

# Machine Learning

## DA220

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Office: PB405

# ML Class schedule

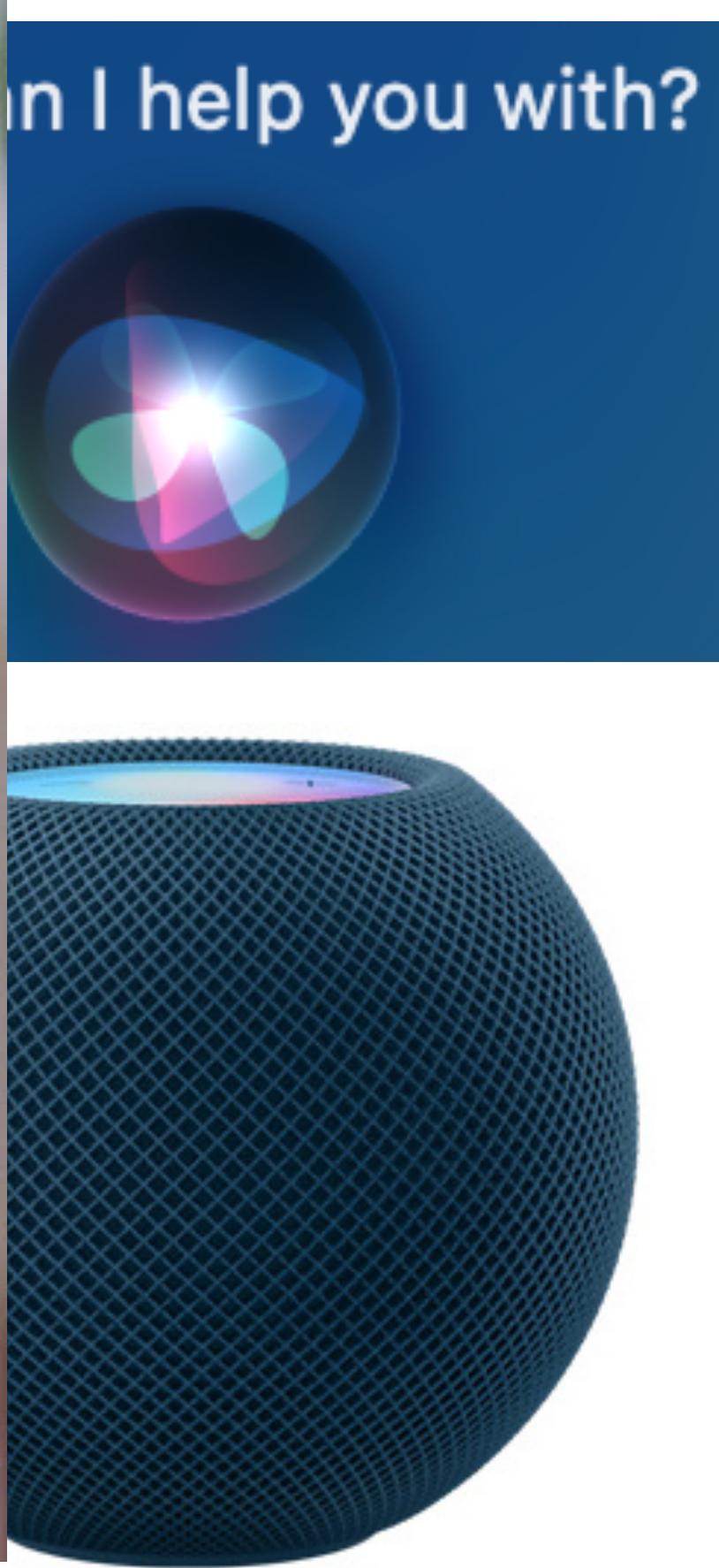
- Tuesday - 10:00 AM - 12:00 PM (Arya lab)
- Thursday - 10:00 AM - 12:00 PM (Arya lab)
- Programming lab
- TA:
  - ▶ Rajdeep Mondal (2nd yr. PhD student)
    - Room no.- PB412 or MB214
  - ▶ Suvajit Patra (1st yr. PhD student)
    - Room no.- MB214



What is machine learning ?

# Some applications and motivation

- Virtual assis-

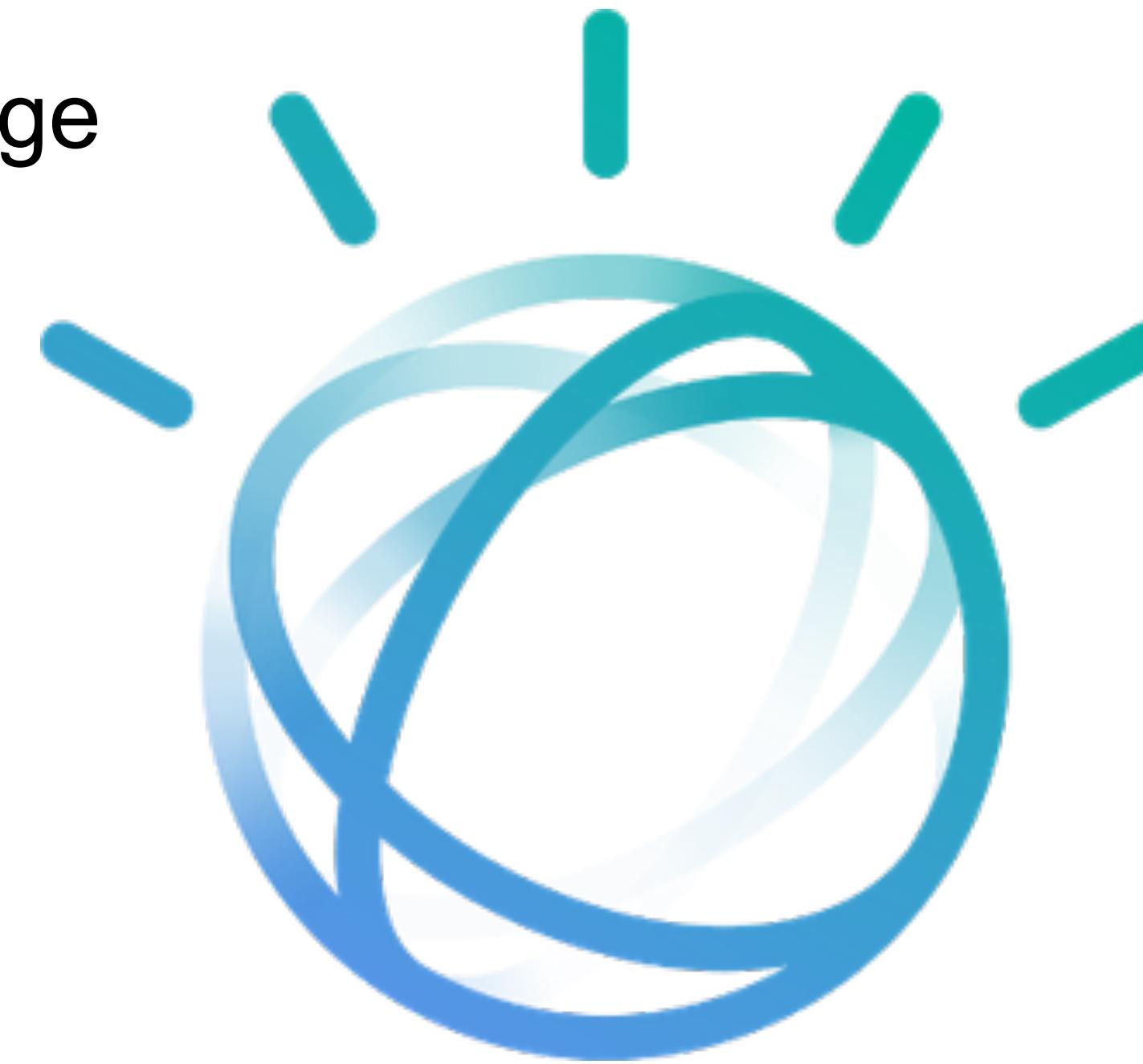


Images: Wikipedia, Amazon, Apple and Google

Video: YouTube

# Language processing

- Question-answering system in natural language
  - ▶ IBM Watson
    - Won first prize in **Jeopardy**, 2011



# Some applications and motivation (Cont.)

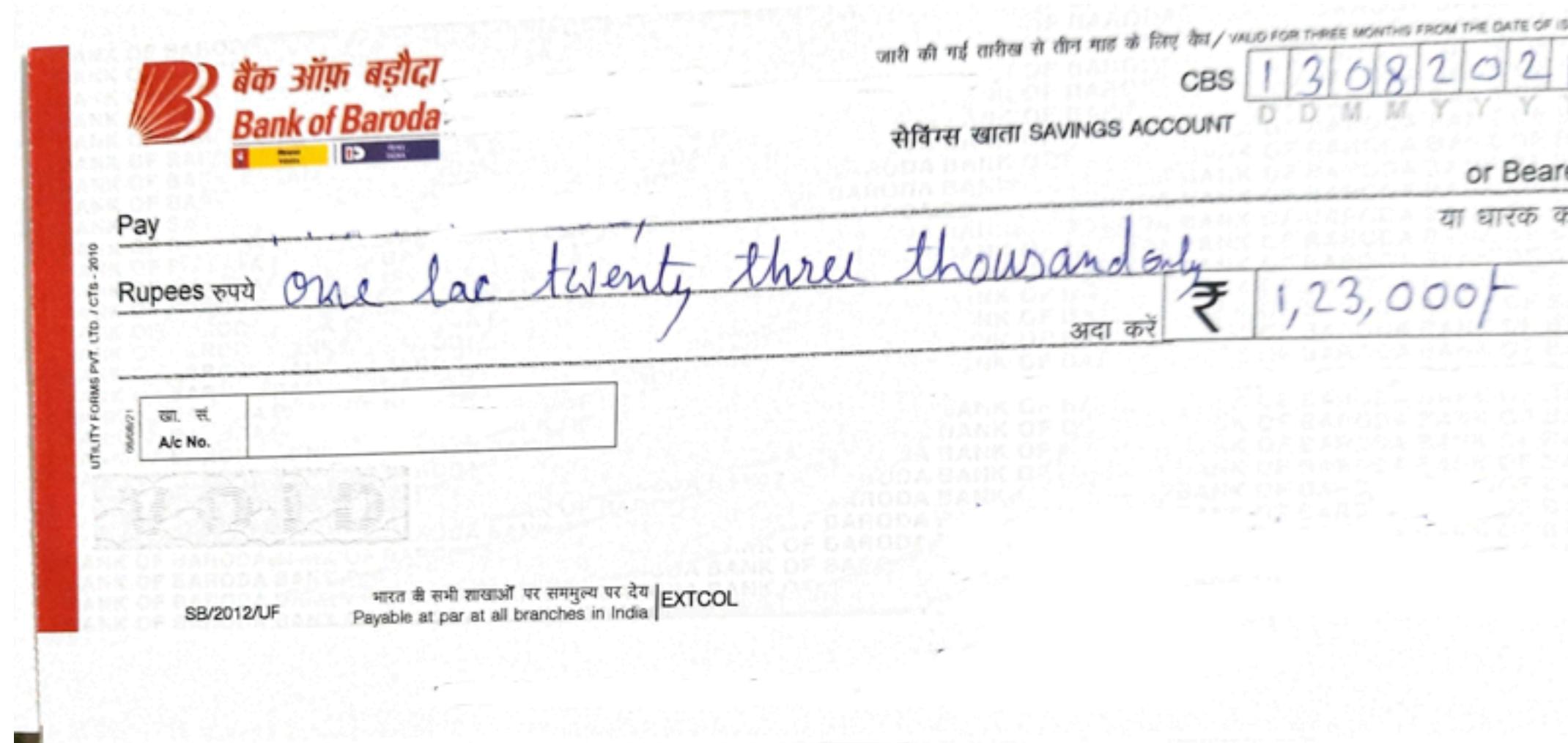


# Hand-written character recognition

0,1,2,3,4,5,...

