Neural Nets and the Perceptron

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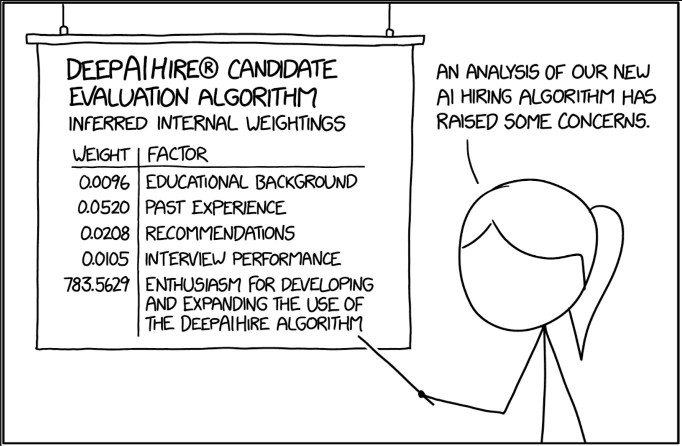
Lecture 07.1 (v2.1.1)

Signposting

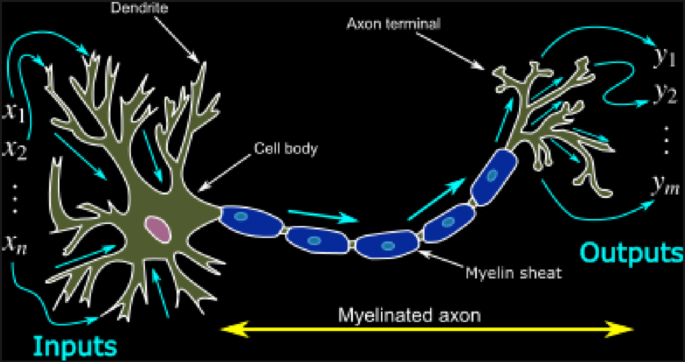


https://xkcd.com/2237/

Questions

- What makes a neural network **deep**?
- Does **deep** matter?
- How can we learn parameters for a neural net?

Neurons



- Dendrites take inputs
- Axons fire on activation
- Form a **dynamical system**

Artificial Neurons

- Take a number of input signals
- Activation function transforms to output
- Output sent as input to downstream neurons
- (Typically) constructed to form a **directed system** for learning

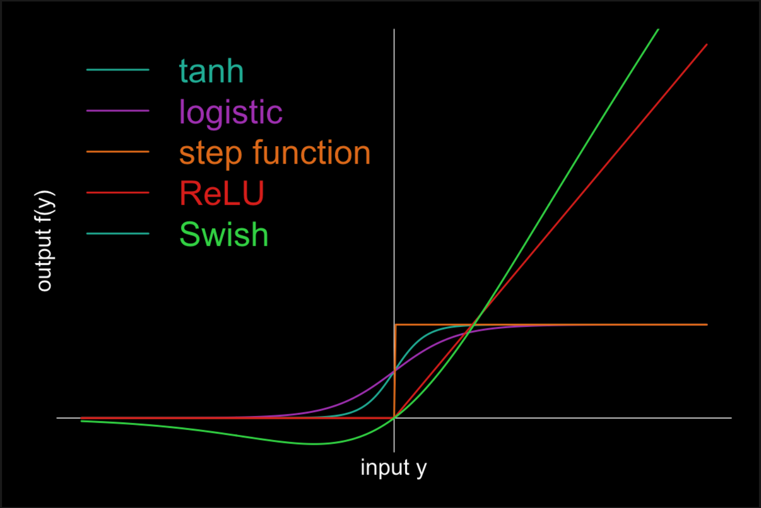
Activation functions

- Neuron i is modelled as:
  - A nonlinear **activation function** f:
  - a base rate $W_{0,i}$,
  - and weights $W_{j,i}$ for each input neuron a_j with output x_{a_j}:

$$f\left(W_{0,i} + \sum_{j=1} W_{j,i} x_{a_j}\right),$$

- f is a mapping $\mathbb{R} \to [r_{min}, r_{max}]$ (which may not be bounded).
- There are many common choices, e.g.:
  - tanh: $f(y) = (1 + \tanh(y))/2$
  - logistic: $f(y) = 1/(1 + e^{-y})$
  - Step function: $f(y) = \mathbb{I}(y > 0)$
  - Rectified linear unit (ReLU): $f(y) = \mathbb{I}(y > 0)y$

Activation functions



Activation functions

- The important features of activation functions are:
  - **Non-linearity**. A deep neural network can be trivially replicated by a one layer neural network if the activations are linear.
  - **Derivatives**. Learning requires evaluating derivatives, which should be *cheap*, and *informative*.
  - **Smoothness**. Simple discontinuities can be handled, complex ones make learning slow.

