1 - Introduction

André Lamúrias

Summary

- Course structure and assessment
- AI and the origin of Artificial Neural Networks
- Machine Learning
- The power of nonlinear transformations
- What deep learning offers

Course Overview

Overview

Objectives

- Overview of two important AI fields in biology
- A practical introduction (some theory, some practice)

Two parts

- Deep learning (sub-symbolic)
  - Build and train deep neural networks
  - Apply to (semi) realistic problems (realistic take more computation power)
- Ontologies (symbolic)
  - Understand and use tools for inference with biological knowledge
  - E.g. Gene Ontology

Overview

Instructor

- André Lamúrias (a.lamurias@fct.unl.pt)

Assessment:

- 2 short assignments, one for each part (25% each)
- 1 test (or exam), on April 22th (during the classes - date and time to be confirmed)

Website

- tiab.ssdi.di.fct.unl.pt

Main Bibliography (part 1)

- B. Goodfellow et. al., Deep Learning, MIT Press, 2016
- S. Skansi, Introduction to Deep Learning: From Logical Calculus to Artificial Intelligence , Springer, 2018
- A. Géron, Hands-on machine learning with Scikit-Learn and TensorFlow, O'Reilly Media, Inc, 2017
- P. Singh and A. Manure, Learn TensorFlow 2.0, Springer 2020

Main Bibliography (part 2)

- P. Robinson and S. Bauer, Introduction to Bio-Ontologies, Chapman & Hall, 2011
- C. Dessimoz and N. Skunca, The Gene Ontology Handbook, Springer, 2017
- G. Antoniou et al., A Semantic Web Primer, MIT Press, 2012
- F: Baader et al., The Description Logic Handbook, Cambridge University Press, 2010
- S. Russell and P. Norvig, Artificial Intelligence: A Modern Approach, Pearson, 2020

Overview

Software

- Python 3.x + Tensorflow 2

- Options
- virtualenv
- Anaconda
- Docker
- Windows Subsystem for Linux (Ubuntu on Windows)
- Google Colab

Artificial Intelligence

The beginning of AI

- 1956: Dartmouth Summer Research Project on Artificial Intelligence
  - John McCarthy, Marvin Minsky, Nathaniel Rochester and Claude Shannon
  - "proceed on the basis of the conjecture that every aspect of learning or any other feature of intelligence can in principle be so precisely described that a machine can be made to simulate it"
- Initially, most successful approach of AI was to process rules
  - Expert systems, logic programming, ...
- Rule-based expert systems
  - Rules provided by humans
  - Computer does inference to reach conclusions

The beginning of AI

- Rule-based expert systems

- Rules provided by humans
- Computer does inference to reach conclusions
- E.g. MYCIN, 1975 (Shortliffe, A model of inexact reasoning in medicine)

```
If:
(1) the stain of the organism is gram positive, and
(2) the morphology of the organism is coccus, and
(3) the growth conformation of the organism is chains
Then :
there is suggestive evidence (0.7) that the identity of
the organism is streptococcus
```

- Such systems were initially quite successful in specific areas

The beginning of AI

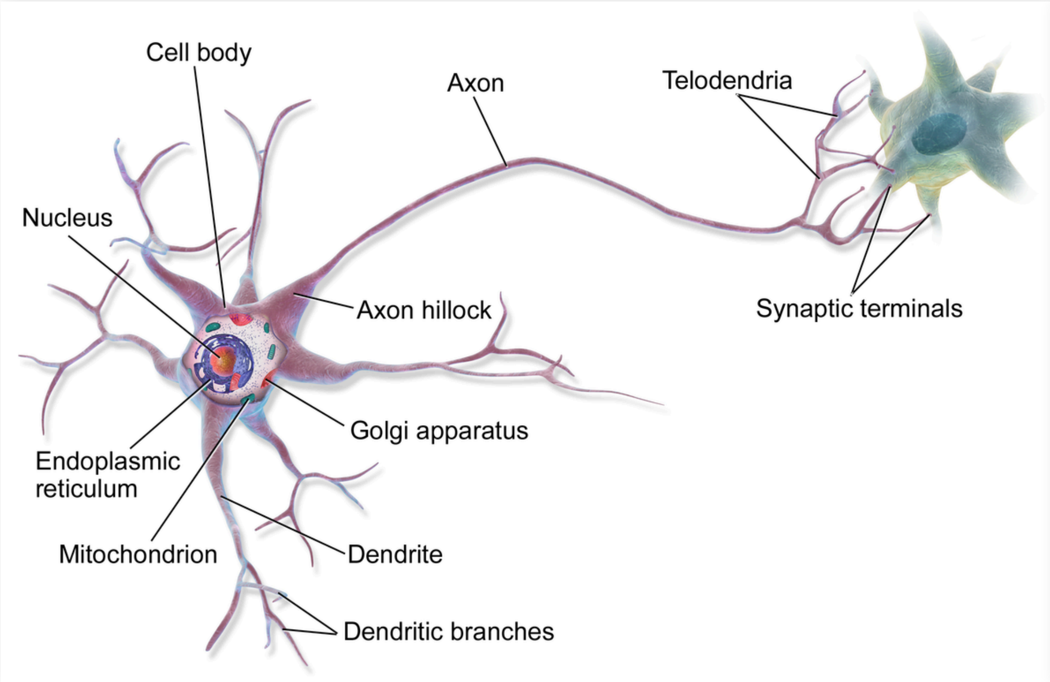
- Problems with rule-based expert systems

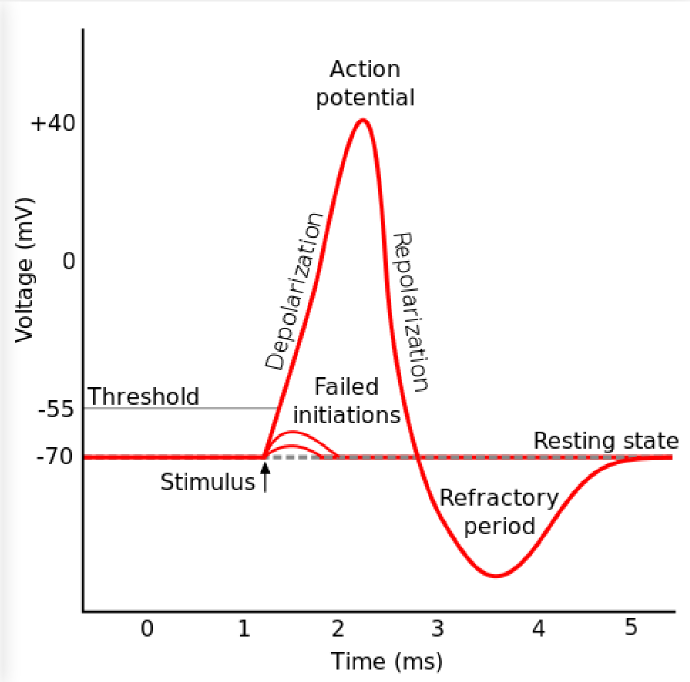
- Computational complexity
- Rigid rules, less adaptative
- Knowledge aquisition problem