Person-1

Hello everyone, today is our first ML class and we will start from a motivating example.



0.1.2.3.4.5,...

Person-2

Hello everyone, today is our first ML class and we will start from a motivating example.

# Hand-written digit recognition

- MNIST digit dataset<sup>1</sup>
  - Image:  $28 \times 28$



## THE MNIST DATABASE of handwritten digits

[Yann LeCun](#), Courant Institute, NYU  
[Corinna Cortes](#), Google Labs, New York  
[Christopher J.C. Burges](#), Microsoft Research, Redmond

*Please refrain from accessing these files from automated scripts with high frequency. Make copies!*

The MNIST database of handwritten digits, available from this page, has a training set of 60,000 examples, and a test set of 10,000 examples. It is a subset of a larger set available from NIST. The digits have been size-normalized and centered in a fixed-size image.

It is a good database for people who want to try learning techniques and pattern recognition methods on real-world data while spending minimal efforts on preprocessing and formatting.

Four files are available on this site:

[train-images-idx3-ubyte.gz](#): training set images (9912422 bytes)  
[train-labels-idx1-ubyte.gz](#): training set labels (28881 bytes)  
[t10k-images-idx3-ubyte.gz](#): test set images (1648877 bytes)  
[t10k-labels-idx1-ubyte.gz](#): test set labels (4542 bytes)

**please note that your browser may uncompress these files without telling you.** If the files you downloaded have a larger size than the above, they have been uncompressed by your browser. Simply rename them to remove the .gz extension. Some people have asked me "my application can't open your image files". These files are not in any standard image format. You have to write your own (very simple) program to read them. The file format is described at the bottom of this page.

The original black and white (bilevel) images from NIST were size normalized to fit in a 20x20 pixel box while preserving their aspect ratio. The resulting images contain grey levels as a result of the anti-aliasing technique used by the normalization algorithm. The images were centered in a 28x28 image by computing the center of mass of the pixels, and translating the image so as to position this point at the center of the 28x28 field.

- Extended MNIST<sup>2</sup>

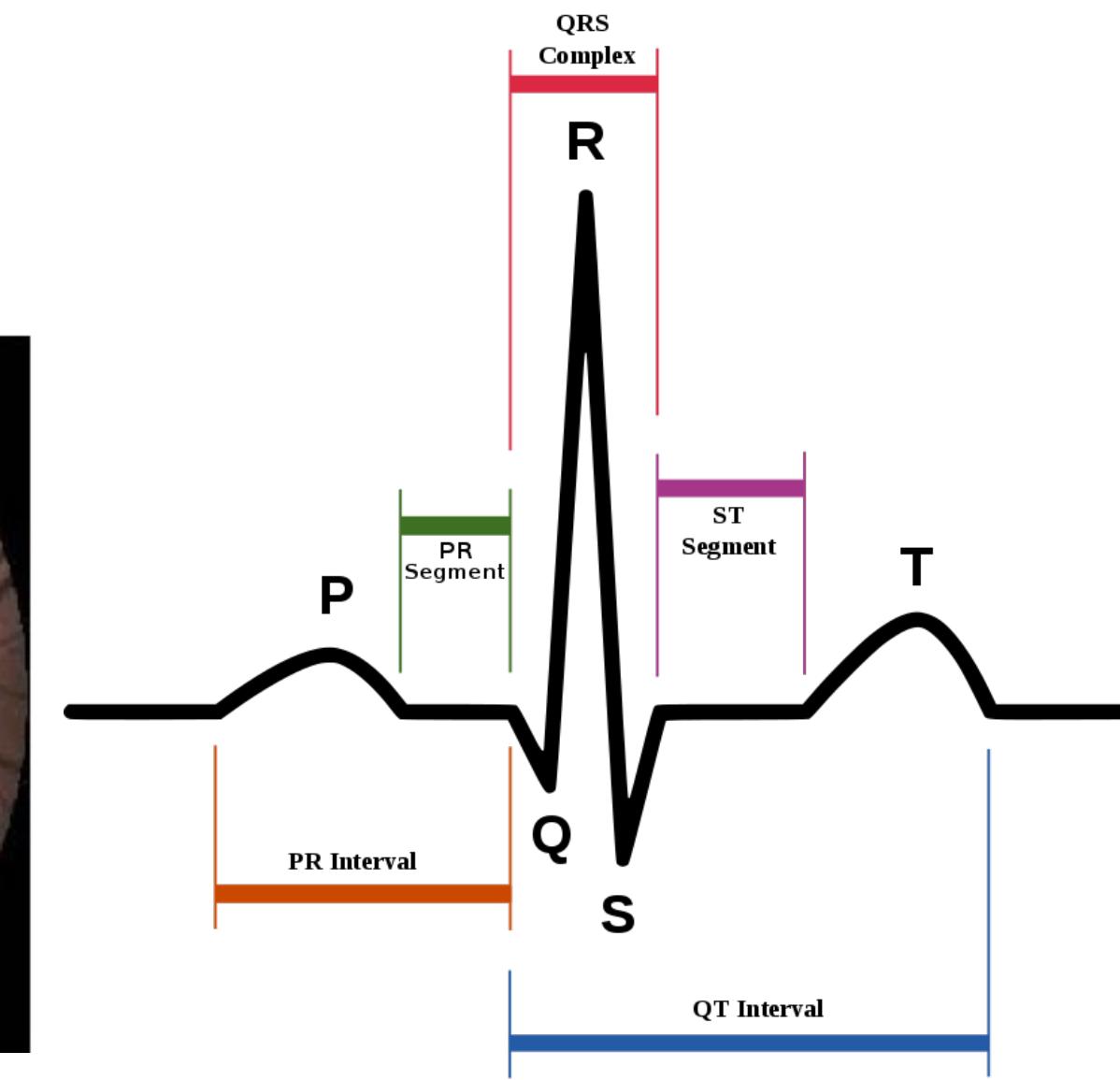
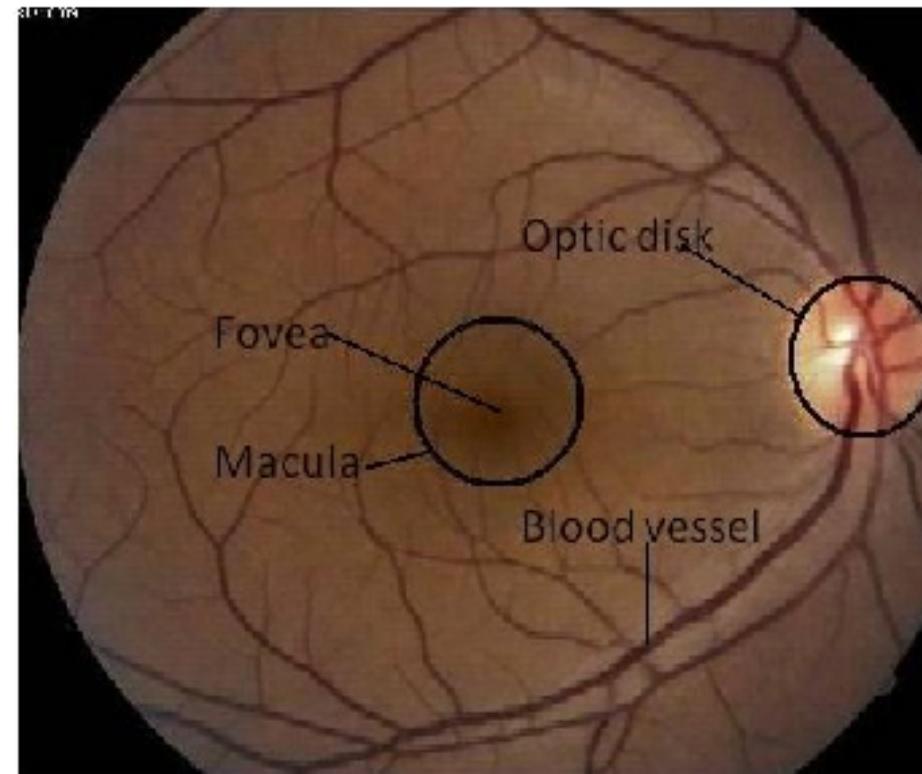
<sup>1</sup><http://yann.lecun.com/exdb/mnist/>

<sup>2</sup><https://www.nist.gov/itl/products-and-services/emnist-dataset>

<https://cs.stanford.edu/people/karpathy/convnetjs/demo/mnist.html>

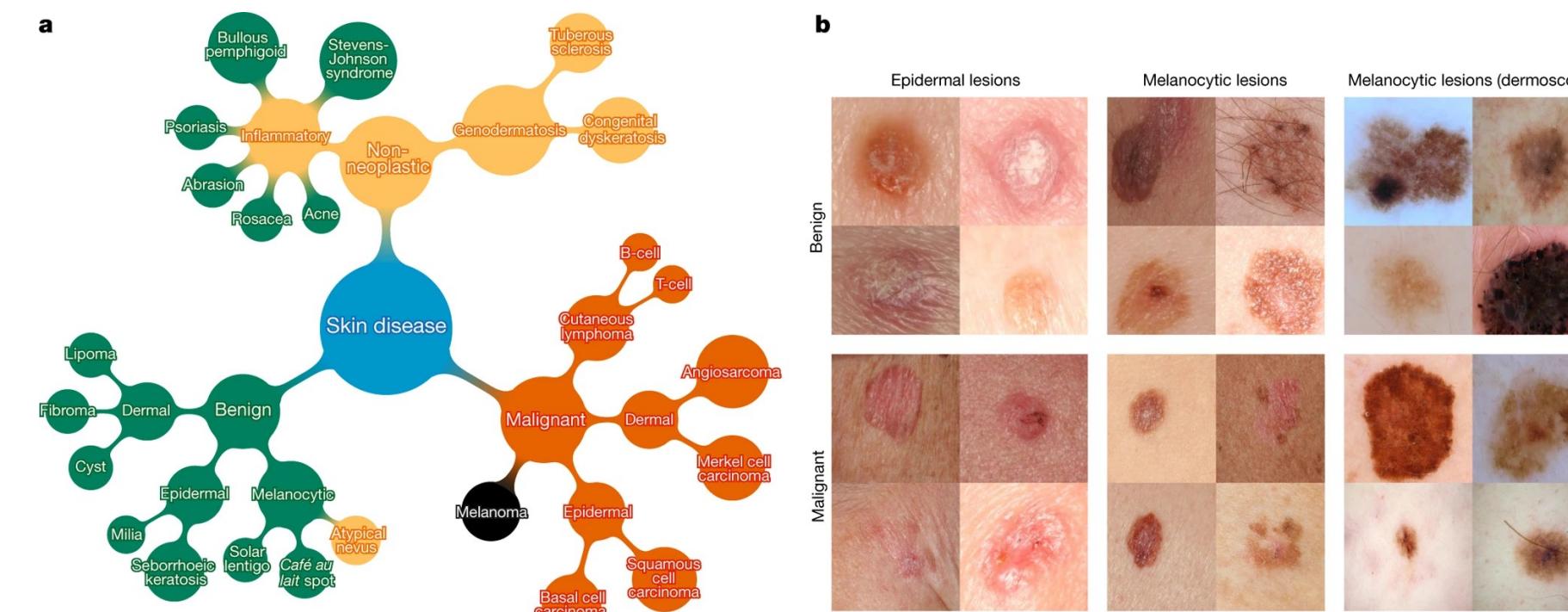
# Computer aided diagnosis

- Automation understanding of biosignals
  - ▶ EEG, ECG, EGG etc.