Activation functions in practice

- ReLU contains the important complexity whilst being very fast to learn;
- It may exhibit convergence problems when $y << 0$;
- For small networks, complex activation helps.
- A notable modern alternative is **Swish**[1]:
  - $f(y) = y / \left(1 + \exp(-\beta y)\right)$
  - **ReLU-like**: Converges to zero for $x \to -\infty$ and to x for $x \to \infty$
  - Has **unbounded derivative** for $x < 0$ so learning still works
  - Strangely, monotonicity seems not to be important?

[1] Ramachandran, Zoph and Le Searching for Activation Functions

Logical functions

- Every boolean function can be implemented by a neural network[2].
- For simplicity $f(x \leq 0) = 0$, and $f(x > 0) = 1$, i.e. the neuron "fires" on activation. Then, the following can be implemented on a single node:
  - AND: $f(x_1, x_2) = -1.5 + x_1 + x_2$
  - OR: $f(x_1, x_2) = -0.5 + x_1 + x_2$
  - NOT: $f(x_1) = 0.5 - x_1$
- Neural networks with more general activation functions can still implement these functions.

[2] McCulloch and Pitts (1943) A logical calculus of the ideas immanent in nervous activity

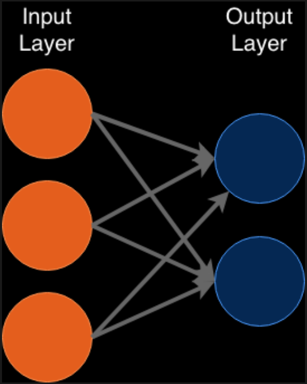
Logical function problems

- But not every function can be implemented in a single layer perceptron[3]:
  - XOR: only x_1 or x_2 can be active

For a two-point space $R = \{x, y\}$, the class $L(\{x, y\})$ of functions linear in the two one-point predicates includes 14 of the $16 = 2^{2^2}$ possible Boolean functions. For larger numbers of points, the fraction of functions linear in the one-point predicates decreases very rapidly toward zero.

[3] Minsky and Papert 1969 Perceptrons

Single Layer perceptron (SLP)



- Has just two layers:
  - data layer (e.g. features)
  - output layer (e.g. classes)
- No **hidden** layers!
- Weights learned
- Making a linear classification rule

Mathematical description of SLP

- N Inputs x_i and M outputs y_j
- Activation function f and with weights W_{ij}:

$$f(\mathbf{x}) = f\left(W_{0j} + \sum_{i=1}^{N} W_{ij}x_i\right)$$

- W_{0j} allows for an offset (mean) in the activation, just like in linear regression
- Loss is the square error over all output variables j:

$$L(W) = \sum_{j=1}^{M} L_j = \sum_{j=1}^{M} \left[y_j - f\left(W_{0j} + \sum_{i=1}^{N} W_{ij}x_i\right)\right]^2$$

$$= \sum_{j=1}^{M} \delta_{ij}^2(\mathbf{w}_j)$$

  - $\delta_{ij}(\mathbf{w}_j)$ is the error for input i output j.

Learning through Gradient Descent

- Learn through Gradient Descent:
  - i.e. Differentiate the loss with respect to the **weights** for $i = 0, \ldots, N$:

$$\nabla_W L = \left(\frac{\partial L}{\partial W_{10}}, \ldots, \frac{\partial L}{\partial W_{ij}} \ldots, \frac{\partial L}{\partial W_{NM}} \right)^T$$

  - where:

