Deep Learning

Foundations of Deep Neural Networks

Kurt Rinnert

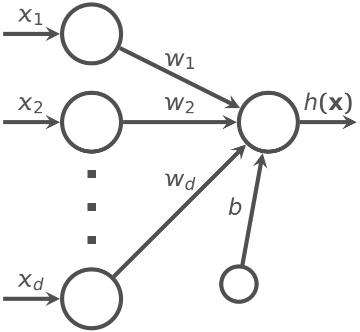
Liverpool
13.06.2018

Overview

We can only cover some basics here.

Artificial Neuron

- Neuron pre-ativation (or input activation)
  $a(x) = b + \sum_i w_i x_i = b + \mathbf{w}^T \mathbf{x}$
- Neuron (output) activation
  $h(\mathbf{x}) = g(a(\mathbf{x})) = g(b + \sum_i w_i x_i)$
- $\mathbf{w}$ are the connection weights
- b is the neuron bias
- $g()$ is the activation function

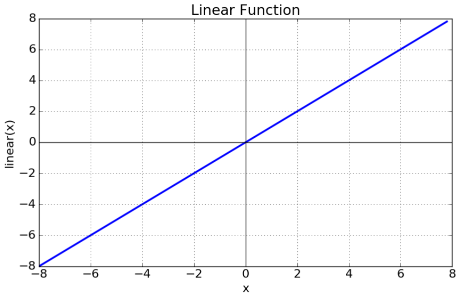


This is the basic building block of all that follows.

Activation Functions

Linear Function: $g(a) = a$

- Range of g same as domain
- Not very interesting

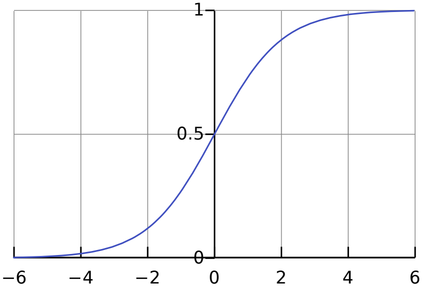


Only linear transformations can be modeled.

Activation Functions

Sigmoid Function: $g(a) = \mathrm{sigm}(a) = \frac{1}{1+\exp(-a)}$

- Maps the pre-activation a to $[0, 1]$
- Always positive
- Bounded
- Strictly increasing

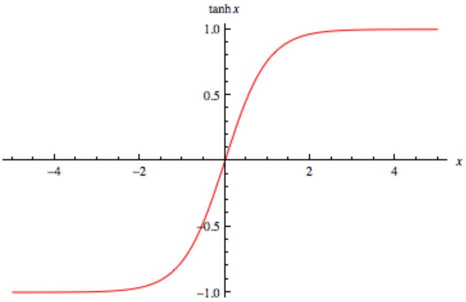


Non-linear models possible.

Activation Functions

tanh Function: $g(a) = \tanh(a) = \frac{\exp(a)-\exp(-a}{\exp(a)+\exp(-a)}$

- Maps the pre-activation a to $[-1, 1]$
- Positive and negative
- Bounded
- Strictly increasing

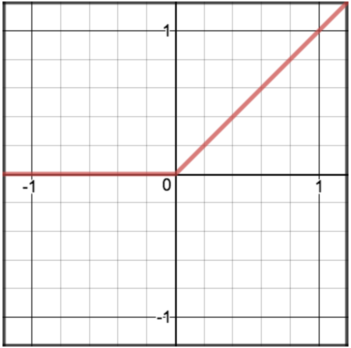


Non-linear models possible.

Activation Functions

Rectified Linear Function (Unit): $g(a) = \mathrm{reclin}(a) = \mathrm{relu}(a) = \max(0, a)$

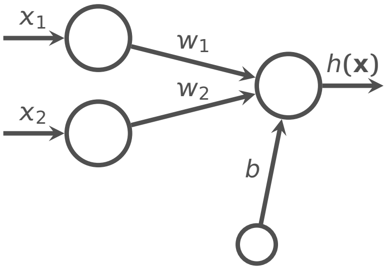
- Bound below by 0
- No upper bound
- Monotonically increasing
- Tends to create "sparse" neurons



A very popular choice.