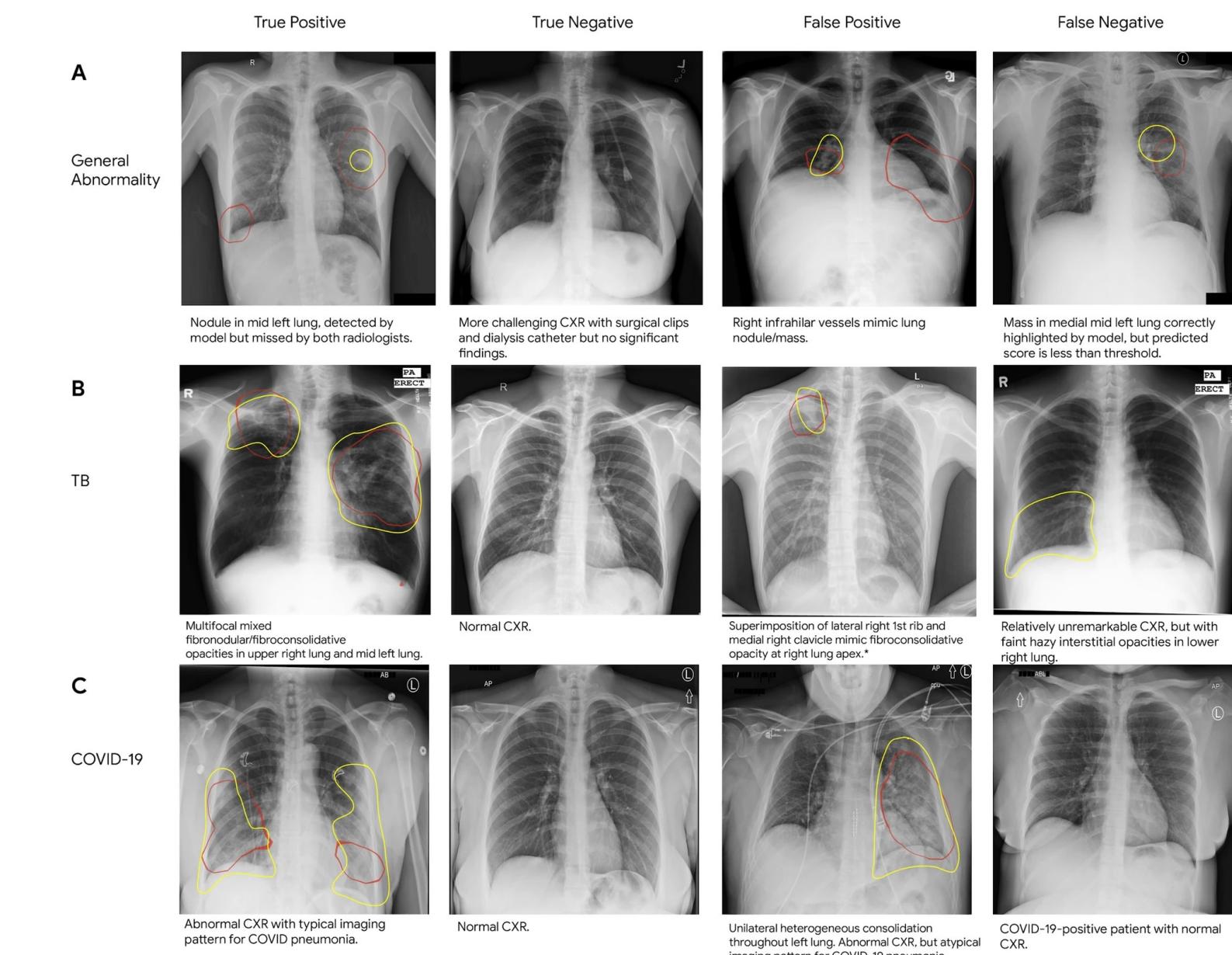


- Diabetic retinopathy

- Skin cancer detection

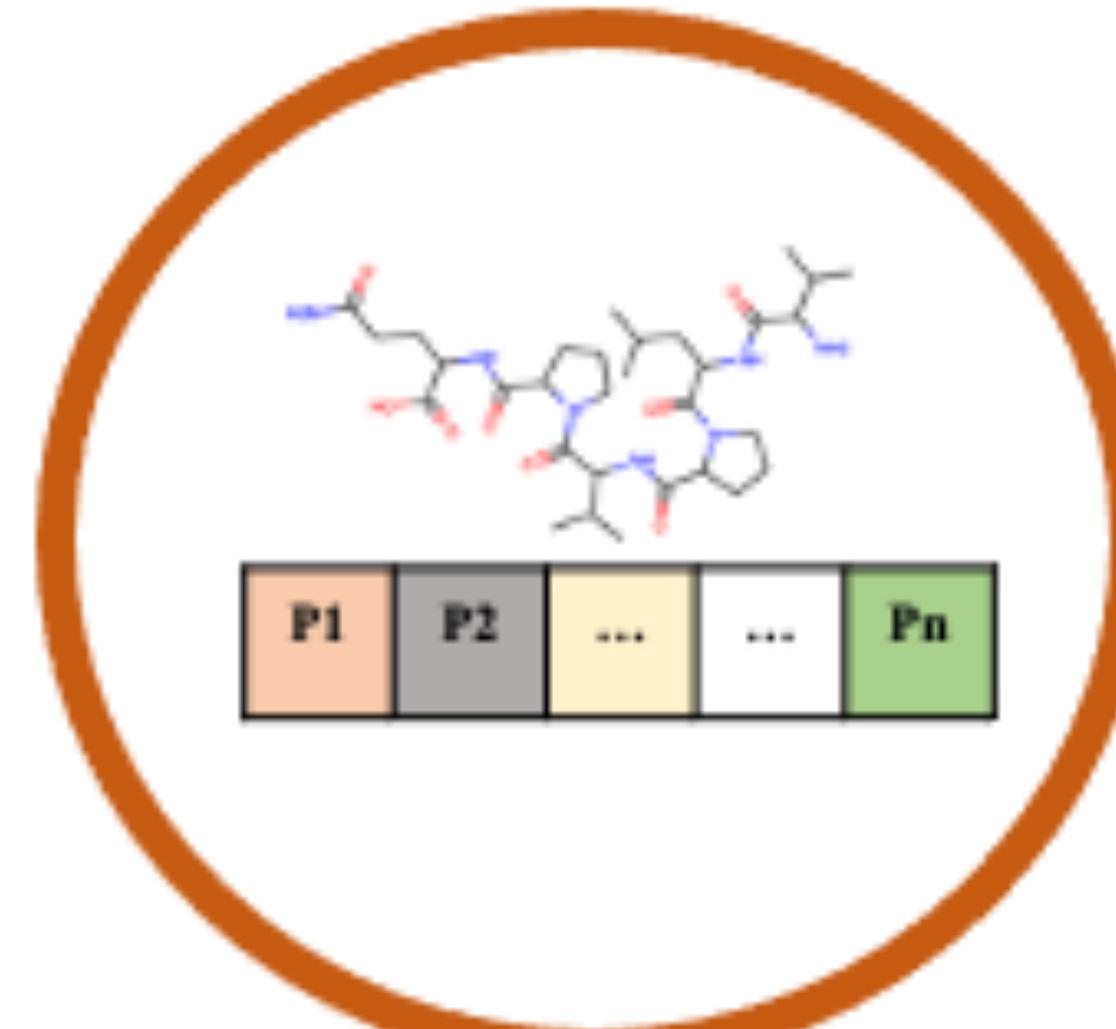


- Abnormal chest x-ray detection
- Designed to assist (**not replace**) physicians