The beginning of Neural Networks

- The modelling of neurons predates modern AI

- 1943: McCulloch & Pitts, model of neuron

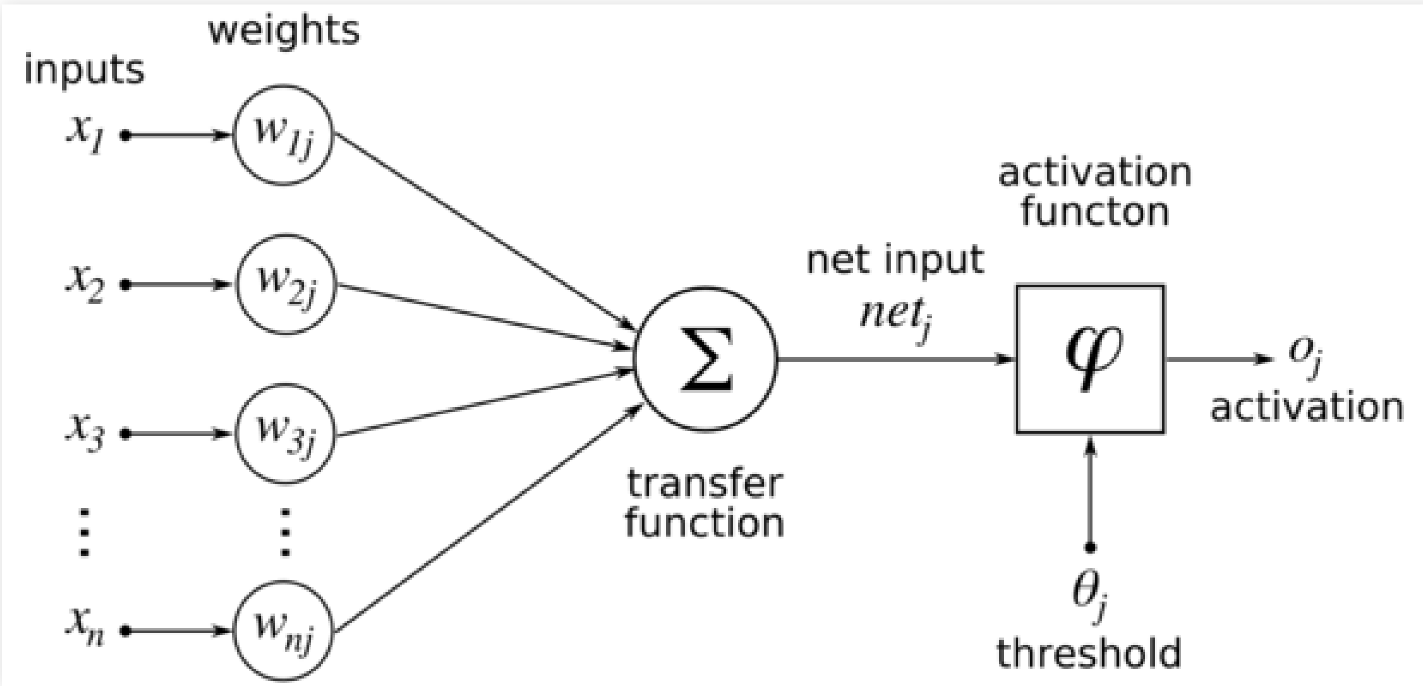




The beginning of Neural Networks

- The modelling of neurons predates modern AI

- 1943: McCulloch & Pitts, model of neuron

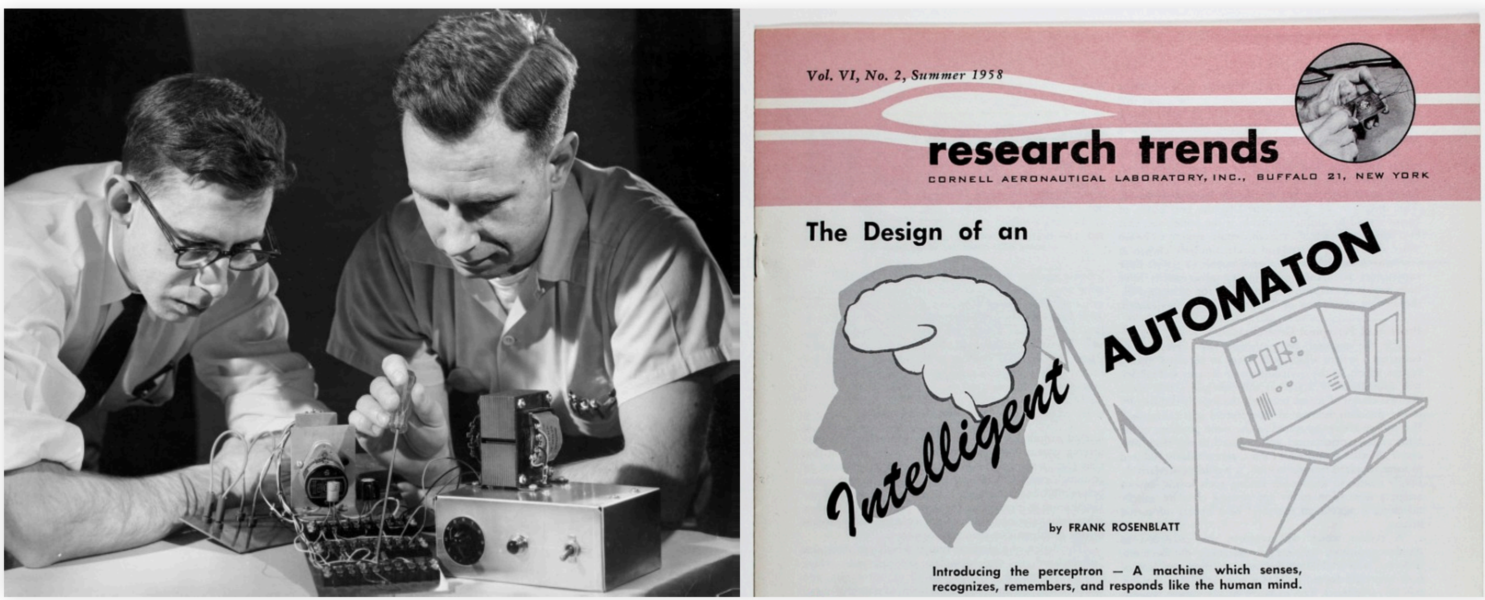


Chrislb, CC-BY, source Wikipedia

The perceptron, the first learning machine

- 1958: Rosenblatt, perceptron could learn to distinguish examples

«the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.»
New York Times, 1958



Wightman and Rosenblatt. Source: Cornell Chronicle

Perceptron

- Linear combination of the d inputs and a threshold function:

$$y = \sum_{j=1}^{d} w_j x_j + w_0 \qquad s(y) = \begin{cases} 1, & y > 0 \\ 0, & y \leq 0 \end{cases}$$

- Training rule for the perceptron:

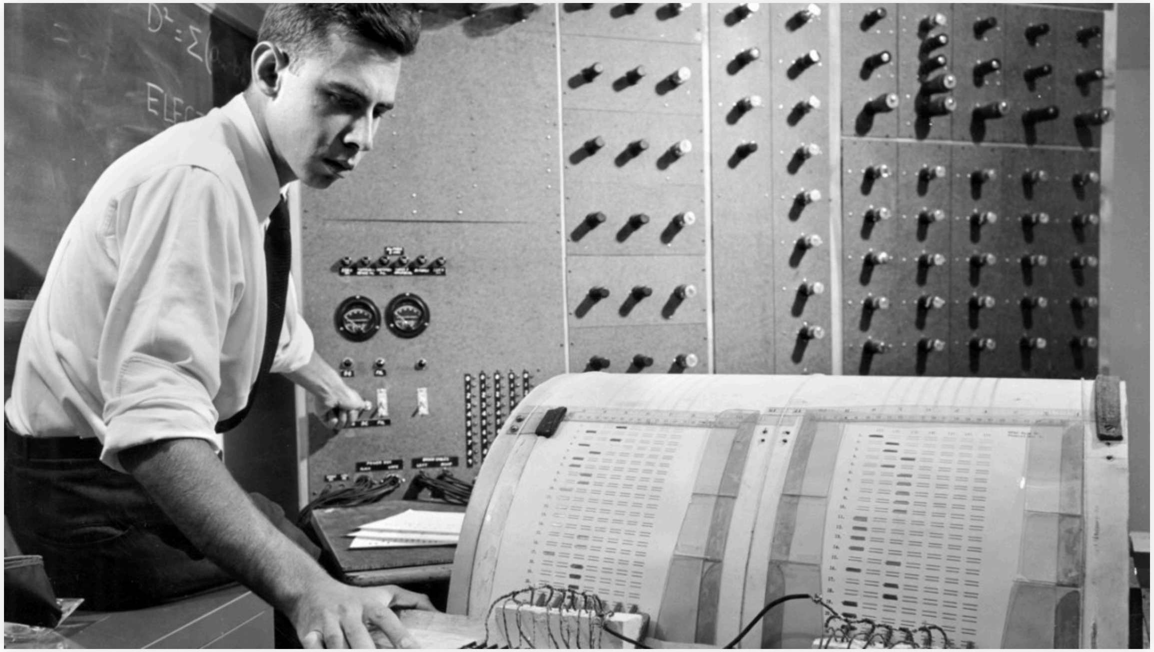
$$w_i = w_i + \Delta w_i \qquad \Delta w_i = \eta(t - o)x_i$$

- Adjust weights slightly to correct misclassified examples.
- Greater adjustment to those with larger inputs.

Perceptron

- First implemented on an IBM 704, 1958

- Learned to distinguish between cards punched on the right and punched on the left after 50 examples



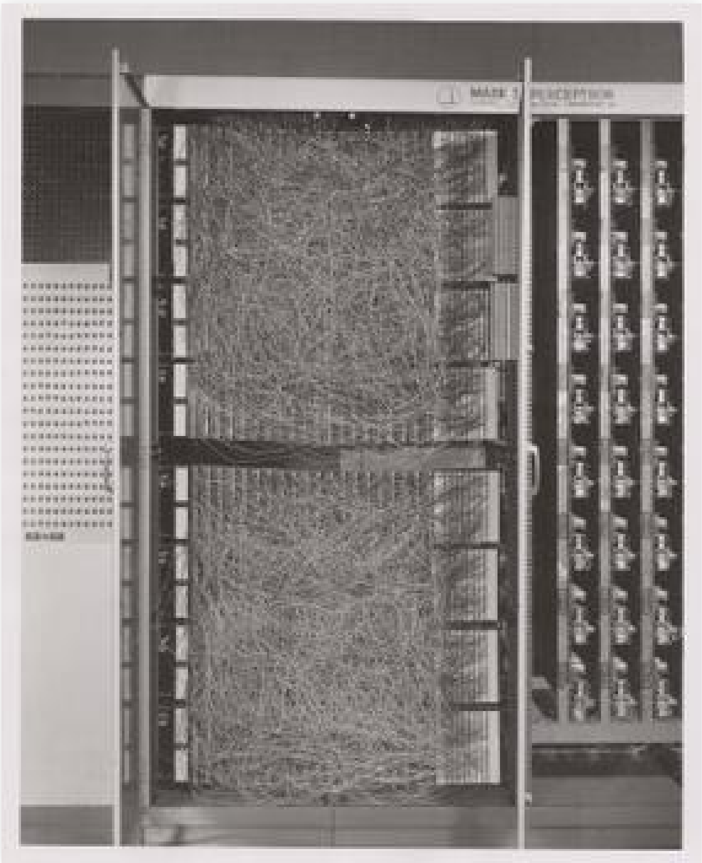
Rosenblatt and IBM 704. Source: Cornell Chronicle

Perceptron

- But then was actually built as a machine

Camera with 20x20 pixels, for image recognition

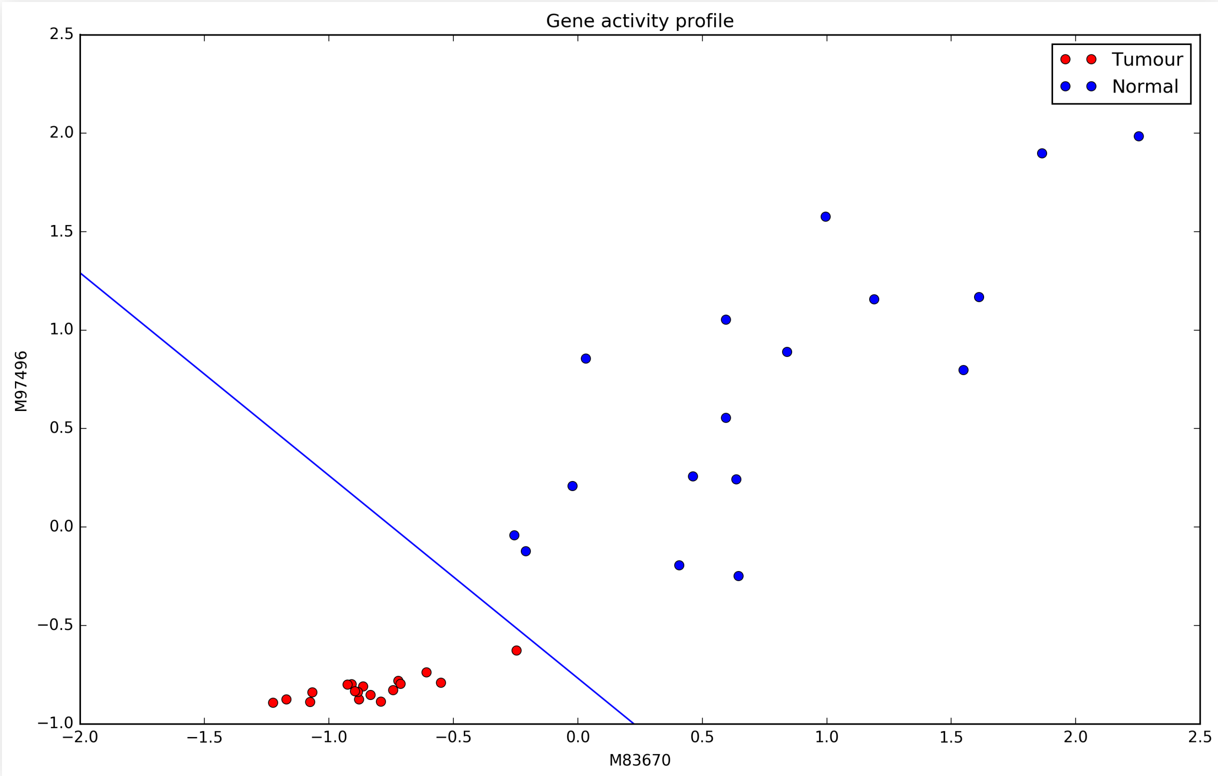
Electric motors to adjust potentiometers for the weights of the inputs