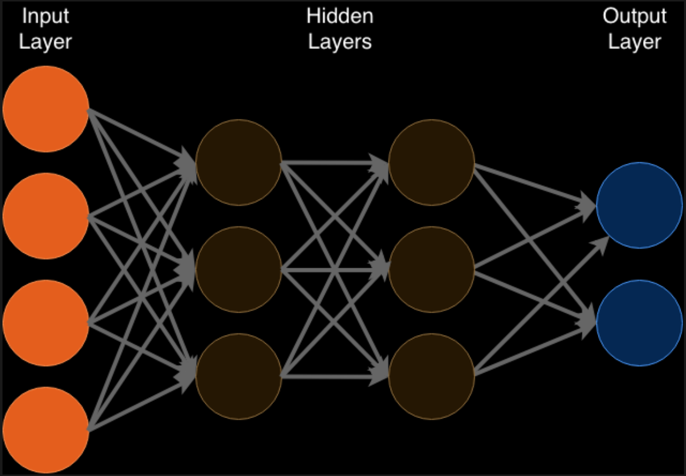
$$\frac{\partial L}{\partial W_{ij}} = \frac{\partial L}{\partial f} \frac{\partial f}{\partial W_{ij}} = -2\delta_{ij} \frac{\partial f}{\partial W_{ij}},$$

- Leading to the update rule:

$$W_{ij} \leftarrow W_{ij} + \alpha \frac{\partial f}{\partial W_{ij}} \delta_{ij}$$

  - We are taking a step of size α in a direction towards the multivariate **minima of the loss**
  - Choose step size α to take steps that move *fast enough* whilst not *overshooting*.
  - In practice α is learned adaptively.

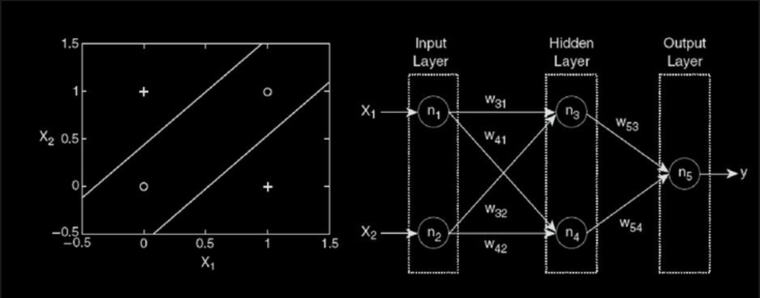
Multilayer Perceptrons / Feed Forward Neural Networks



Multilayer Perceptrons / Feed Forward Neural Networks

- A Neural Network's power is in **hidden layers**
  - Hidden layers can be treated exactly as the layers we have observed
  - Maths allowing modularly that is transformative
- **Architecture** choices include the number of layers and the connectedness:
  - Completely connected layers?
  - Locality towards data?
  - Number of neurons in each layer?
- These choices are somewhat manual and define your **model**
- Architecture is robust, i.e. many choices will lead to similar predictions...
- But they are **not** arbitrary!

Universal Approximation Theorem



(a) Decision boundary. (b) Neural network topology.

Figure 5.19. A two-layer, feed-forward neural network for the XOR problem.

- Any[4] function of n inputs can be approximated
- By using **non-linear** activation functions (e.g. ReLU)
- Using a **single hidden layer**, with an **exponential width** (number of nodes, scale with n)
- Or a (linear in n) **deep network with finite width**

[4] continuous, compact function on $\mathbb{R}^n$

Back Propagation

- Learning Neural networks was an art until **back propagation** was discovered[5].
- This is a method to compute all derivatives of all weights, exactly and efficiently.
- Notation:
  - Index the current layer as k (of K) with node labels i, the next layer with labels j.
  - Activation function $x_j^k = f(a_j^k)$
  - $a_j^k = W_{0j}^k + \sum_{i=1}^{n_k} W_{ij}^k x_i^k$
- Output layer: W_{ij}^K is learned as a Single Layer Perceptron
- Work backwards from there...

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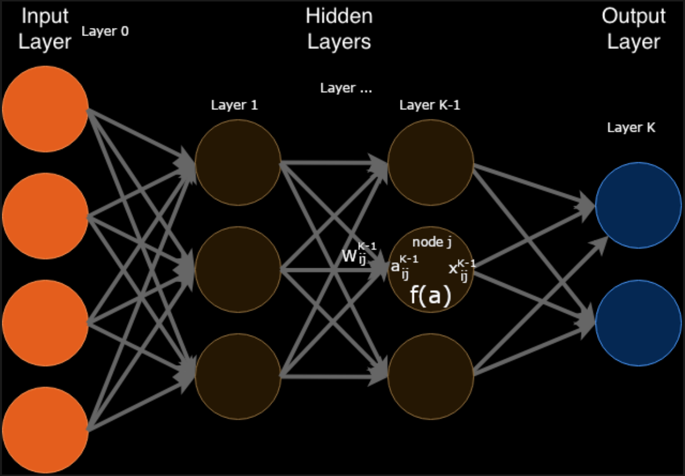
[5] Hecht-Nielsen, Robert. "Theory of the backpropagation neural network." Neural networks for perception. Academic Press, 1992. 65-93.