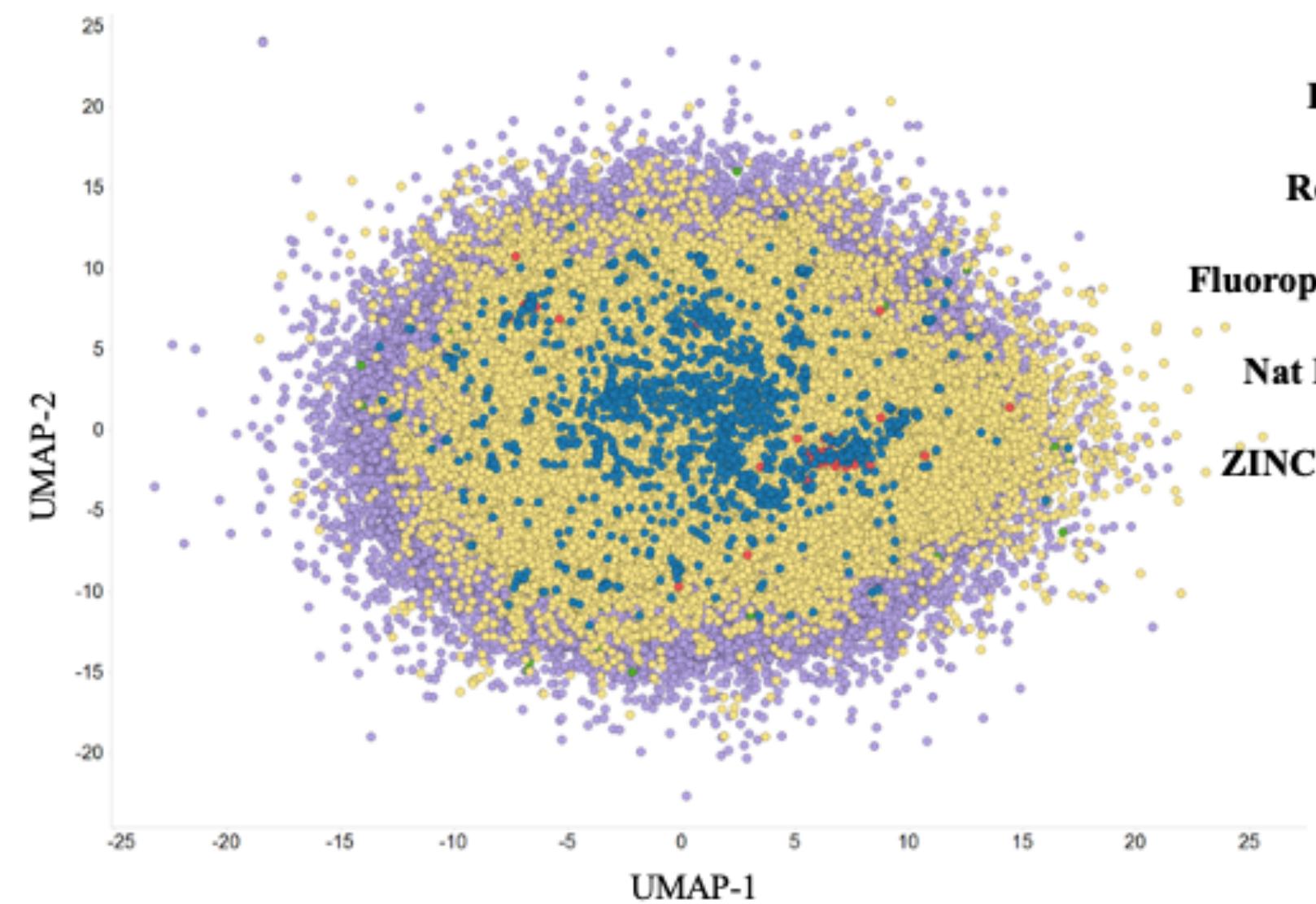


# Drug discovery

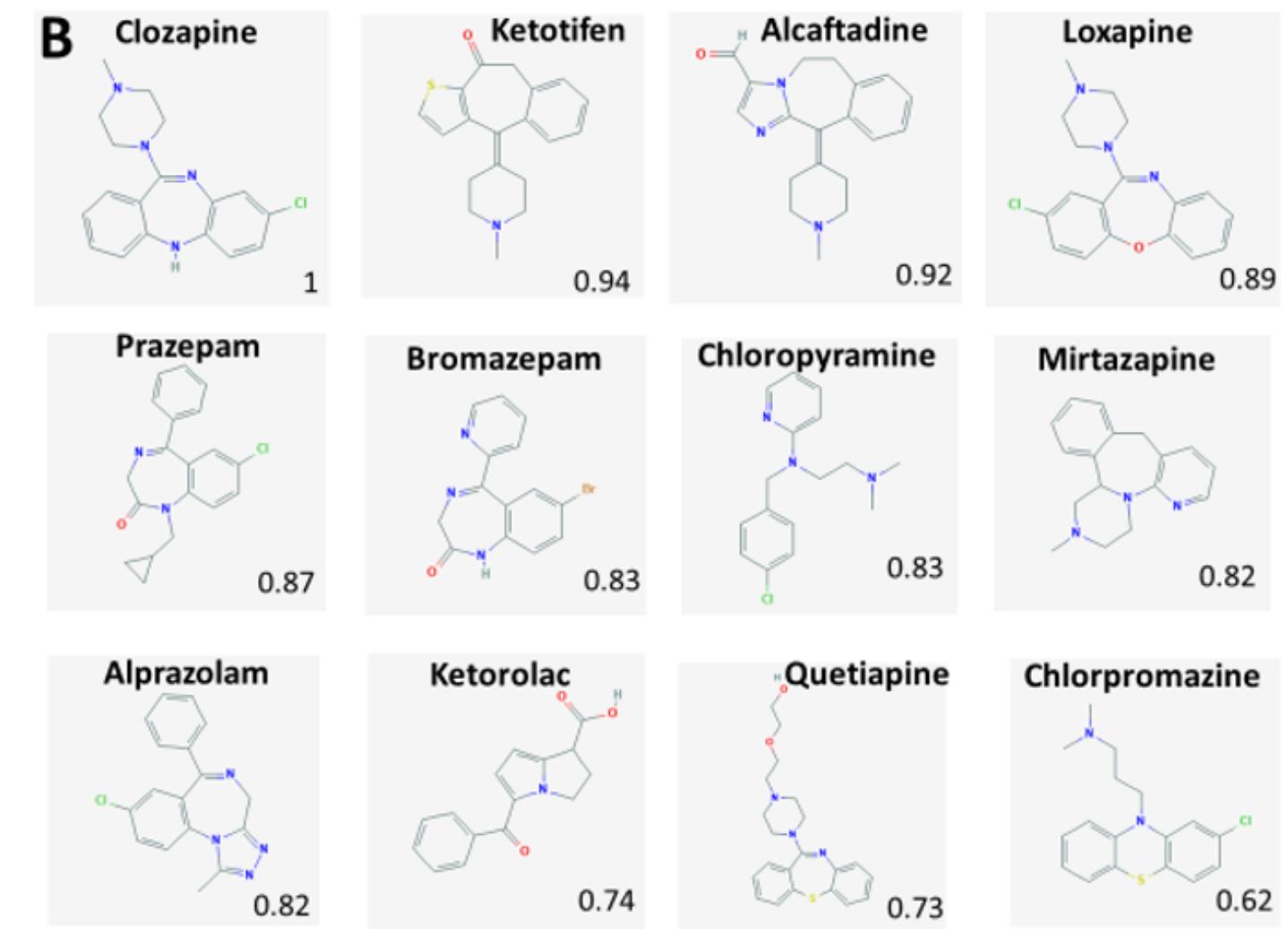
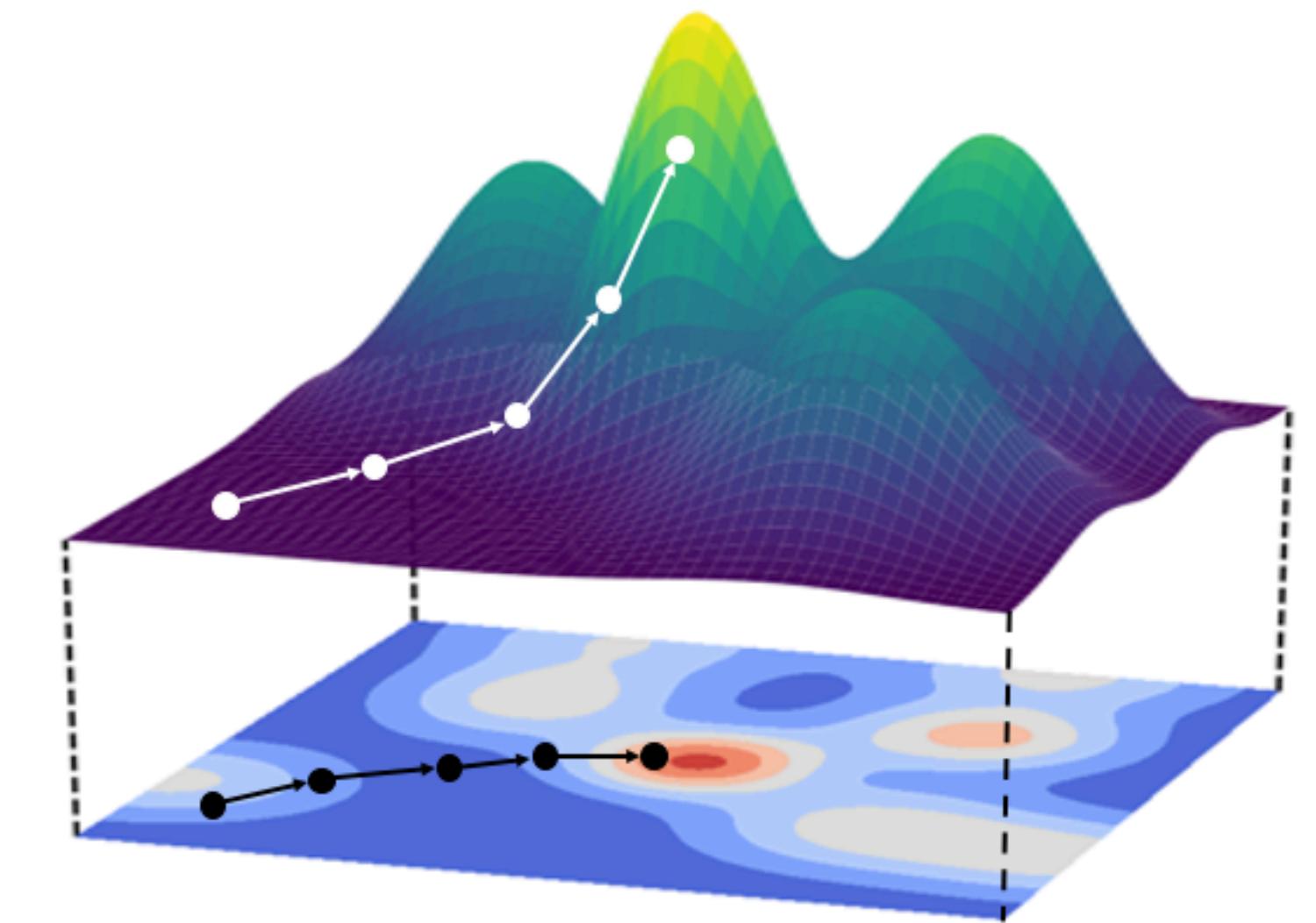
- Search (drug) molecule with desired properties



Nearest molecules (new) search?

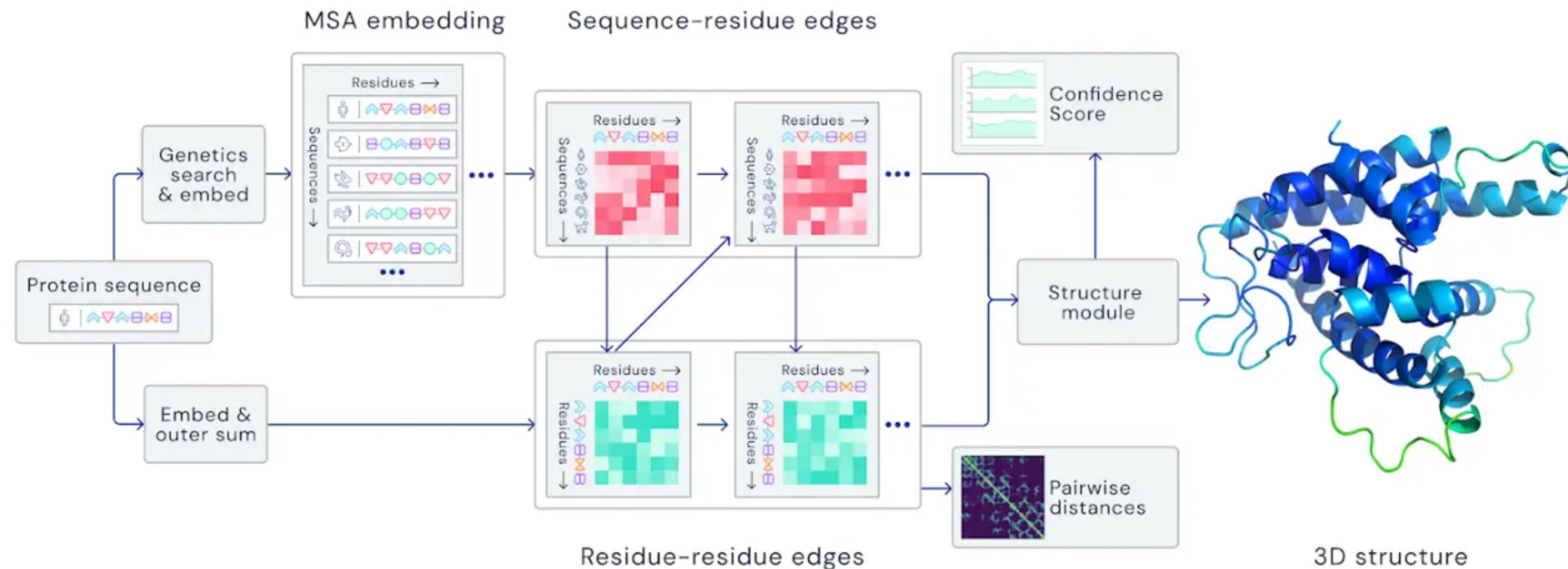


Drugs  
Recon2  
Fluorophores  
Nat Prods  
ZINC (6M)