Mark I Perceptron (Wikipedia)

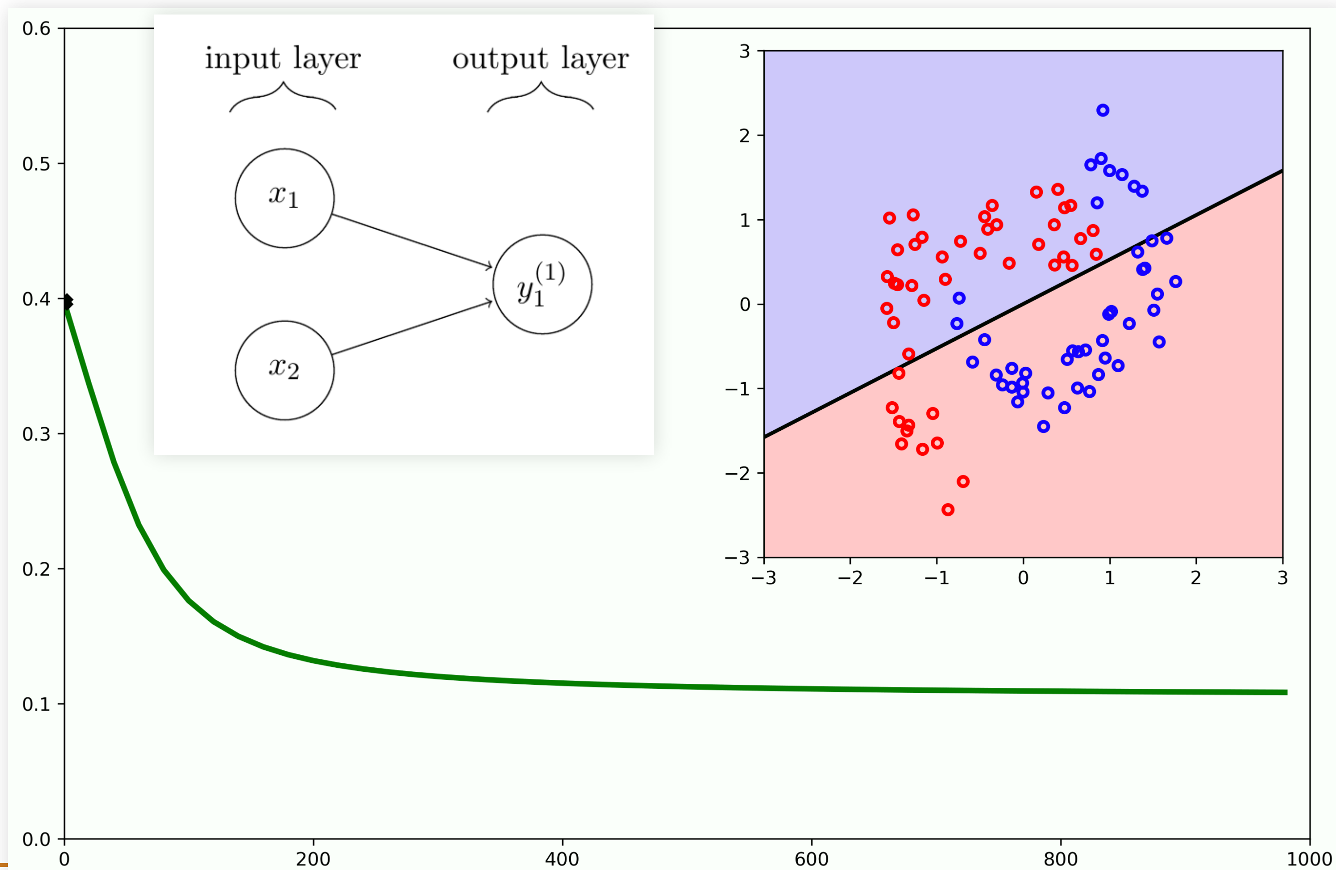
Perceptron

- Seemed a promising start
- But the perceptron is just a linear model



Perceptron

- It's a single neuron, so a linear classifier
- similar to logistic regression that was already known



Neural Networks

- A very promising early start with neuron and perceptron:
  - 1943: McCulloch & Pitts, model of neuron
  - 1958: Rosenblatt, perceptron and learning algorithm
- But these turned out to be equivalent to generalized linear models
  - And in 1969 Perceptrons (Minsky, Papert): need fully connected networks

1960-mid 1980s: "AI Winter", in particular ANN

- Logic systems ruled AI for the larger part of this period
- But eventually funding was cut drastically
- 1986: Rumelhart, Hinton, Williams, backpropagation can be used for multi-layer networks

Machine Learning

What is machine learning?

- "Field of study that gives computers the ability to learn without being explicitly programmed"
  (Samuel, 1959)
- "A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E"
  (Mitchell, 1997)

Machine Learning problem

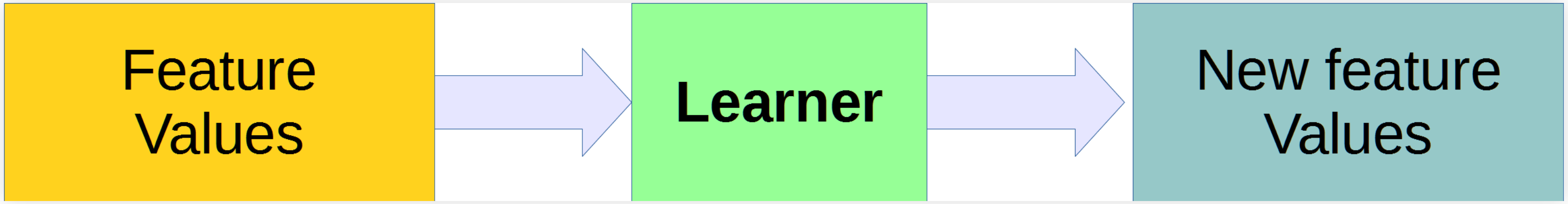
- A task that the system must perform.
- A measure of its performance
- The data used to improve its performance
- Examples:

- Spam filtering
- Image classification
- Medical diagnosis
- Speech recognition
- Autonomous driving
- Clustering, feature representation, ...

Basic kinds of ML problems

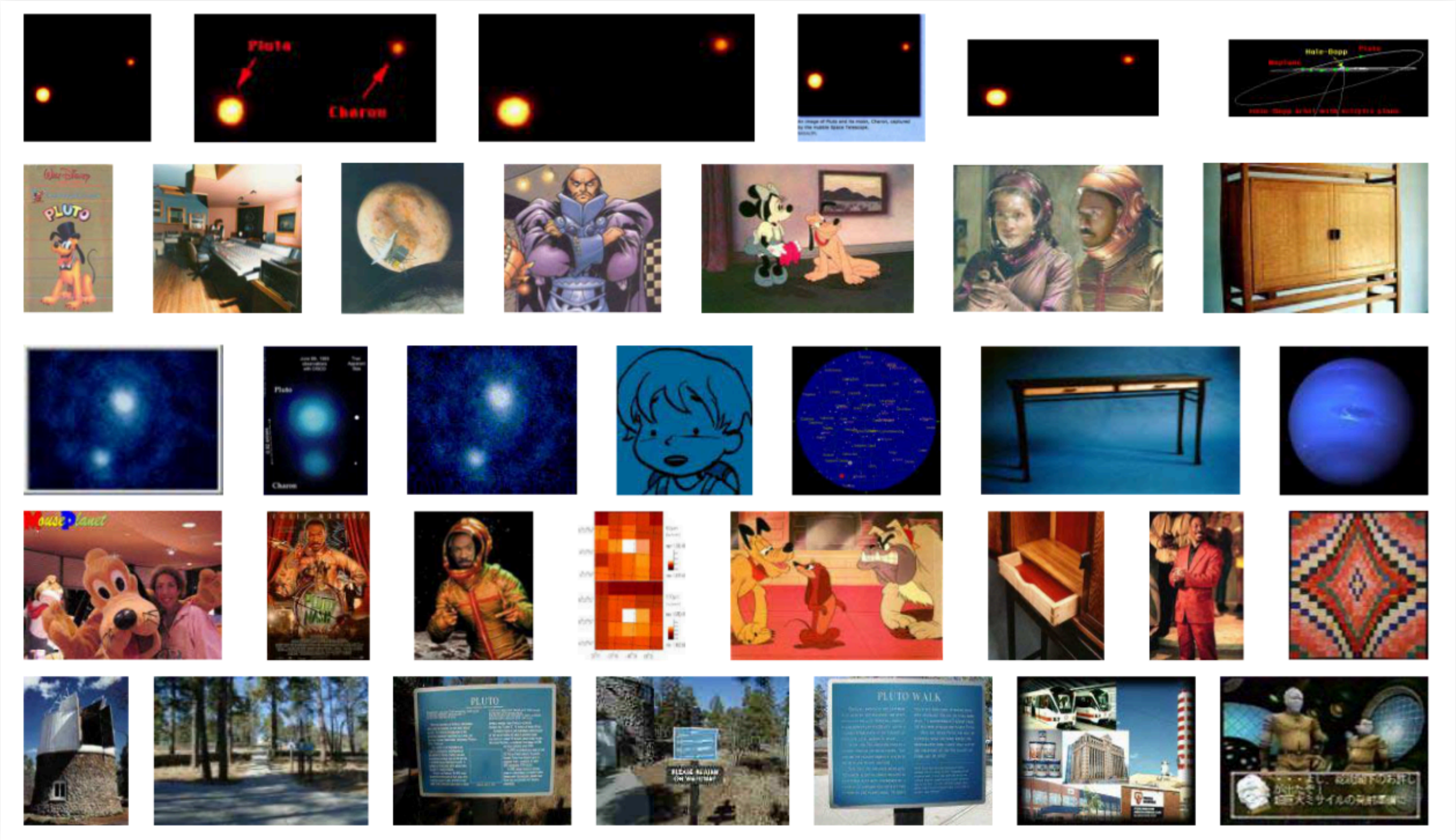
- Unsupervised learning

- No need for labels in data;
- Find structure in data
- Clustering is a common example, but we will see applications in deep learning