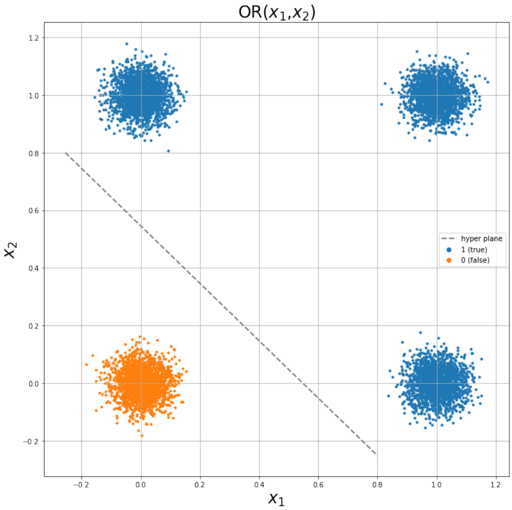
Capacity of a Single Neuron

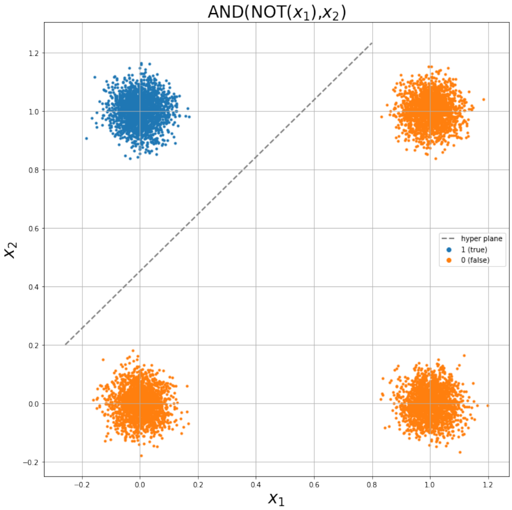
- Can separate two classes…
- …if separation is linear (hyperplane)
- Sigmoid activation allows for probability interpretation
- Cut at 0.5 for classification



A single neuron can act as a binary classifier.

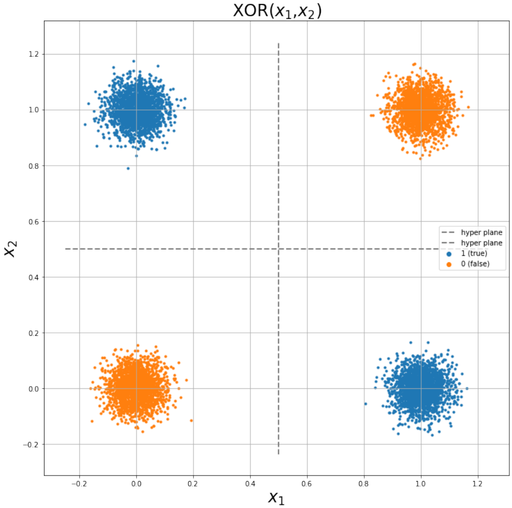
Linear Classification Examples

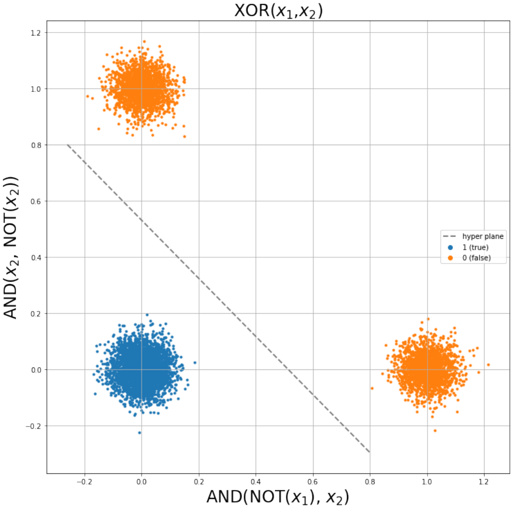




Can be separated by a single neuron.

Non-Linear Example

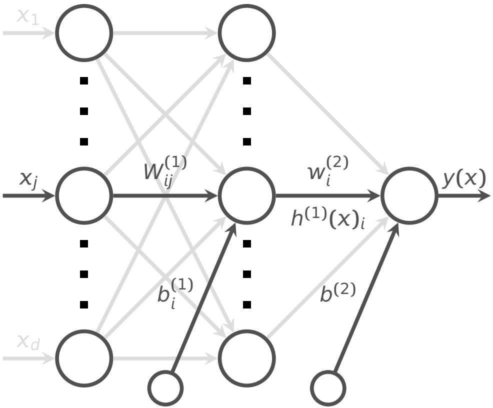




Additional neurons can encode the transformation!

One Hidden Layer

- Hidden layer pre-activation:
  $\mathbf{a}(\mathbf{x}) = \mathbf{b}^{(1)} + \mathbf{W}^{(1)}\mathbf{x}$
- Hidden layer activation:
  $\mathbf{h}^{(1)}(\mathbf{x}) = \mathbf{h}^{(1)}(\mathbf{a}(\mathbf{x}))$
- Output Layer:
  $\mathbf{y}(\mathbf{x}) = \mathbf{o}(\mathbf{b}^{(2)} + \mathbf{w}^{(2)T}\mathbf{h}^{(1)}\mathbf{x})$



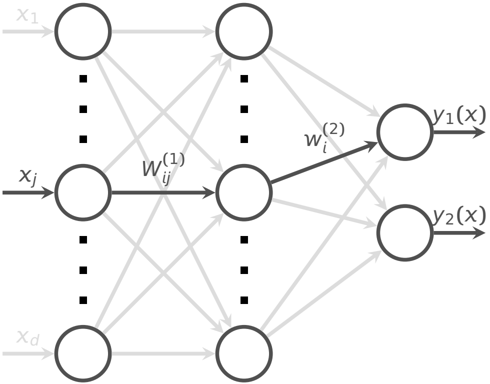
The function $o()$ is the output layer activation.