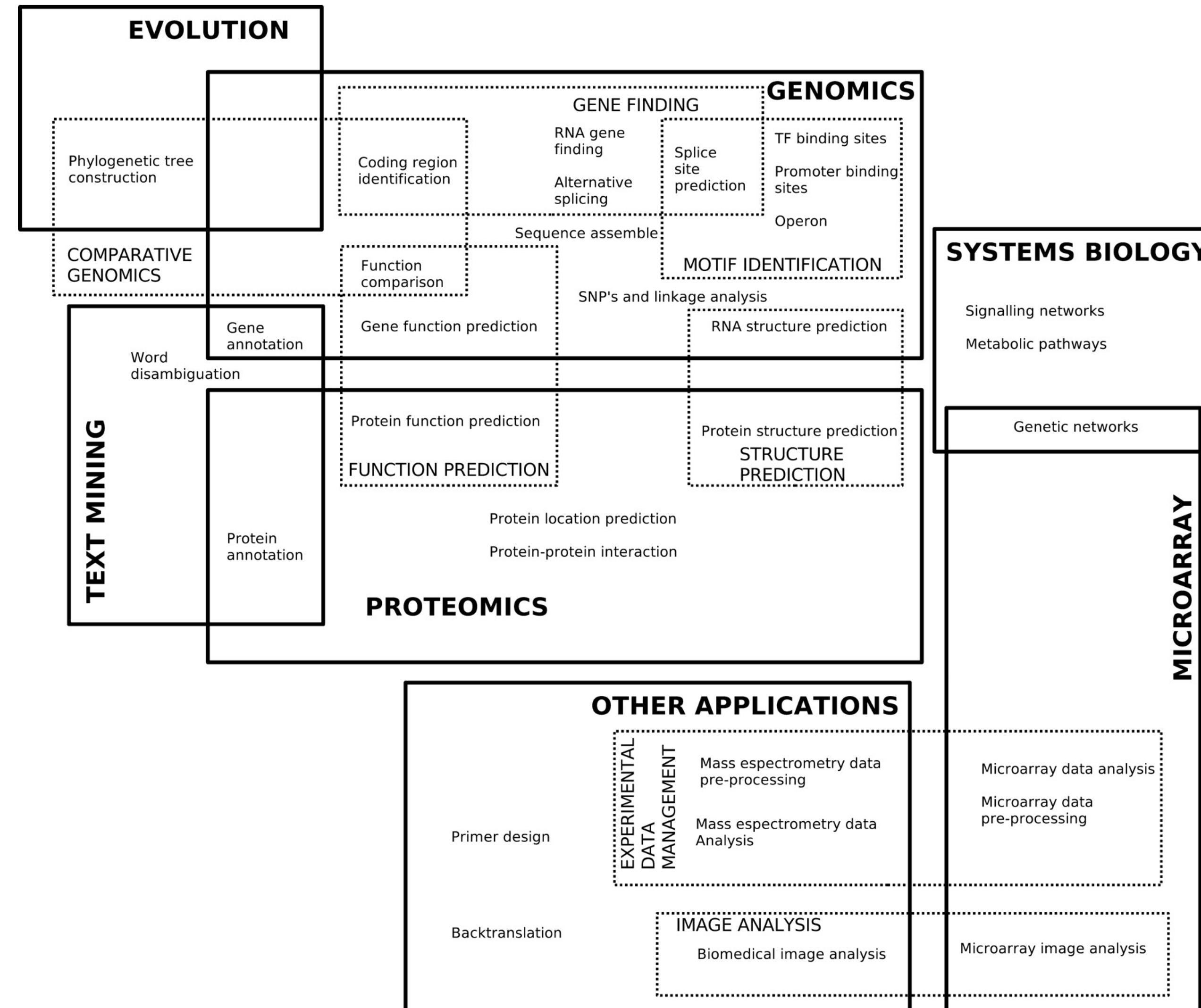


# Protein-folding

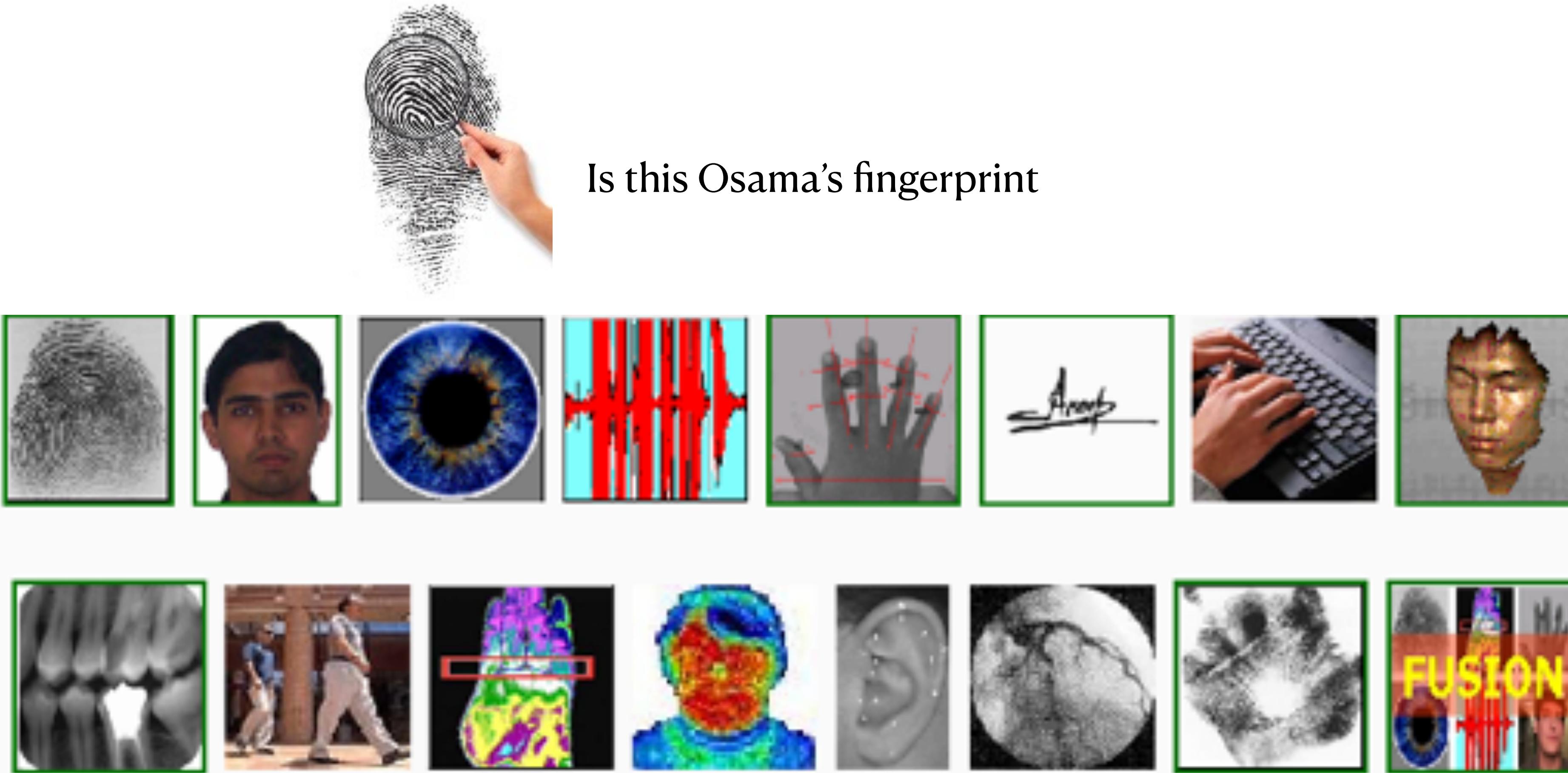
- Prediction of protein structure
  - ▶ CASP: <https://predictioncenter.org/casp15/index.cgi>
  - ▶ AlphaFold2 (DeepMind)- CASP-14, 2020



