Neural Networks – Part II

PHYS 250 (Autumn 2025) – Lecture 14

David Miller

Department of Physics and the Enrico Fermi Institute
University of Chicago

November 19, 2024

Outline

1. *Reminders*
   - Reminders from Lecture 13
2. *Historical perspective*
   - Brief History of Machine Learning Generally
   - Brief History of Neural Networks
3. *Structure of Neural Networks*
   - Single layer perceptron
   - Training a single layer perceptron
   - Training a Multi-Layer Perceptron (MLP)
4. *Classification tasks with NN*
   - What is classification?
   - Example of binary classification
   - More realistic case of classification

Reminders from last time

We embarked on a whirlwind introduction to neural networks.

Neural networks and machine learning

- **Context and perspective**
  - We discussed the general issue of training computers to **discover, identify, and analyze patterns** of interest in datasets
  - Categorized tasks that make use of this idea: **classification, regression, generation, clustering, anomaly detection**
- **Neural networks as a tool**
  - Introduced both the **modeling** perspective as well as the **biological** perspective on what a neural network achieves
  - Described the **structure and function** of a neuron
  - Began discussing the **mathematical properties** of a neural network

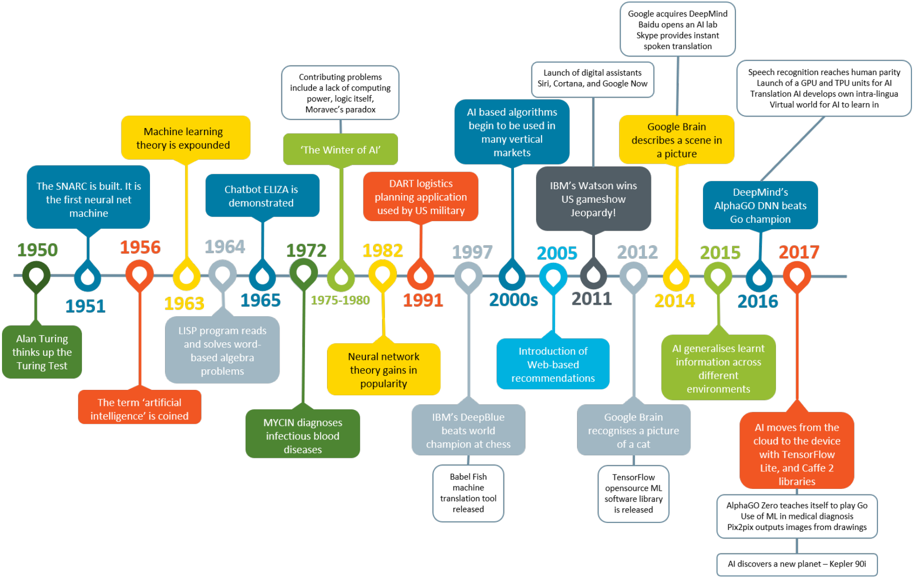
Today we will build our own networks! But first, I just wanted to follow-up on some points and questions from last time.

Outline

1. *Reminders*
   - Reminders from Lecture 13
2. *Historical perspective*
   - Brief History of Machine Learning Generally
   - Brief History of Neural Networks
3. *Structure of Neural Networks*
   - Single layer perceptron
   - Training a single layer perceptron
   - Training a Multi-Layer Perceptron (MLP)
4. *Classification tasks with NN*
   - What is classification?
   - Example of binary classification
   - More realistic case of classification

Brief history of machine learning

Taken from Harry Ide on InnovationLaboratory.com (18 May 2018):



Brief history of machine learning

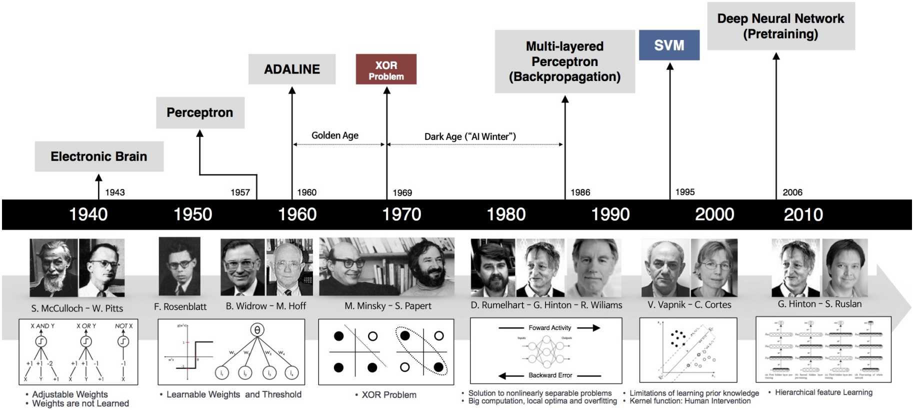
Taken from Harry Ide on InnovationLaboratory.com (18 May 2018):

Quote from Harry Ide on "AI"

"The cutting edge might not be as sharp as many believe. AI has a nearly 70-year long history with some surprising back-tracks and re-emergences among it."