ML Problems

- Example: clustering images

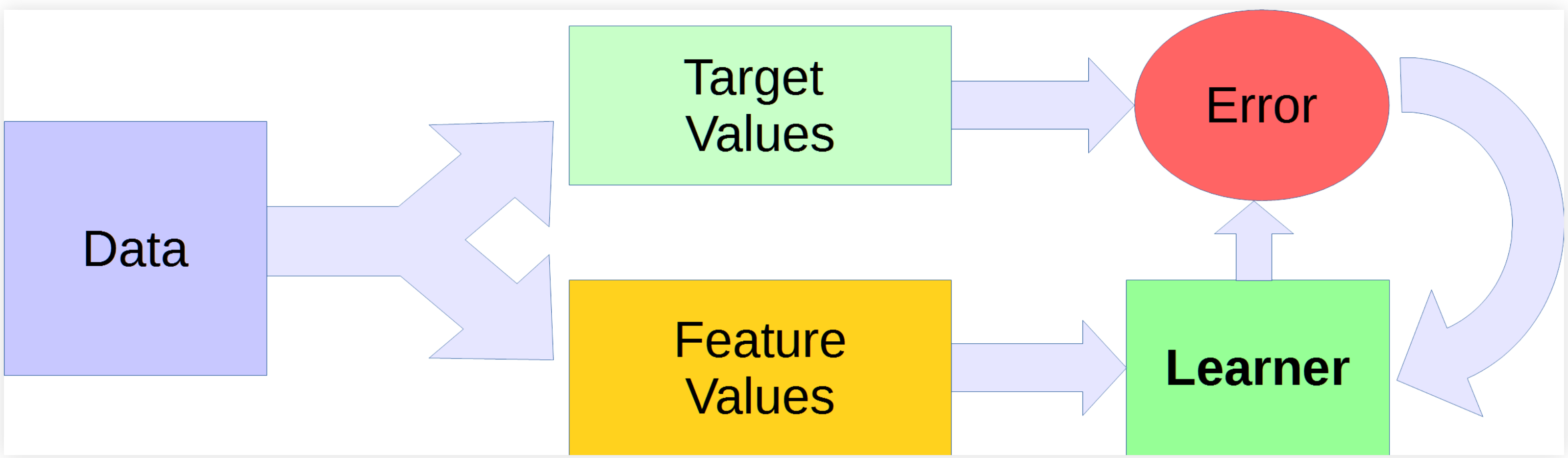


Group searches with features from image and HTML (Cai et al, Clustering of WWW Image Search Results, 2004)

Basic kinds of ML problems

- Unsupervised learning
- Supervised learning

- Uses labelled data and aims at predicting classes or values
- Continuous values: Regression
- Discrete classes: Classification



ML Problems

Supervised learning

- Example: face identification

Valenti et al, Machine Learning Techniques for Face Analysis, 2008

Basic kinds of ML problems

- Unsupervised learning
- Supervised learning
- Semi-supervised learning
- Mixes labeled and unlabeled data
- Can be useful to increase size of data set

Basic kinds of ML problems

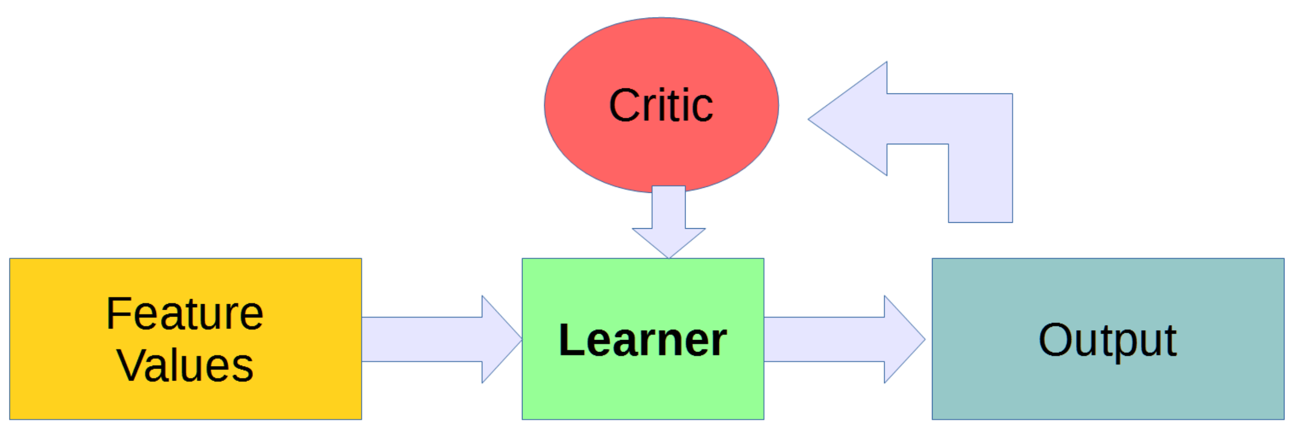
- Unsupervised learning
- Supervised learning
- Semi-supervised learning
- Self-supervised Learning

- Labels are intrinsic to the data

Basic kinds of ML problems

- Unsupervised learning
- Supervised learning
- Semi-supervised learning
- Self-supervised Learning
- Reinforcement learning

- Optimize output without immediate feedback for each instance



Can solve different kinds of problems

- Extracting new features and finding relations
  - Unsupervised learning
- Approximating a target
  - Supervised learning
- Optimizing policy
  - Reinforcement learning

Traditional approach:

- Use very different models, optimizations, etc.

The rise of machine learning

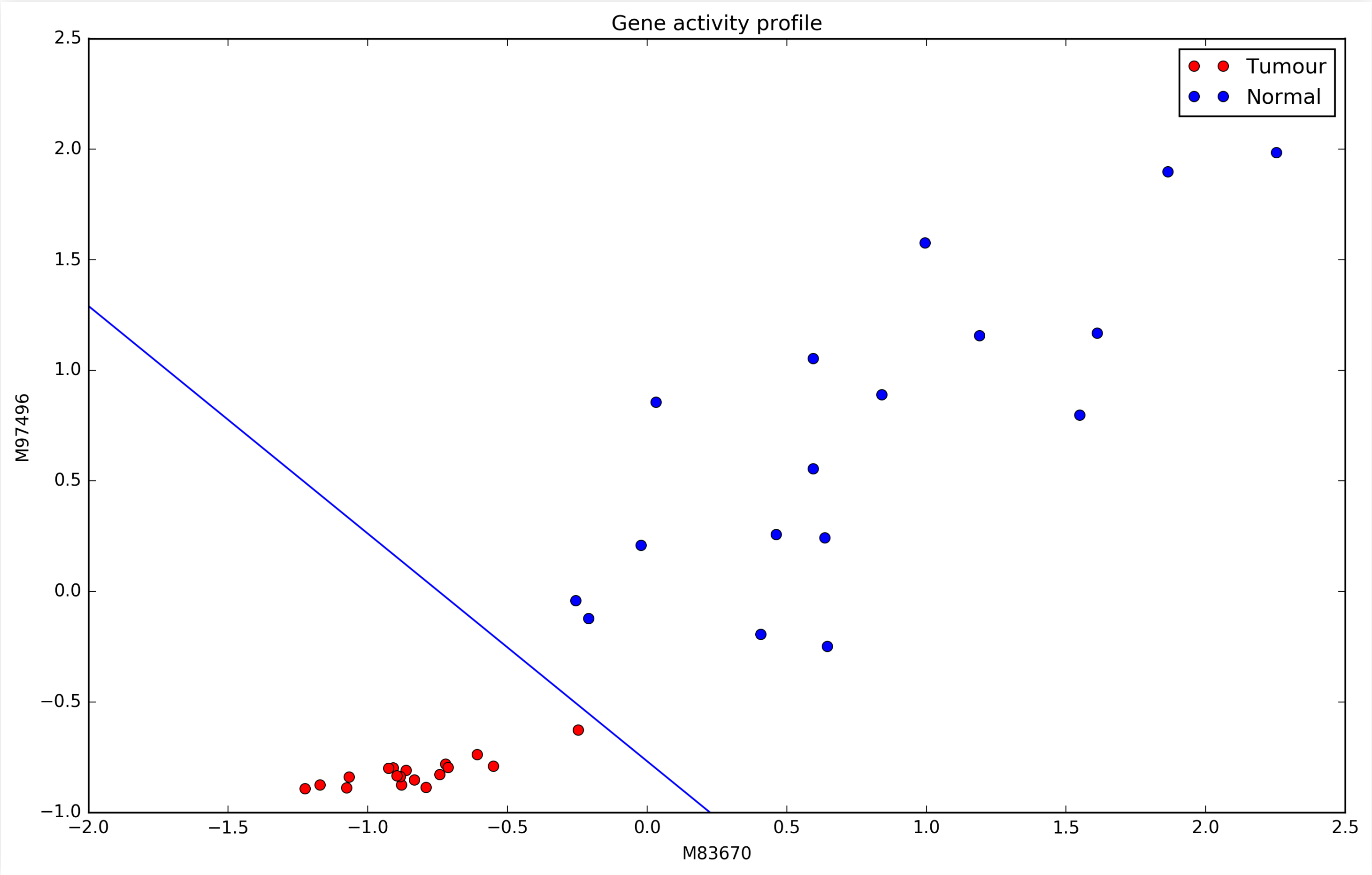
- In the 1990s, AI shifted from knowledge-driven to data-driven with new ML algorithms
  - E.g. 1992 Vapnik et. al. publish the kernel trick for SVM

- 1995: SVM (Cortes & Vapnik), Random Forest (Ho)
- 1997: Multi-layered and convolution networks for check processing USA (leCun)
- 1998: MNIST database (LeCun). Benchmarks, libraries and competitions