# Bioinformatics

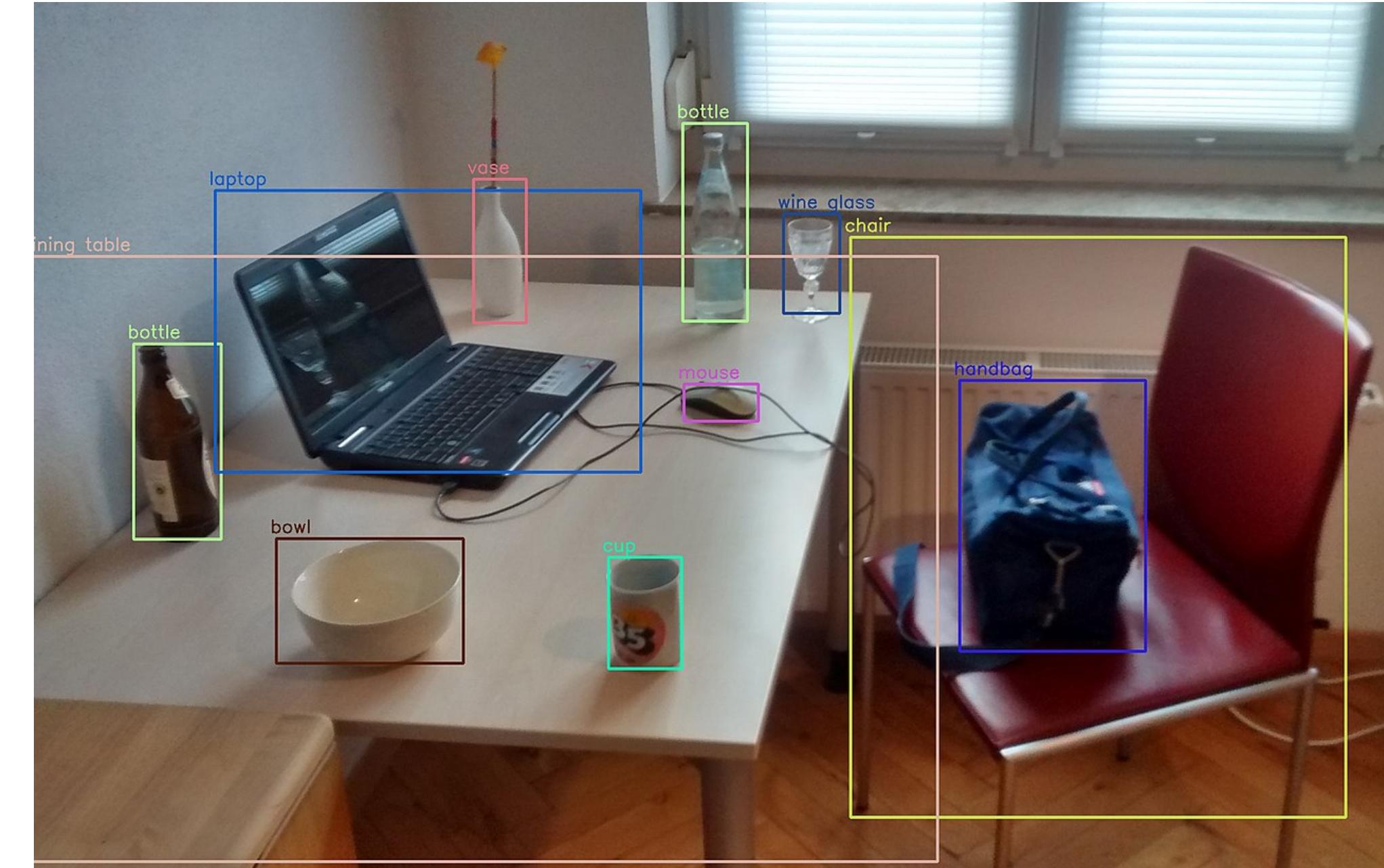
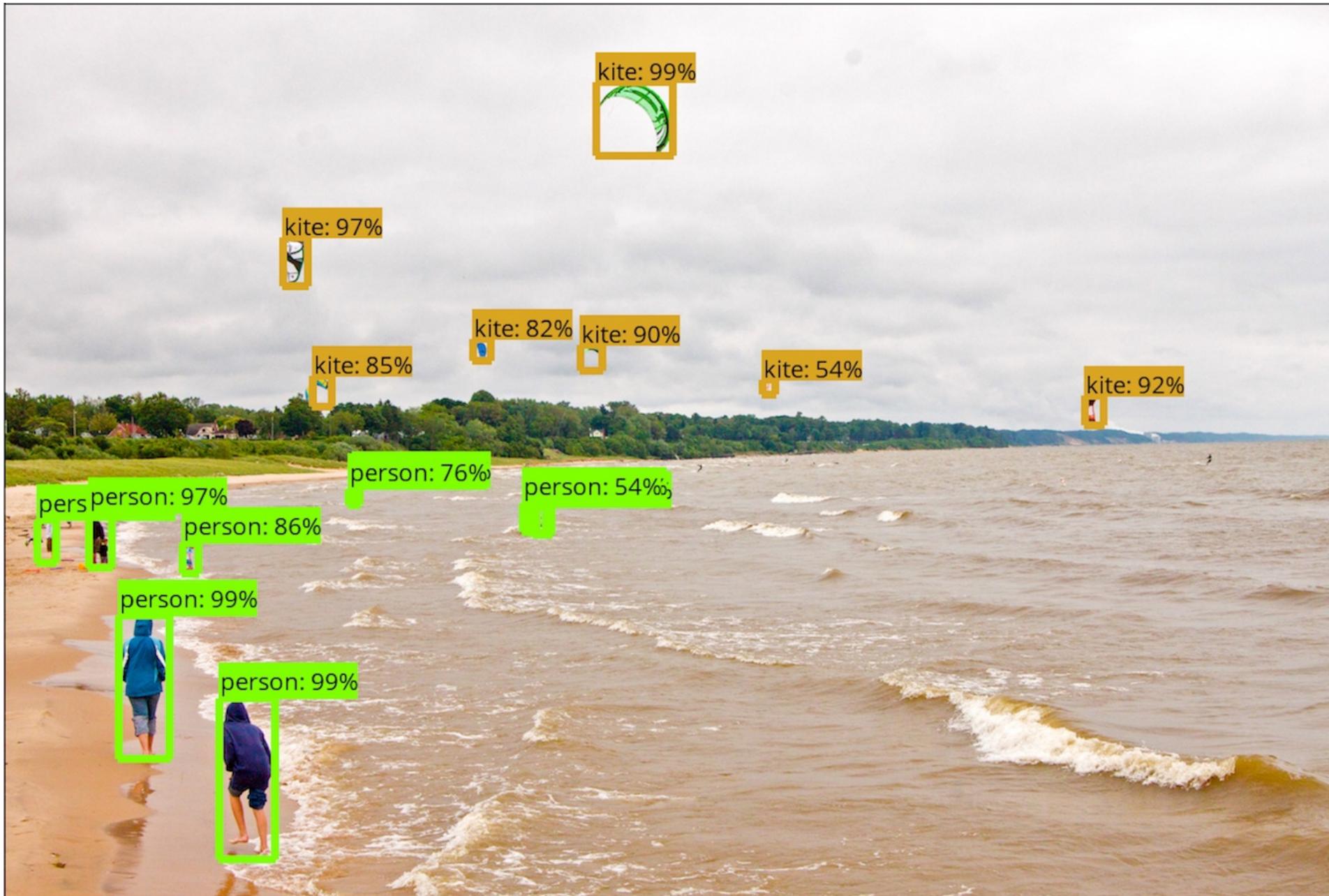