Multiple Classes

- Softmax as output activation:

  $$y_j(\mathbf{x}) = o(\boldsymbol{\alpha})_j = \frac{e^{a_j}}{\sum_{k=1}^{K} e^{a_k}}$$

  for $j = 1, \ldots, K$
- Strictly positive
- Sums to one



Softmax provides normalized probabilities.

Feedforward Neural Networks

Training Neural Networks

Deep Neural Networks

Practical Considerations

Further Reading

Empirical Risk Minimization

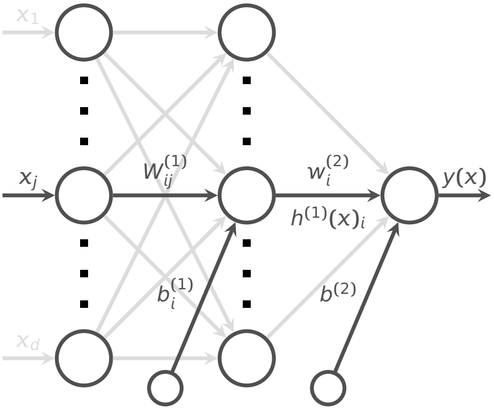
- Framework to design learning algorithms
  $\arg\min \frac{1}{T}\sum_t l(y(\mathbf{x}^{(t)};\boldsymbol{\theta}), y^{(t)}) + \lambda\Omega(\boldsymbol{\theta})$
- $\boldsymbol{\theta}$ is the set of all parameters
- $l(y(\mathbf{x}^{(t)};\boldsymbol{\theta}), y^{(t)})$ is the loss function
- $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)
- the loss function is an upper bound on the classification error

Learning is cast as optimization.

Stochastic Gradient Descent (SDG)

Algorithm for update after each seen example:

- initialize $\boldsymbol{\theta}$ (all parameters)
- Then, for N iterations (epochs):
- For each training example $(\mathbf{x}^{(t)}, \mathbf{x}^{(t)})$:
- $\Delta = -\Delta_\theta l(f(x^{(t)}, \theta), y^{(t)}) - \lambda \Delta_\theta \Omega(\theta)$
- $\theta \leftarrow \theta + \alpha \Delta$

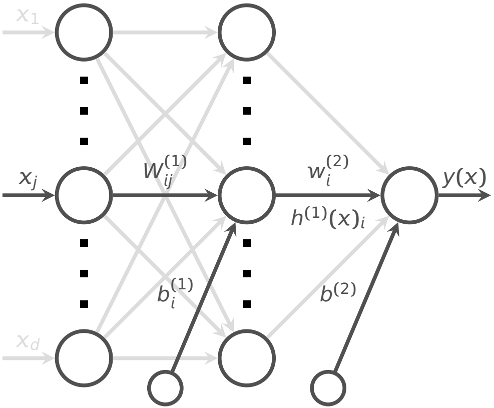


Meta parameters like α are not optimized!

Ingredients for SDG

To apply the algorithm wee need:

- The loss function $l(f(x^{(t)}, \theta), y^{(t)})$
- The parameter gradients, $\Delta_\theta l(f(x^{(t)}, \theta), y^{(t)})$ etc.
- The regularizer Ω and its gradiend $\Delta_\theta \Omega$
- An initialization method
- A method to compute the gradients in practice



Gradient computation is done by back-propagation.

Regularization

L2 Regularization

$$\Omega(\theta) = \sum_k \sum_i \sum_j (W_{i,j}^{(k)})^2$$

- Only applied to weights, not biases
- Causes weights to decay

Can be interpreted as a Gaussian prior.