The power of nonlinearity

Nonlinearity

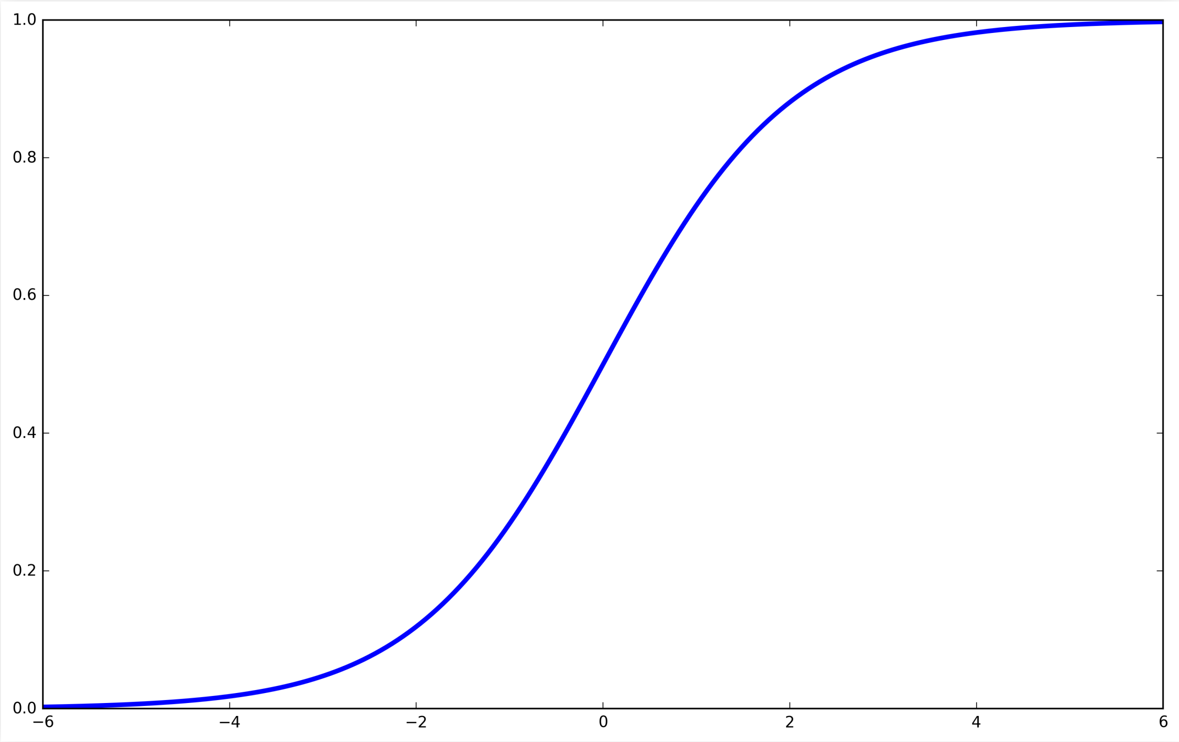
Linear classification



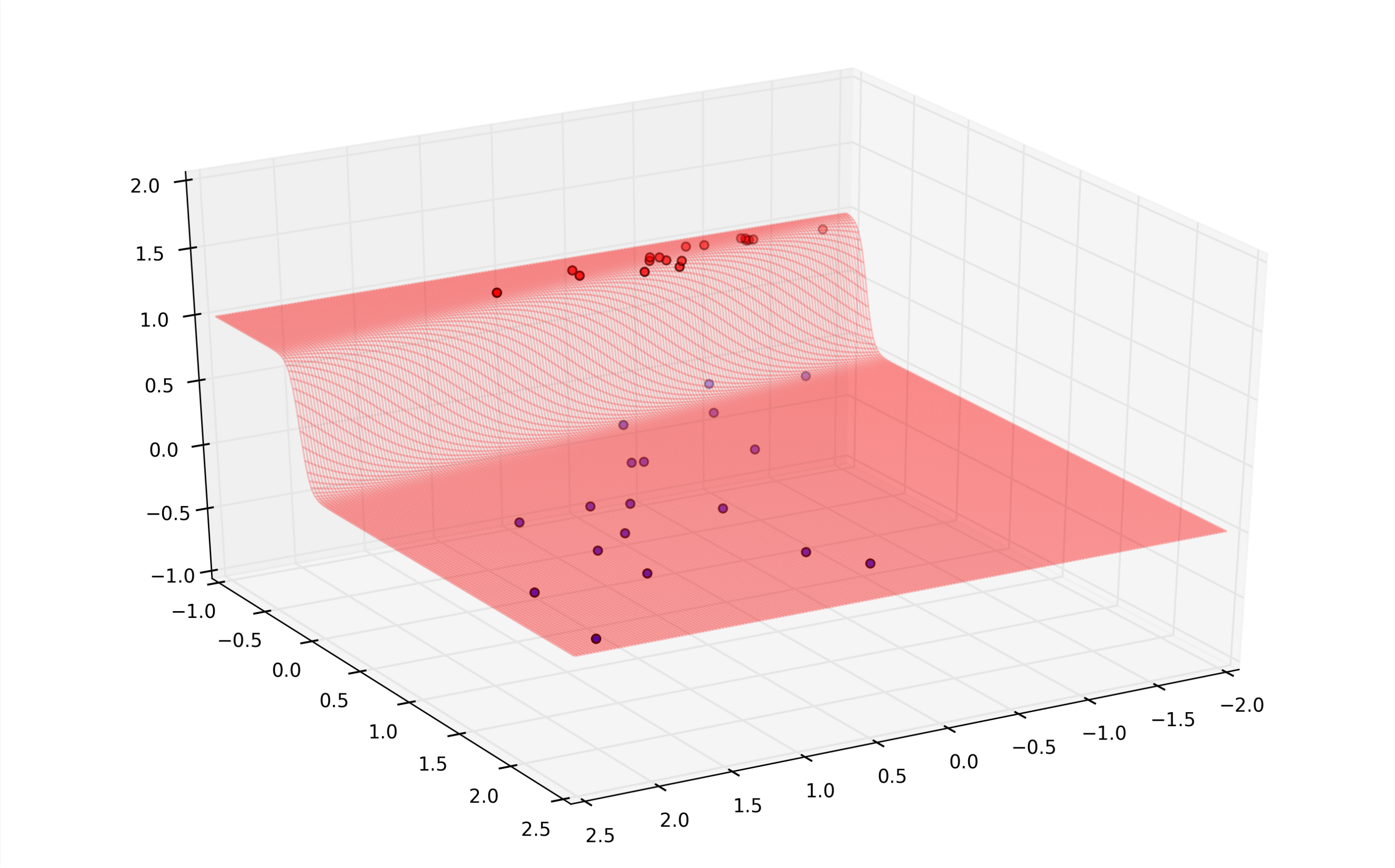
Nonlinearity

Linear classification, e.g. Logistic Regression

$$g(\vec{x}, \widetilde{w}) = P(C_1|\vec{x}) \qquad g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-(\vec{w}^T\vec{x} + w_0)}}$$

