbf{x}_i)\ldots\big)\Big)$

Given a matrix $M = (m_{ij}) \in \mathbb{R}^{m\times n}$, the Frobenius norm is defined as $\|M\|_{\text{Fro}}^2 = \sum_{ij} m_{ij}^2$

Conclusion

Artificial neural networks (ANN)

- motivated by how the brain works
- consisting of neurons organized in multiple layers with (feed-forward) connections
- learning feature representation (network weights) and classifier at the same time

Next video: ANNs on images (CNNs)

References I

W. S. McCulloch and W. Pitts, A logical calculus of the ideas immanent in nervous activity, *The bulletin of mathematical biophysics*, vol. 5, no. 4, pp. 115–133, 1943.