Regularization

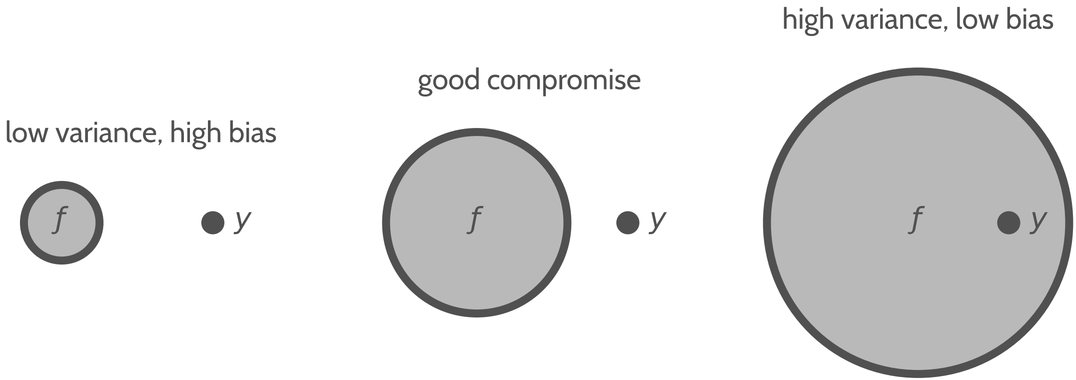
L1 Regularization

$$\Omega(\theta) = \sum_k \sum_i \sum_j |W_{i,j}^{(k)}|$$

- Only applied to weights, not biases
- Will push some weiths to exactly zero

Can be interpreted as a Laplacian prior.

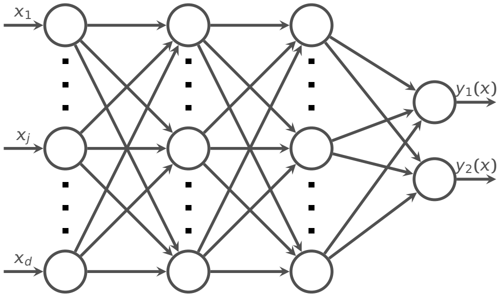
Variance vs. Bias



This intuitively motivates regularization.

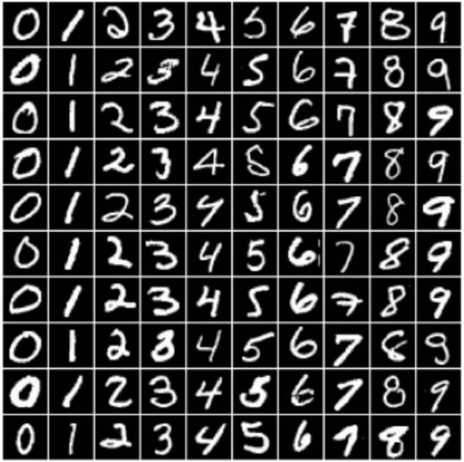
Deep Neural Networks

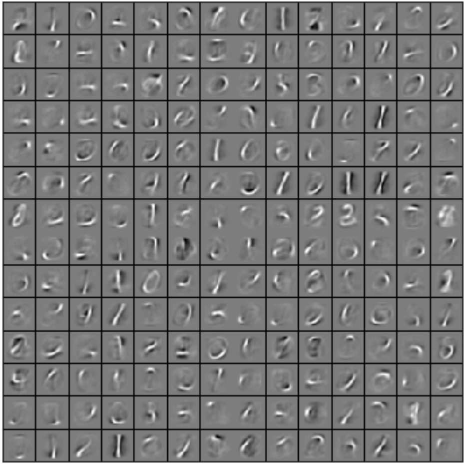
- Instance of multilayer representation
- Each layer corresponds to "distributed" representation
- There motivations from biology (visual cortex)
- Feature extraction
- Grouping of features
- Recognition of classes



More compact representation that single layer.

Example: MNIST, Handwritten Digits





Multiple classes. Feature extraction.

Training Difficulties

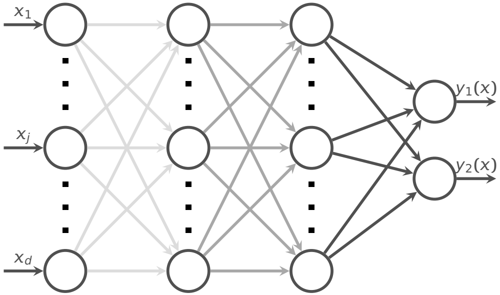
Harder optimization problem

- $\rightarrow$ vanishing gradient problem
- Underfitting
- Saturated units block propagation
- Can be mitigated by pre-training followed by refining

High variance / low bias situation

- Many parameters
- Complex function space
- Overfitting

Pre-training can be unsupervised!



Practical Considerations

- There many frameworks avaialable that do most of the tedious work for you:
  - Tensorflow/Keras
  - Theano/Keras
  - SciKit Learn
  - PyTorch
  - ...
- With various levels of abstraction
- And programming styles
- Most are GPU enabled
- I prefer PyTorch (for now)

If you want to dive, you need to know python.

Let’s look at a simple example!

Feedforward Neural Networks

Training Neural Networks

Deep Neural Networks

Practical Considerations

Further Reading

Further Reading

- A very accessible series of lectures:
  youtube video series
- Books:
  "Introduction to Statistical Learning"
  "The Elements of Statistical Learning"
  "Bayesian Reasoning and Machine Learning"

Getting to the bottom of this will take time.