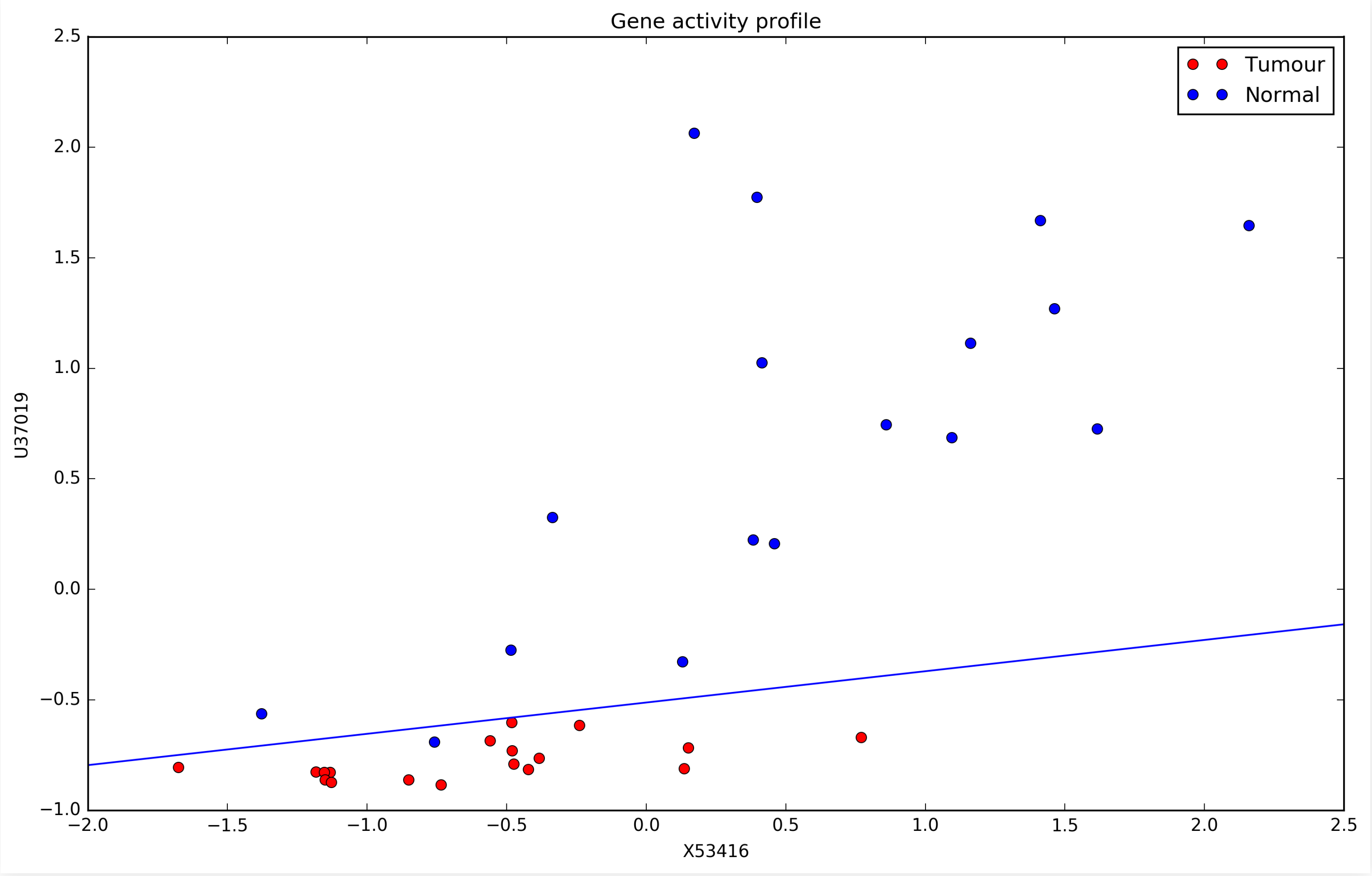


Linear classification, e.g. Logistic Regression



Nonlinearity

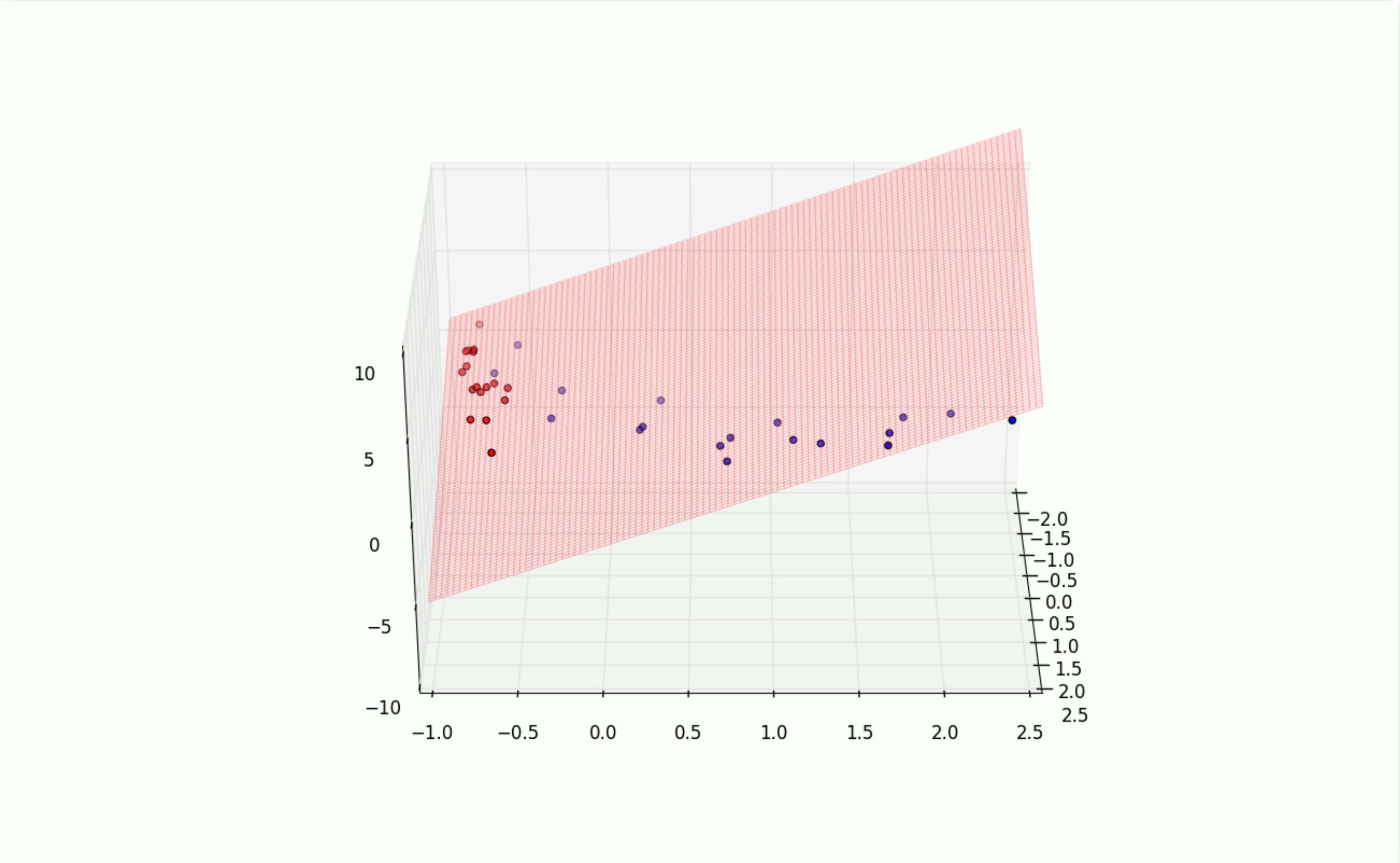
Linear classification, e.g. Logistic Regression



Nonlinearity

Nonlinear expansion of attributes

- We can expand the attributes non-linearly ($x_1 \times x_2$)



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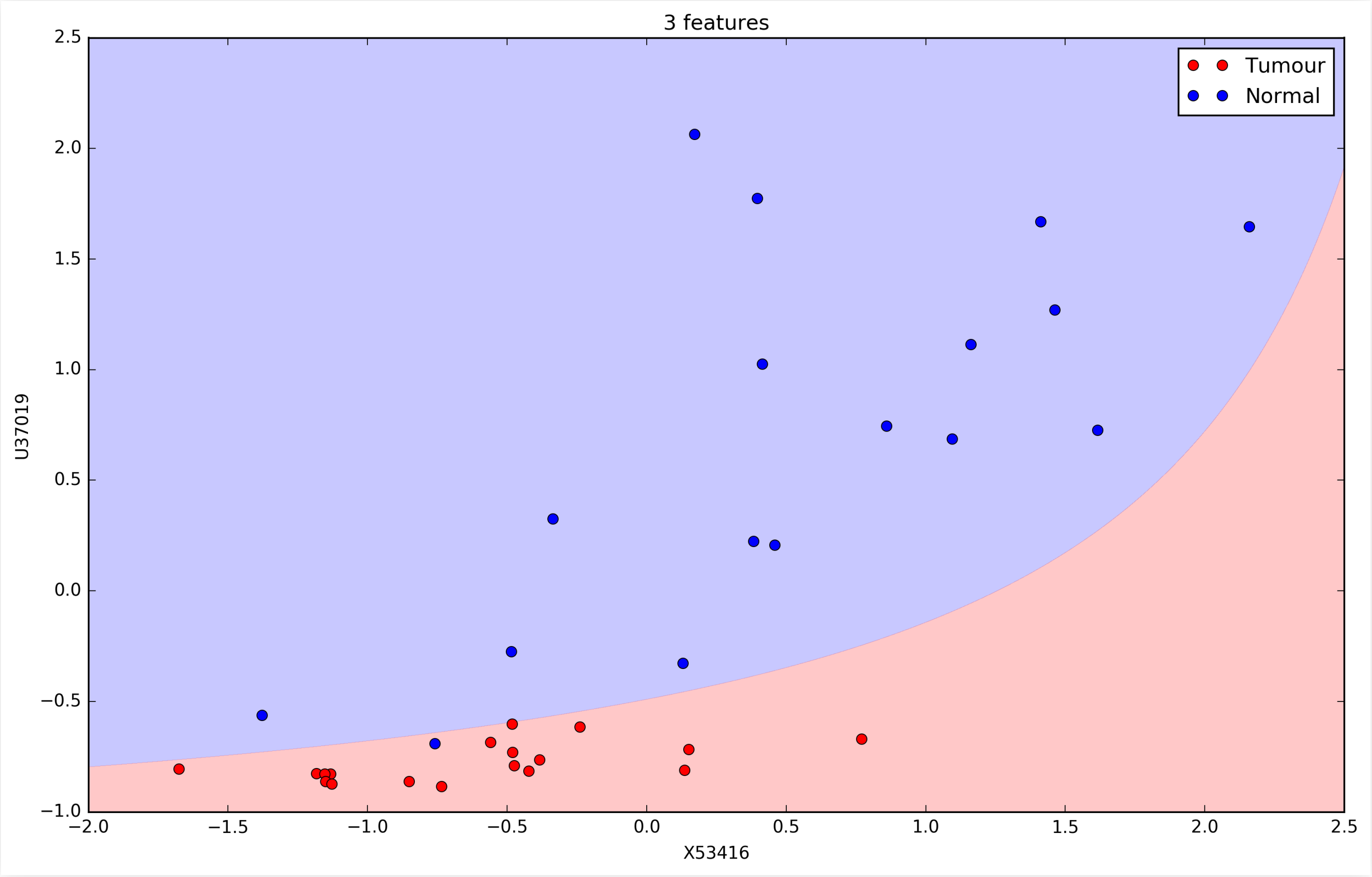
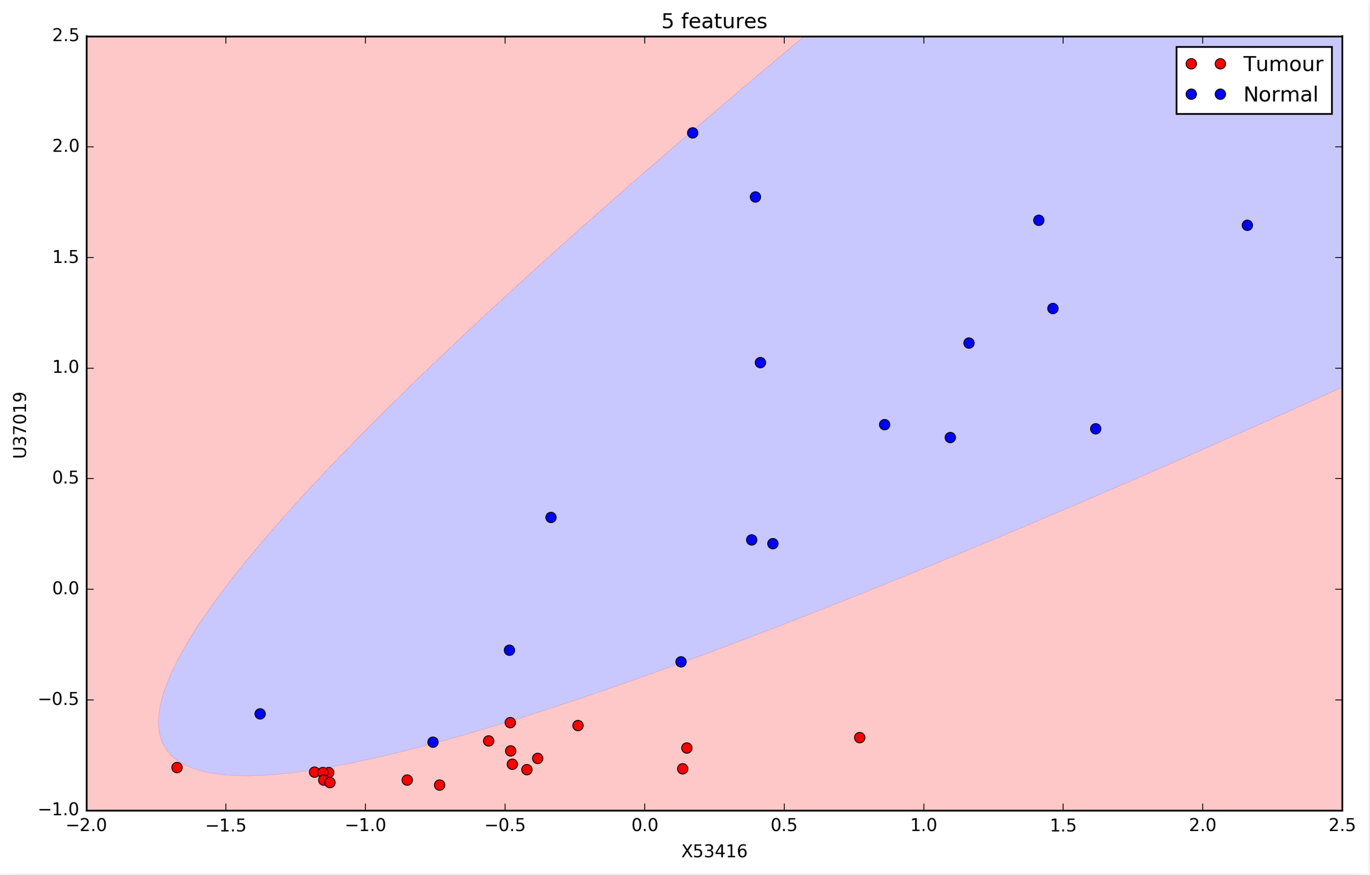