Brief history of neural networks

Taken from this talk on SlideShare:



Outline

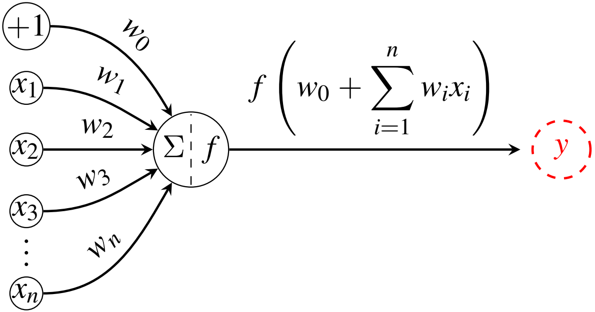
1 *Reminders*
- Reminders from Lecture 13

2 *Historical perspective*
- Brief History of Machine Learning Generally
- Brief History of Neural Networks

3 *Structure of Neural Networks*
- Single layer perceptron
- Training a single layer perceptron
- Training a Multi-Layer Perceptron (MLP)

4 *Classification tasks with NN*
- What is classification?
- Example of binary classification
- More realistic case of classification

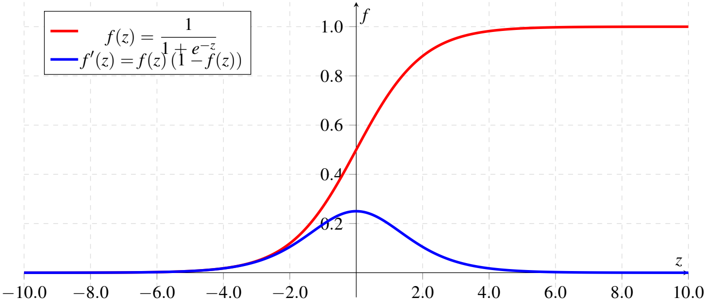
Single layer perceptron



- $\vec{x} = (x_1, x_2, \cdots, x_n)$ **is an input feature vector of length** n
  i.e. the attributes of the data, e.g. voltages
- $\vec{w} = (w_1, w_2, \cdots, w_n)$ **is the weight vector with** w_0 **reserved as a bias**
  - becomes a matrix for multiple layers
- Σ **indicates summation (or matrix mult.):** $z = \sum w_i x_i$ $(x_0 = 1)$
- f **is the activation function, or non-linearity:** $f(z)$
- $y = f(z)$ **is the output**

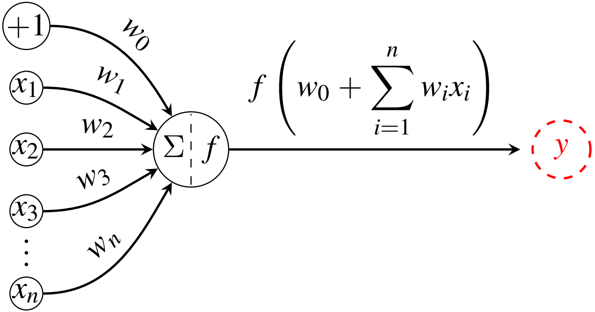
Sigmoid as activation function

As we discussed, a typical function for a **single layer perceptron** is the **sigmoid**.



Here, we plot both the function itself, as well as its derivative, since that will be important when evaluating the **backpropagation** of weights in order to update the neural network.