Backpropagation network



Back Propagation

- Hidden layers: back-propagate the error from the **next layer** to the **current**, using the chain rule:

$$\frac{\partial L}{\partial W_{ij}^{k}} = \sum_{j=1}^{n_{(k+1)}} \frac{\partial L}{\partial x_j^{(k+1)}} \frac{\partial x_j^{(k+1)}}{\partial a_{ij}^{(k+1)}} \frac{\partial a_j^{(k+1)}}{\partial W_{ij}^{k}}$$

- i.e. we compute the activation function for one layer as a (sum over) two components:
  - **error** : $\delta_j^{k+1} = \frac{\partial L}{\partial x_j^{(k+1)}}$
  - **response** : $\frac{\partial x_j^{(k+1)}}{\partial a_{ij}^{(k+1)}} = \frac{\partial f(a)}{\partial a}$
  - **response rate** : $\frac{\partial a_j^{(k+1)}}{\partial W_{ij}^{k}}$
- The last two are often combined, but this representation separates the activation function from the weights.

Stochastic Gradient Descent

- **Gradient Descent** is just the beginning. It is appropriate for:
    1. **Smooth** or **convex** error functions, so that we do not become trapped in a local optima;
    2. **Small data regimes**, where we can afford to compute the entire gradient every update.
- **Stochastic Gradient Descent** addresses local minima and computational cost together.
    - It uses **mini-batches** of data for a gradient update.
    - This makes each update **random**, creating a type of **annealing** in the algorithm:
    - We can take large random steps when we are far from the optima (large step size),
    - And much shorter and hence on average reliable steps when we are closer (small step size).

Interpreting classifier output

- Neural networks output a set of **activations**
- It is standard to apply **softmax** $p(\mathbf{z}) : \mathcal{R}^n \rightarrow [0, 1]$ s.t. $\sum_{i=1}^{n} z_i = 1$:
$$p(z_i) = \frac{e^{z_i}}{\sum_j e^{z_j}}$$
- This interprets the activation as a log-likelihood
- This is **almost always wrong**

Interpreting classifier output

- Various sophisticated approaches are available:
  - e.g. Mixture Density Networks[6]
  - Calibrate probabilities in a "post processing" layer[7]
- Neural Networks are **not** (normally) approximating probabilities. They are predicting data, or equivalently, predicting decisions.
  - e.g. A NN driving a car doesn't care about the probability of a person being in the screen.
  - It cares about the Loss function, which in this case would be expressed in terms of **actions**.

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[6] Bishop 1994 Mixture Density Networks

[7] Kull et al 2019 NeurIPS Beyond temperature scaling: Obtaining well-calibrated multiclass probabilities with Dirichlet calibration

References (1)

- Chapter 11 of The Elements of Statistical Learning: Data Mining, Inference, and Prediction (Friedman, Hastie and Tibshirani).
- Russell and Norvig Artificial Intelligence: A Modern Approach
  - Chapter 20 Section 5: Neural Networks
- Swish: Ramachandran, Zoph and Le Searching for Activation Functions
- Important historical papers:
  - McCulloch and Pitts (1943) A logical calculus of the ideas immanent in nervous activity
  - Minsky and Papert 1969 Perceptrons
- Theoretical practicalities:
  - Practical advice from Bengio 2012 Practical Recommendations for Gradient-Based Training of Deep Architectures
  - Kull et al 2019 NeurIPS Beyond temperature scaling: Obtaining well-calibrated multiclass probabilities with Dirichlet calibration

References (2)

- Important historical papers:
  - Hecht-Nielsen, Robert. “Theory of the backpropagation neural network.” Neural networks for perception. Academic Press, 1992. 65-93.
  - Bishop 1994 Mixture Density Networks
- Likelihood and modelling applications of Neural Networks:
  - Chilinski and Silva Neural Likelihoods via Cumulative Distribution Functions
  - Albawi, Mohammed and Al-Zawi Understanding of a convolutional neural network
  - Omi, Ueda and Aihara Fully Neural Network based Model for General Temporal Point Processes