Nonlinearity

Nonlinear expansion of attributes

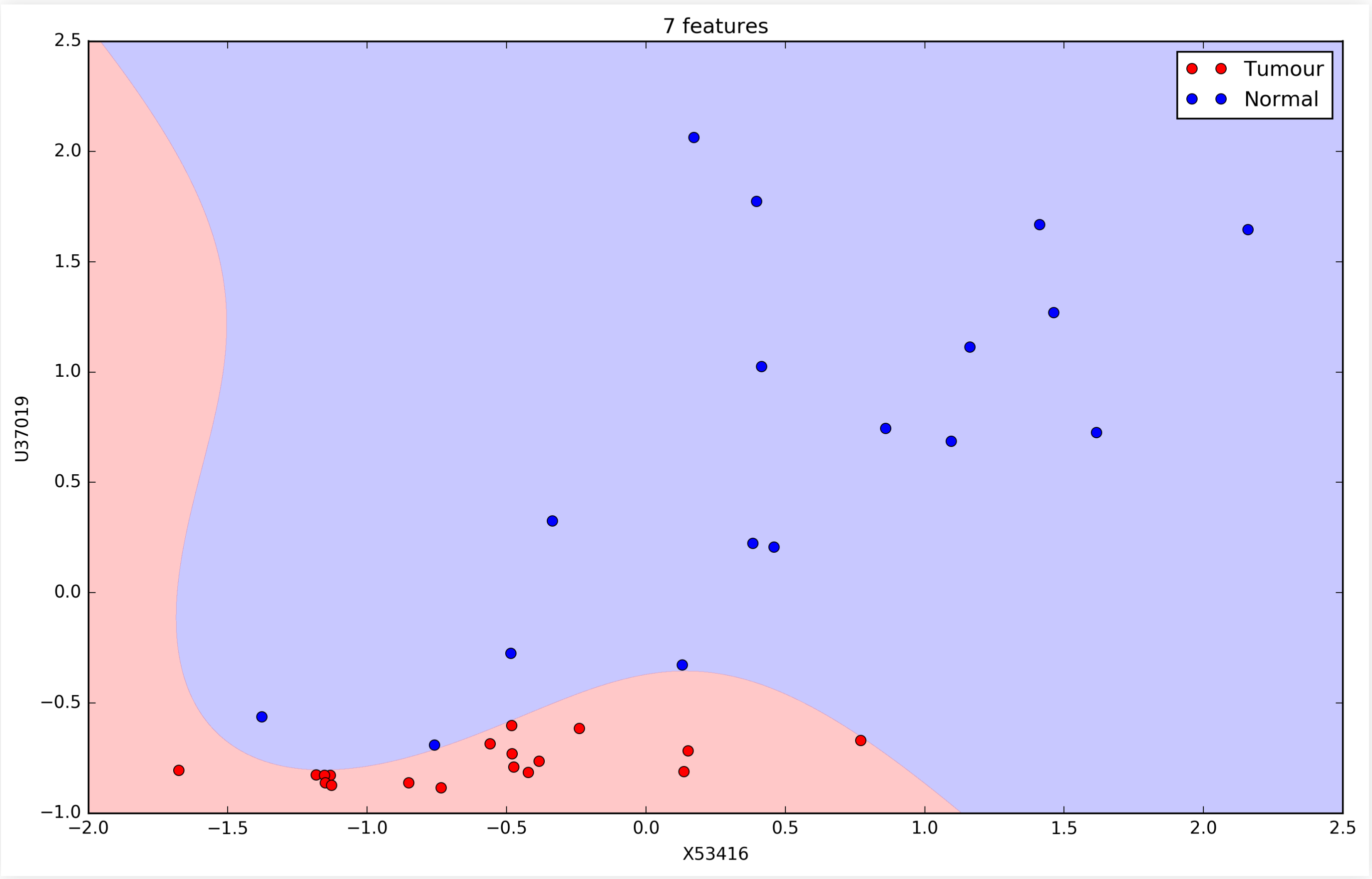
- We can expand further $(x_1, x_2, x_1x_2, x_1^2, x_2^2)$



Nonlinearity

Nonlinear expansion of attributes

- We can expand further $(x_1, x_2, x_1 x_2, x_1^2, x_2^2, x_1^3, x_2^3)$



Nonlinearity

Nonlinear expansion of attributes

- With logistic regression this is not practical
  - We have to do it by hand
- Support Vector Machines do this automatically

$$\arg\max_{\vec{\alpha}} \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} \alpha_n \alpha_m y_n y_m K(\vec{x}_n, \vec{x}_m)$$

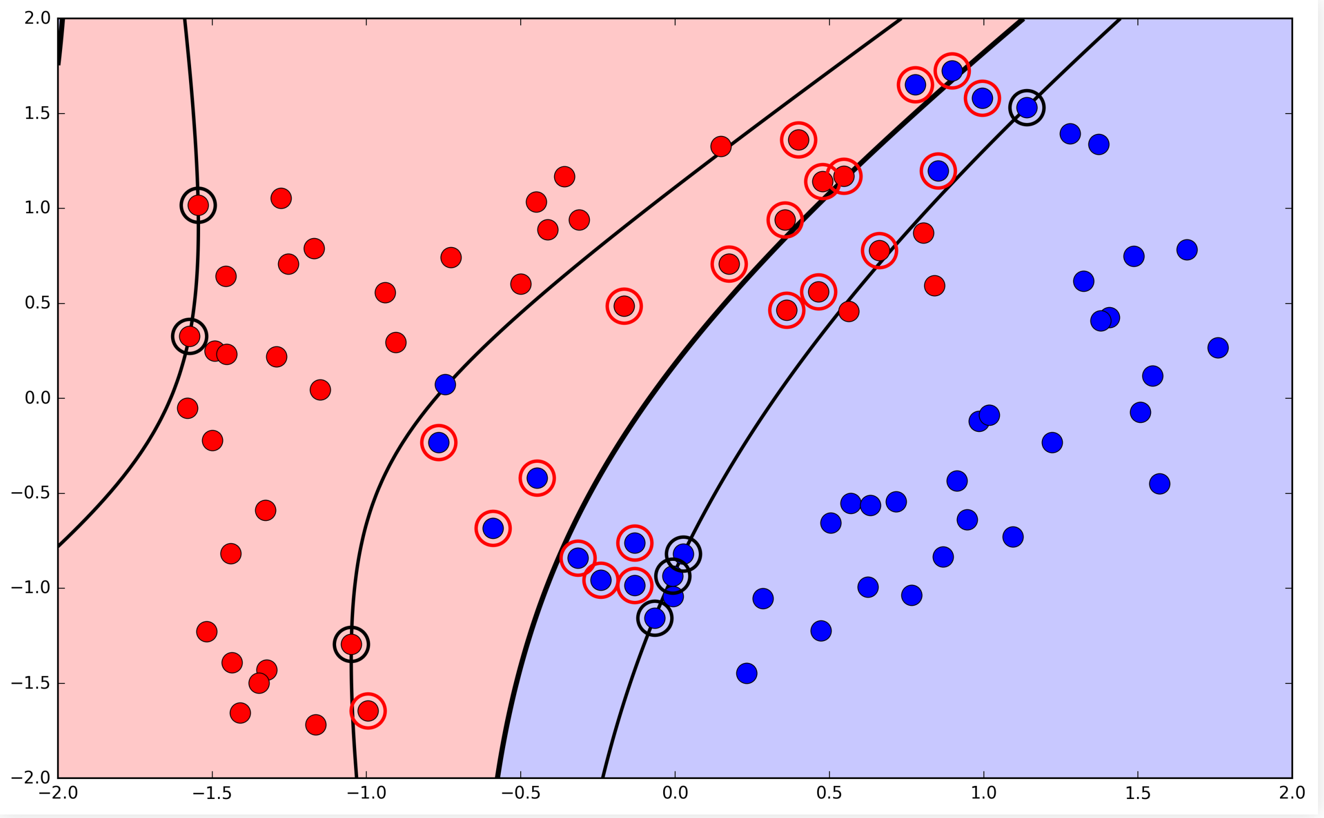
- Where $\vec{\alpha}$ is a vector of coefficients, $K(\vec{x}_n, \vec{x}_m)$ is the kernel function for some non-linear expansion ϕ of our original data

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \cdot \begin{bmatrix} x_1 & x_2 \end{bmatrix} = \begin{bmatrix} x_1^2 & x_1 x_2 \\ x_1 x_2 & x_2^2 \end{bmatrix}$$