# Biometric recognition



Multimodal biometric

# Object detection



Started in 2005,  
4-object class



Started in 2010, 1000-object class

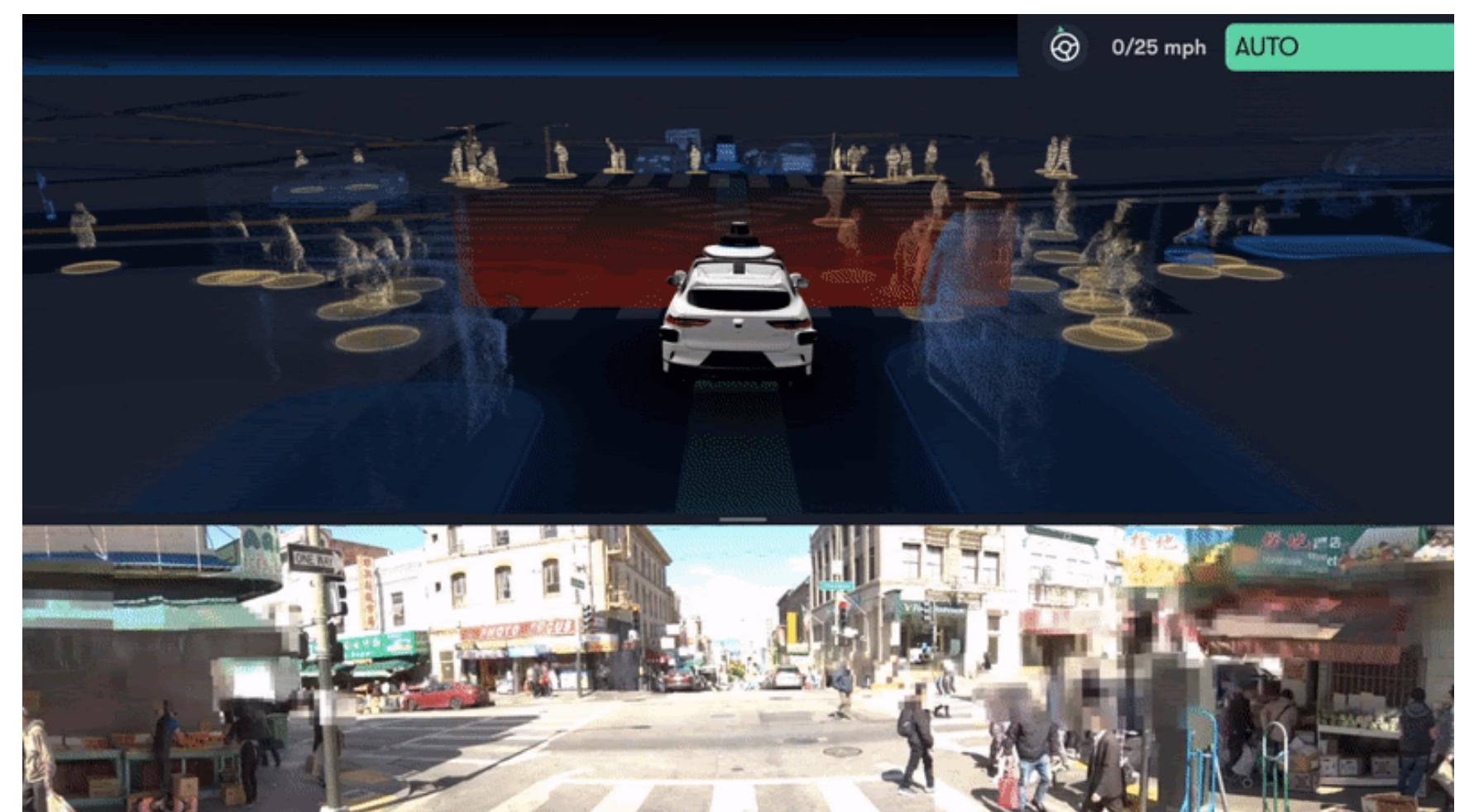


# Self driving car

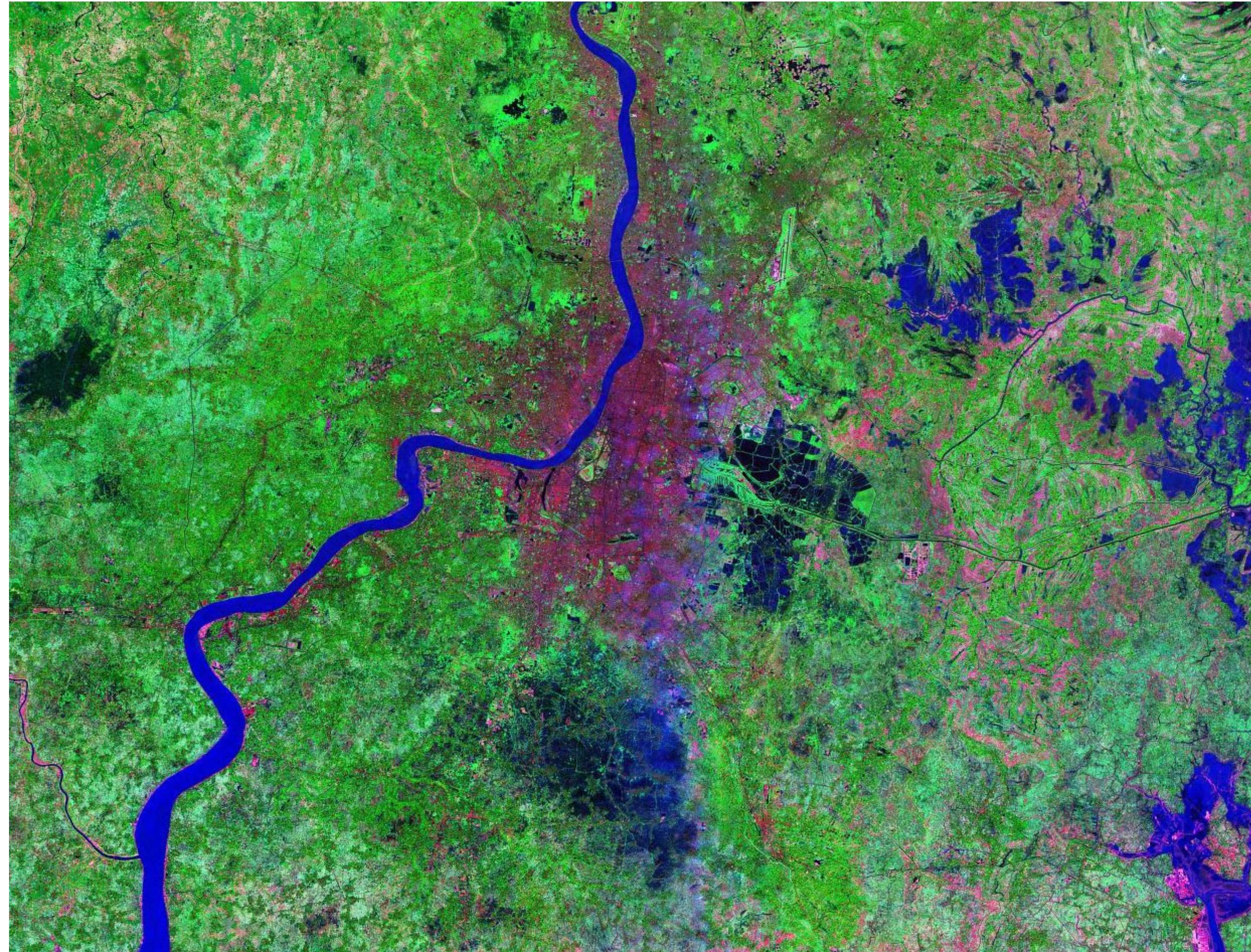
- DARPA grand challenge
  - ▶ 2005- Stanley



- Every car company jump into self driving car
  - ▶ Tata, BMW, GM, Nissan, Mercedes-Benz, etc.
- Big tech company
  - ▶ Google (Waymo), Apple, Uber, Tesla etc.



# Satellite image analysis



Where are water body, concrete, and green area?

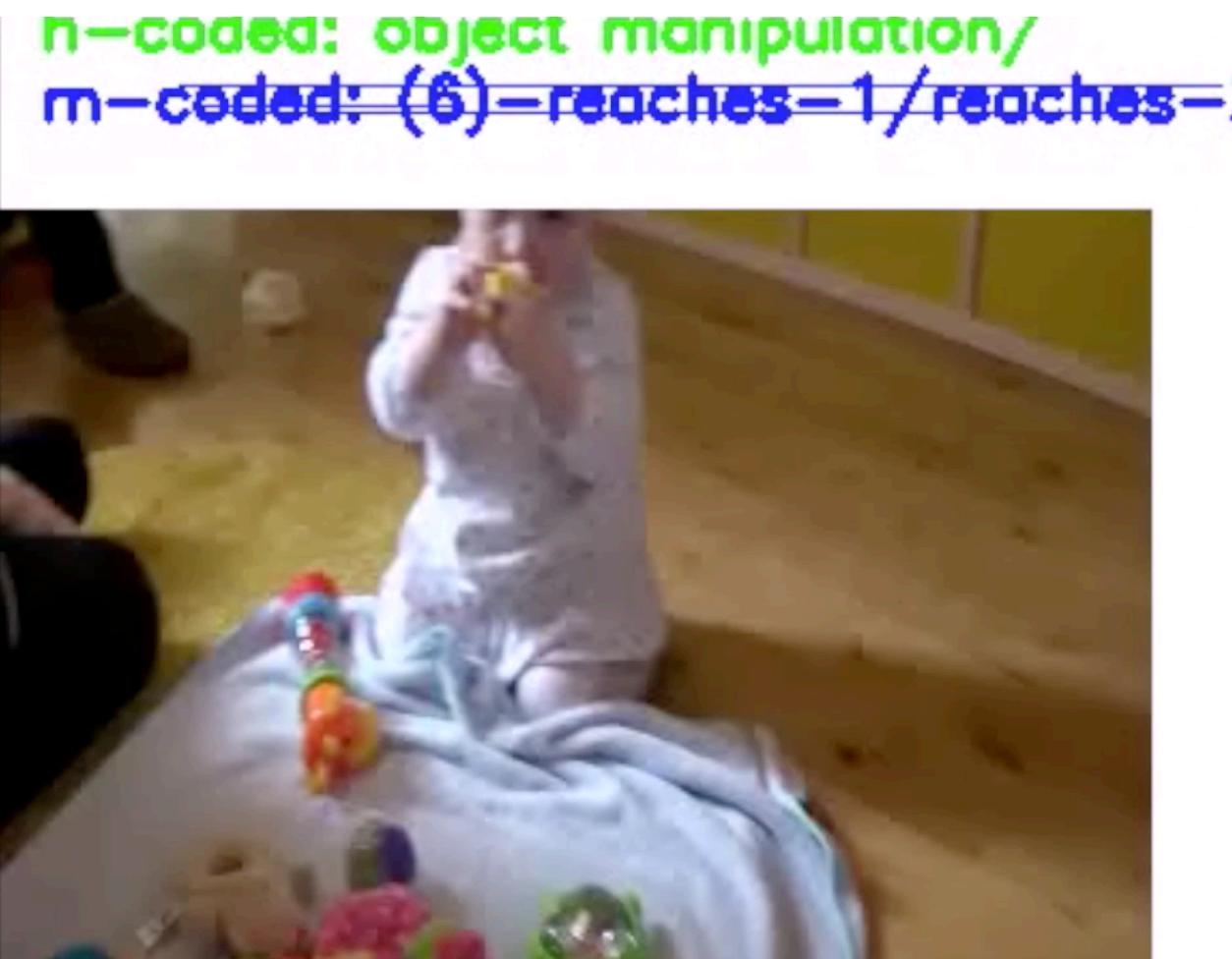
# AlphaGo

- Computer program defeat professional human Go player
  - ▶ Beat
  - ▶ Beat world no 1 Go player Ke Jio, 2017