Training a single layer perceptron

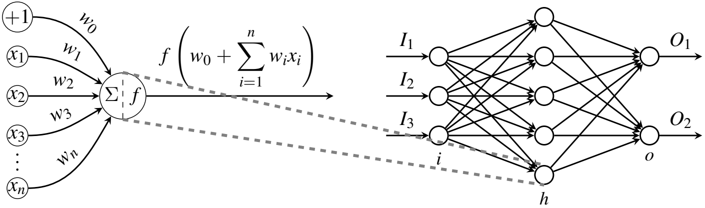


Given j objects $\vec{x}_j$ in dataset, each with **known values of f**, d_j

- **Calculate the output:** $y_j = f(\vec{w} \cdot \vec{x}_j)$
- **Determine the error:** $\epsilon_j = d_j - y_j$
- **Update the weights:** $w_i^{\text{new}} = w_i + r(\epsilon_j \cdot \vec{x}_j)_i$

Choosing the learning rate r is where the derivative is used. It's not important for the single-layer perceptron, but is **essential** for a network.

Multi-layer perceptron (MLP)

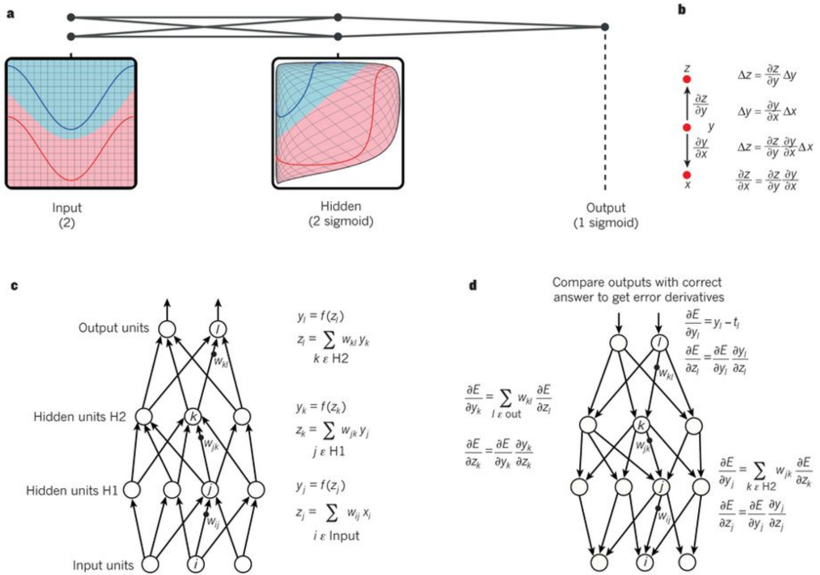


Given j objects $\vec{I}_j$ in dataset, each with features $\vec{I} = (I_1, I_2, \cdots, I_n)$ and **known outputs $\vec{d}_j$ at each output node o**, $\vec{d} = (d_1, d_2, \cdots, d_o)$

- **Calculate the h outputs of hidden layer:** $v_h = f(\sum_i w_{ih} I_i)$
- **Calculate the o outputs of output layer:** $y_o = f(\sum_h w_{ho} v_h)$
- **Determine the error at output each node o:** $\epsilon_o = d_o - y_o$
- **Determine the total error for data object j:** $\mathcal{E}_j = \frac{1}{2}\sum_o \epsilon_o^2$
- **Determine change in weights for output neuron y_o:** $\Delta w_{oh} = -\eta \frac{\partial \mathcal{E}}{\partial z_o} v_h = \eta \epsilon_o f'(z_o)$

LeCun, Bengio, Hinton, “Deep learning”

Nature volume 521, pages 436-444 (28 May 2015)



Outline

1. *Reminders*
   - Reminders from Lecture 13
2. *Historical perspective*
   - Brief History of Machine Learning Generally
   - Brief History of Neural Networks
3. *Structure of Neural Networks*
   - Single layer perceptron
   - Training a single layer perceptron
   - Training a Multi-Layer Perceptron (MLP)
4. *Classification tasks with NN*
   - What is classification?
   - Example of binary classification
   - More realistic case of classification

What is classification?

Slides stolen from colleague Ben Nachmann

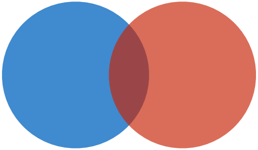
Classification

Goal: Given a *feature vector*, return an integer indexed by the set of possible *classes.*

In most cases, we care about *binary* classification in which there are only two classes (signal versus background)

There are some cases where we care about *multi-class classification*

Feature vector can be many-dimensional



Harder = more overlap between for **S** and **B**

What is classification?