Nonlinearity

Nonlinear expansion of attributes

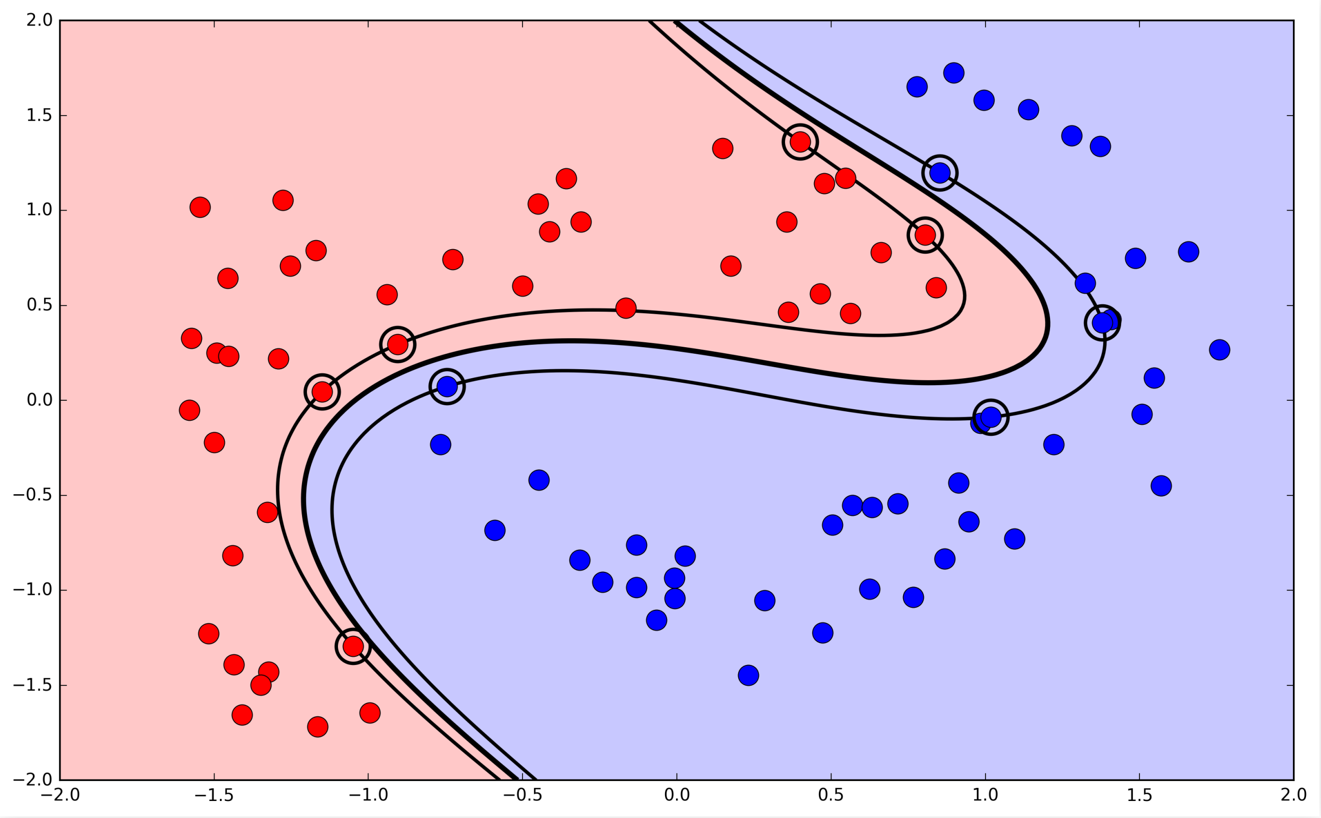
- Example, using a polynomial kernel: $K_{\phi(\vec{x}^n)} = (\vec{x}^T \vec{z} + 1)^2$



Nonlinearity

Nonlinear expansion of attributes

- Example, using a polynomial kernel: $K_{\phi(\vec{x}^n)} = (\vec{x}^T \vec{z} + 1)^3$



No free lunch

No free lunch

No-free-lunch theorems (Wolpert and MacReady, 1997)

"[I]f an algorithm performs well on a certain class of problems then it necessarily pays for that with degraded performance on the set of all remaining problems."

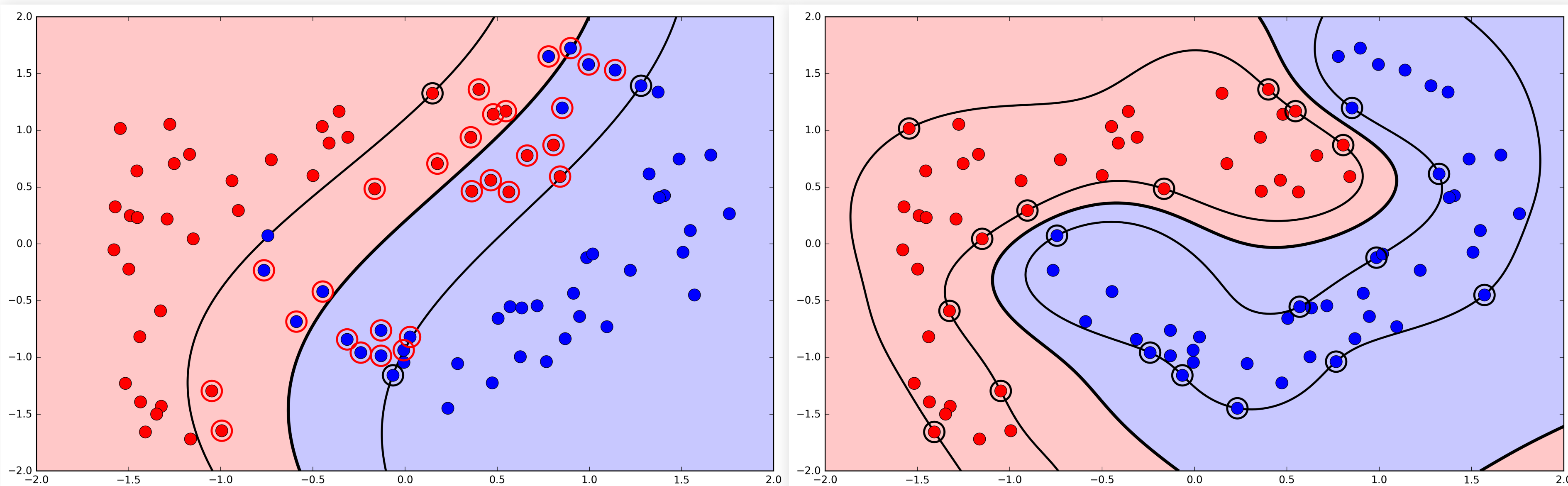
Important for two reasons:

- No single model can be best at all tasks:
  - We need to create different models optimized for different tasks
- Overfitting
  - The hypothesis chosen may be so adjusted to the training data it does not generalize

Overfitting

Nonlinearity is important for capturing patterns in data

- But can lead to loss of generalization



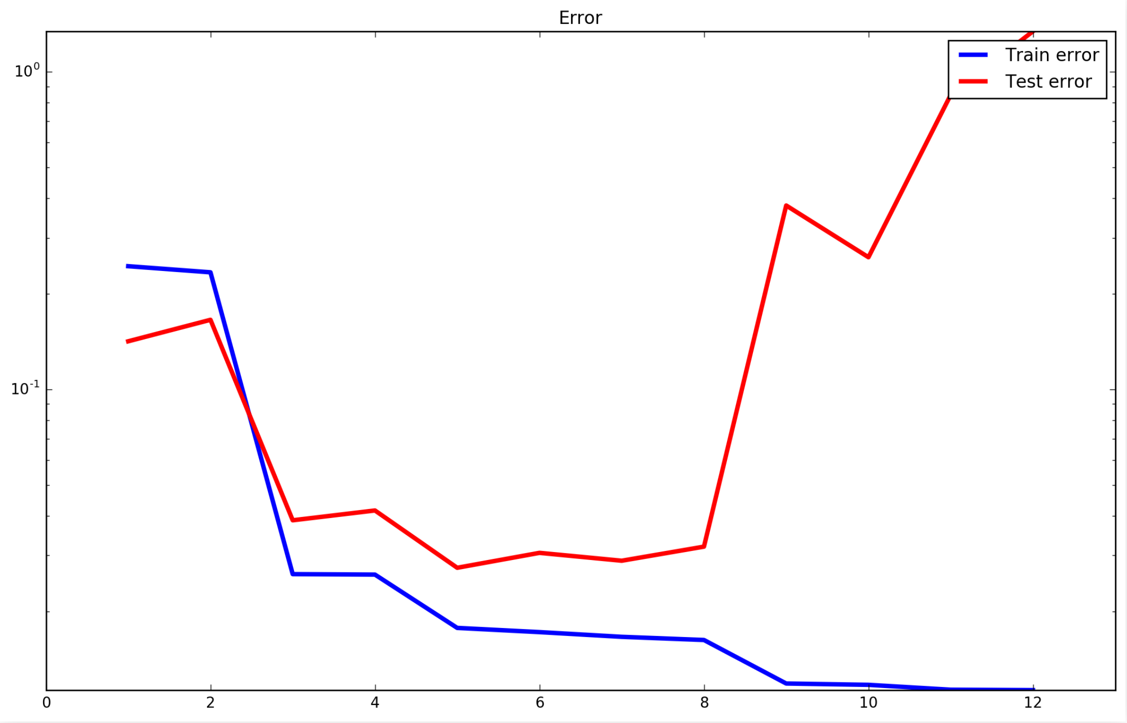
"With great power comes great overfitting"

Benjamin Parker (attributed)

Overfitting

Occurs when model adjusts to noise

- Some details are informative about patterns in the population
- Some are particular to the data sample and do not generalize



Overfitting

Occurs when model adjusts to noise

- Measuring overfitting:
  - Evaluate outside the training set
  - Validation set: used for selecting best model, hyperparameters, ...
  - Test set: used to obtain unbiased estimate of the true error
- Preventing overfitting:
  - Adjust training (regularization)
  - Select adequate model
  - Use more data (allows more powerful models)

What do we have in "classical" machine learning?

- Many algorithms do nonlinear transformations
- Many different models
  - Great diversity, with different algorithms
- The right features
  - Feature extraction usually done by the user
- Preventing overfitting
  - Method depends on the algorithm
- Ability to use large amounts of data
  - Some do, some don't

Deep learning helps solve these problems

- Nonlinear transformations, stacked
- Many different models
  - but all built from artificial neurons
- The right features
  - can be done automatically determined by the model during training
- Preventing overfitting
  - Many ways to regularize
- Ability to use large amounts of data
  - Yes!

Summary

Summary

- Overview of the course
- AI and Machine learning
- Nonlinear transformations and Overfitting
- The promise of deep learning

Further reading:

- Skansi, Introduction to Deep Learning, Chapter 1
- Goodfellow et al, Deep Learning, Chapters 1 and 5