Classification

Goal: Given a *feature vector*, return an integer indexed by the set of possible *classes.*

In practice, we don't just want one classifier, but an entire set of classifiers indexed by:

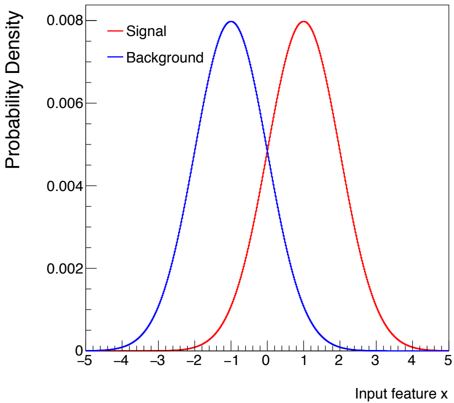
True Positive Rate = signal efficiency = Pr(label signal | signal) = sensitivity

True Negative Rate = 1 - background efficiency = rejection = Pr(label background | background) = specificity

For a given TPR, we want the lowest possible TNR!

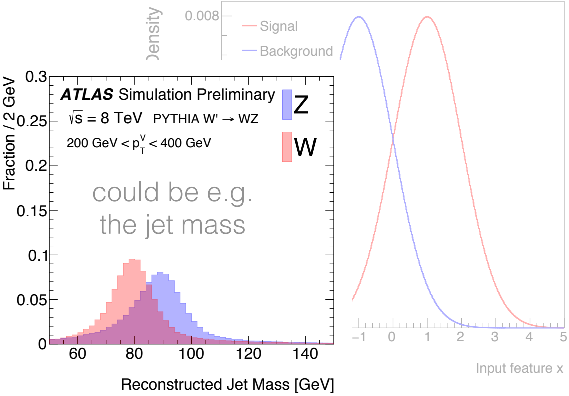
Binary classification (I)

Let's consider an important special case:
binary classification in 1D



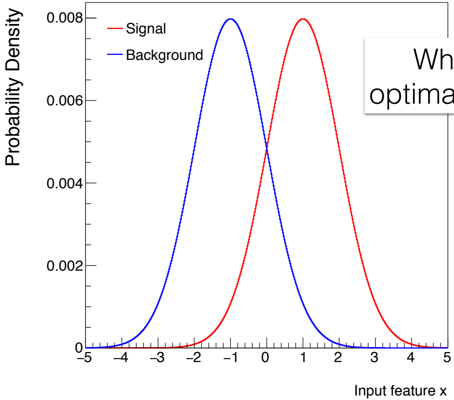
Binary classification (II)

Let's consider an important special case:
binary classification in 1D



Binary classification (III)

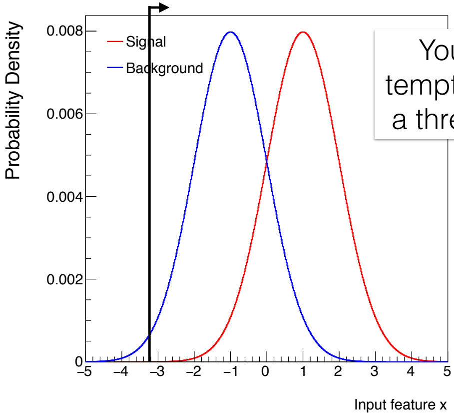
Let's consider an important special case:
binary classification in 1D



What is the optimal classifier?

Binary classification (IV)

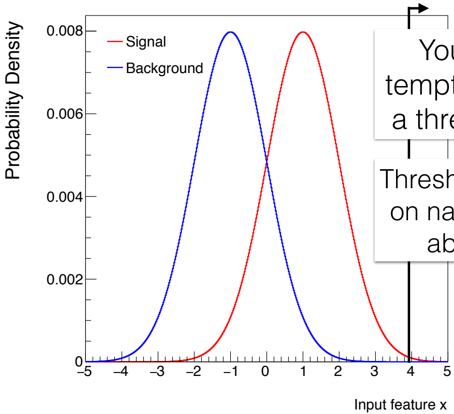
Let's consider an important special case:
binary classification in 1D



You may be tempted to place a threshold on x

Binary classification (V)

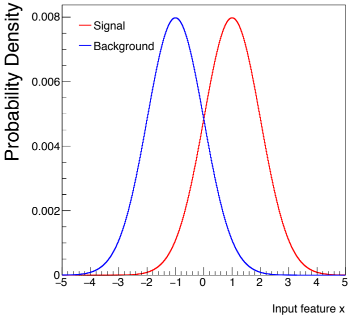
Let's consider an important special case:
binary classification in 1D



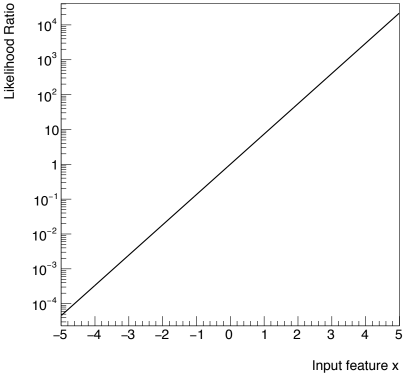
You may be tempted to place a threshold on x

Threshold depends on natural relative abundance

Binary classification (VI)



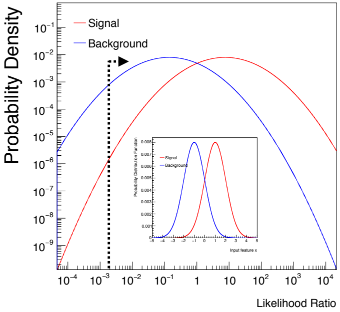
Is the simple threshold cut optimal?



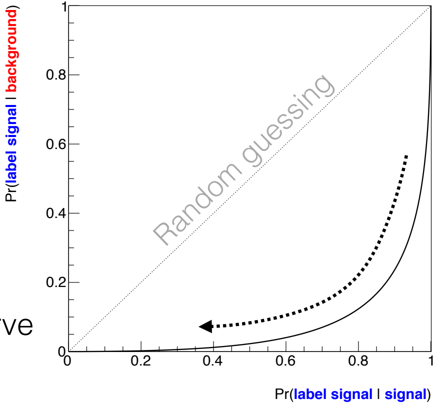
In this simple case, the log LL is proportional to x: **no need for non-linearities**!

Threshold cut is optimal

Binary classification (VII)



The optimal procedure is a threshold on the LL

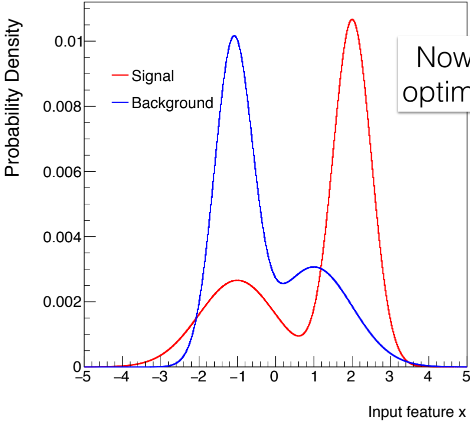


“Receiver Operating Characteristic” (**ROC**) Curve

“Realistic” classification (I)

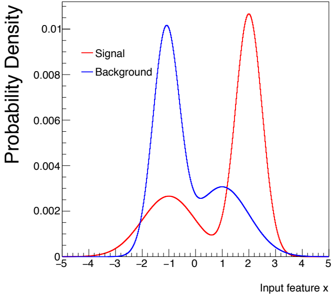
What if the distribution of x is complicated?

Real life is complicated!

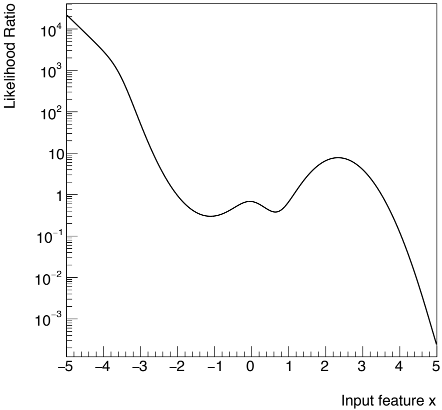


Now what is the optimal classifier?

"Realistic" classification (II)

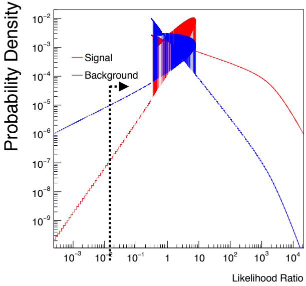


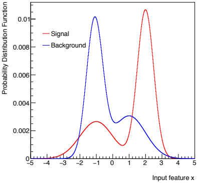
In this case, LL is highly non-linear (**non-monotonic**) function of x



A threshold on x would be sub-optimal

“Realistic” classification (III)





ROC is worse than the Gaussians, but that is expected since the overlap in their PDFs is higher.