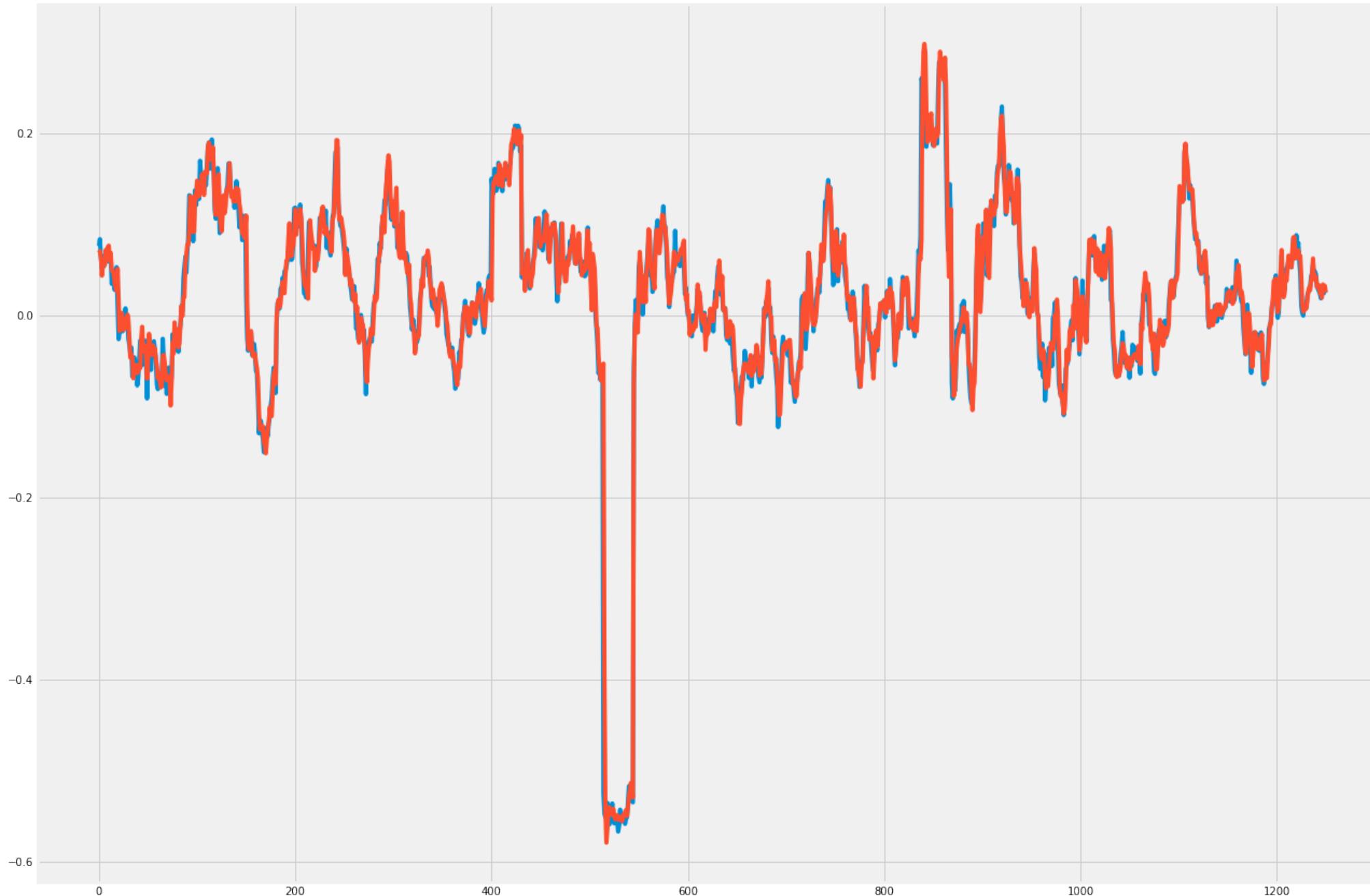
Image: DeepMind  
Video: YouTube

# Human action detection



# Financial forecasting

- Stock market prediction

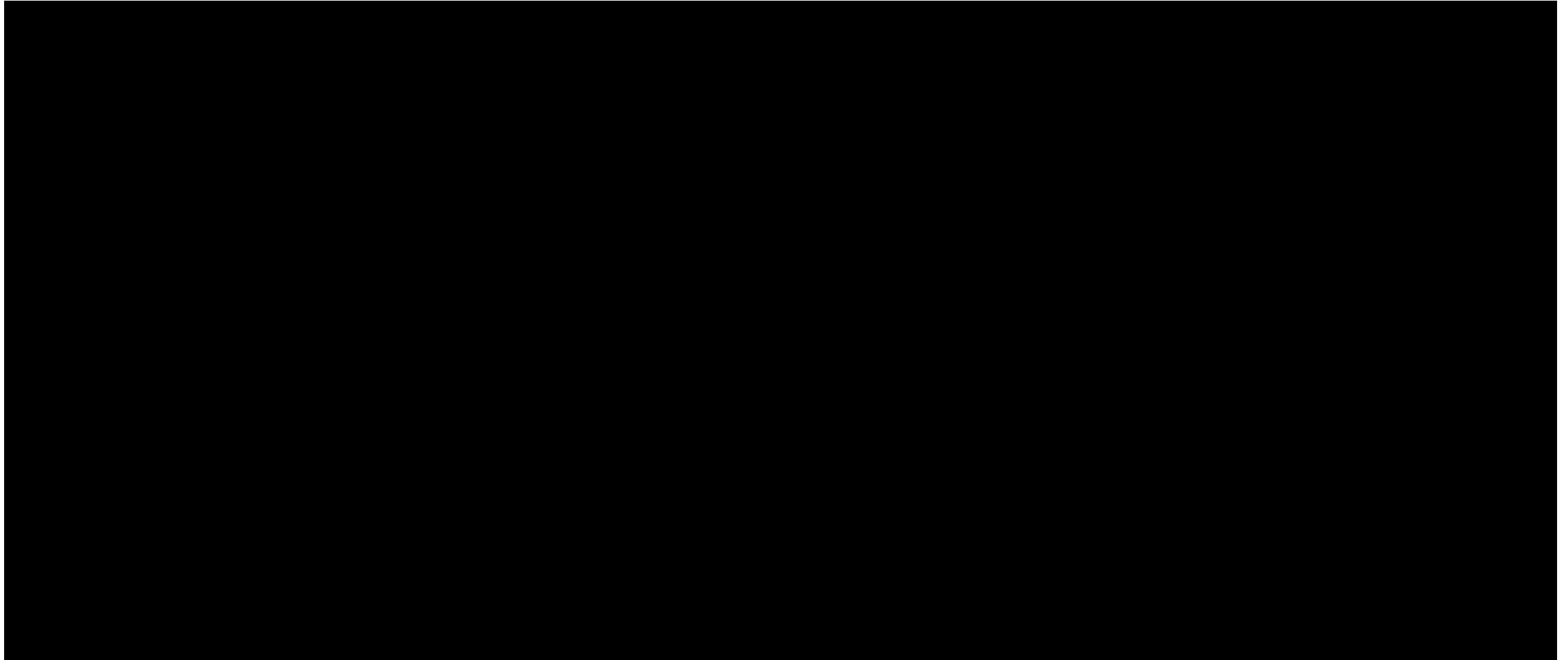


- Unwanted bank transaction (fraud) detection

# Application of ML

- Applications
  - ▶ Image processing
  - ▶ Computer vision
  - ▶ Speech recognition
  - ▶ Natural language processing
  - ▶ Optical character recognition
  - ▶ Financial forecast
  - ▶ Medical diagnosis
  - ▶ ...

# What is ML?



Video: <https://www.youtube.com/watch?v=QHH3jSeDBLo>

# What is machine learning?

- Extract (learn) meaningful information from the examples (training) and answer the query for unseen examples
- Specific task
- How can we allow computer to extract meaningful information from the examples?
  - ▶ Design general rules
  - ▶ Development of algorithms

# Inference

## deductive vs inductive

- Deductive
  - ▶ Process of reasoning from one or more statements (premises) to reach a logical conclusion
- Example-1:
  - ▶ Premises-1: All RKMVERI students are excellent
  - ▶ Premises-2: Amol study in the RKMVERI
  - ▶ Conclusion: Amol is an excellent student
- In general:
  - ▶ If  $A \implies B$  and  $B \implies C$
  - ▶ Then  $A \implies C$
- If premises are correct, then the conclusion is certain

# Inference

## deductive vs inductive

- **Inductive**
  - ▶ Method of reasoning in which a body of observation is synthesised to come up with a general principle
- Example-1:
  - ▶ Very often, we drop lots of things
  - ▶ All the times, the things fall downwards, but not upwards.
  - ▶ We can conclude that, if we drop things, likely they always fall downwards
- The truth of the conclusion is probable, based on the evidence given so far
- So, **conclusion is not certain!**
  - ▶ Example?

# What is machine learning?

- Extract (learn) meaningful information from the examples (training) and answer the query for unseen examples
- Specific task
- How can we allow computer to extract meaningful information from the examples?
  - ▶ Design general rules
  - ▶ Development of algorithms
- Automate the process of **inductive inference**

# Course logistics

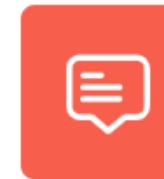
# Course page in xlms

## Machine Learning

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### ▼ General

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FILE

[Suggested reading](#)

[Mark as done](#)

### ▼ 7 February - 13 February

<https://xlms.rkmvu.ac.in/course/view.php?id=47>

# Prerequisites

- Mathematics
  - ▶ Linear Algebra, Multivariate Calculus, Basis Optimisation and Basic probability
  - ▶ No worries, we will touch some background when we need
- Computer programming: Any one from C/C++/**Python (recommended for the class project and assignments)**/MATLAB/Octave
- Basic concept in Algorithms and Data Structure

# Linear Algebra

- Vector space
  - ▶ Definition, Basis, Dimension, Eigen value and Eigen vectors etc.
- Matrix
  - ▶ Addition, Multiplication, Trace, Inverse etc.
  - ▶ Positive definite matrices, Singular value decomposition etc.

# Multivariate Calculus

- Derivative, Partial derivative, Taylor series expansion, Chain rules etc.

# Basic Optimisation

- Convex set, Convex hull, Convex function
- Gradient of a function, Hessian
- Constrained and Unconstrained optimisation problem, Optimality condition

# Probability

- Definition, Random variables, Distribution function and their different variants
- Conditional probability, Independence, Expectation, Variance, Moments, Entropy
- Law of large numbers, Central limit theorem

# Evaluation

- Mid-term: 15%
- End-term: 50%
- Assignments: 15%
- Project: 20%

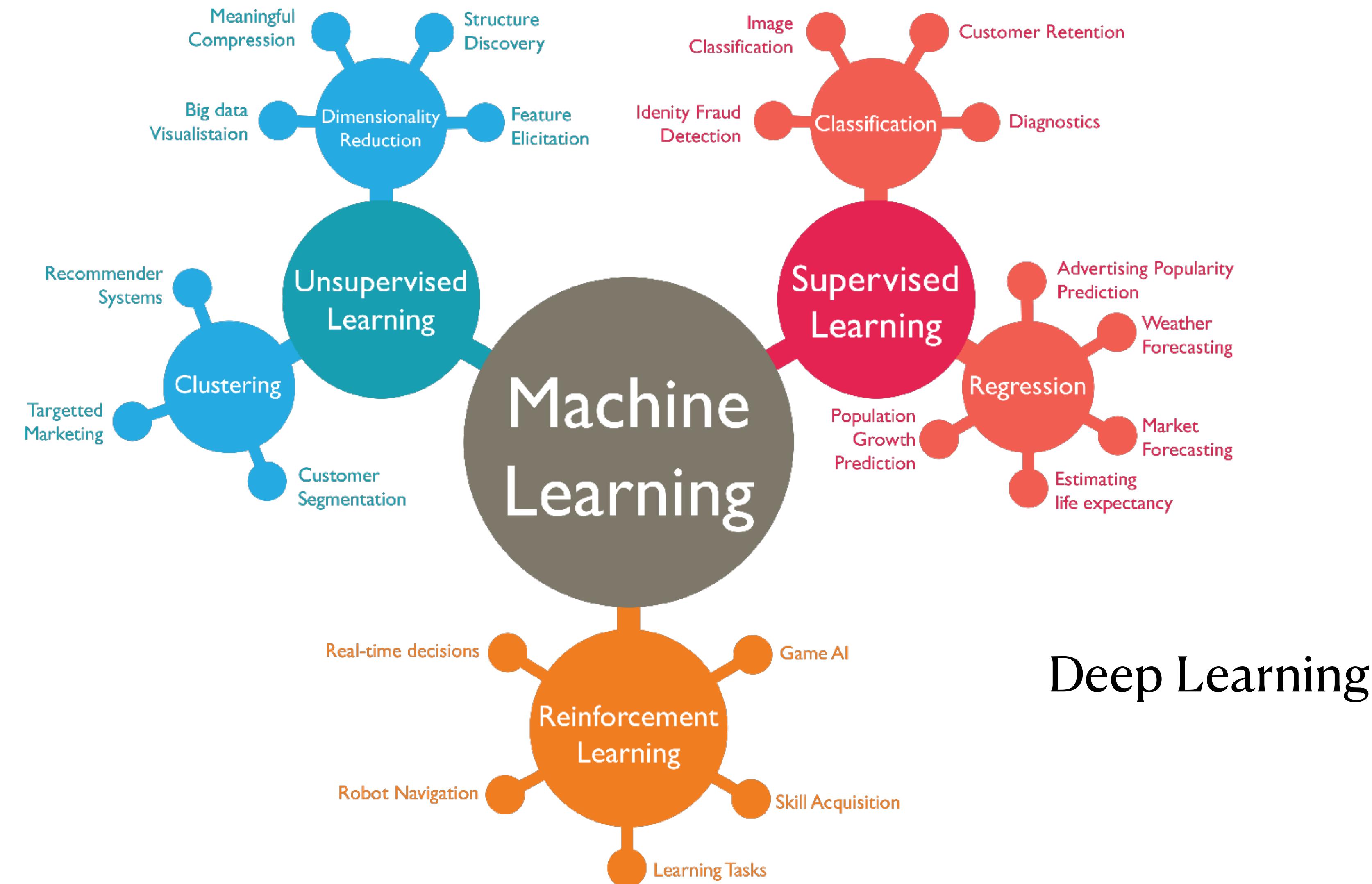
# Assignments

- Mostly implementation of different ML algorithms
  - ▶ **Python (preferable)**/C/C++/MATLAB/Octave
- There might be one-two theoretical assignments
- Submission deadline is strict and weightage reduce to **40%/day** after the deadline
  - ▶ We will consider **11.59PM** as our day end

# Projects

- Can be done in a group (max two students)
- Define your own project
- Submit a one page project proposal- within fixed time (first six weeks) 21-03-2023?
- Finished the work within the time-line
- Report submission
  - ▶ Submission deadline: **5th June, 2023**
  - ▶ We will consider 11:59PM as our day end
- Final presentation
  - ▶ 20 min (divided into group members)/**poster presentation**
  - ▶ **7th June, 2023**

# Course syllabus



# Course materials

- Books: We will follow multiple books for different topics
  - ▶ Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar, Foundations of Machine Learning, MIT Press, Second Edition, 2018
  - ▶ Shai Shalev-Shwartz and Shai Ben-David, Understanding Machine Learning: From Theory to Algorithms, Cambridge University Press, 2014
  - ▶ Christopher M. Bishop, Pattern Recognition and Machine Learning, Springer, 2006
  - ▶ Kevin Patrick Murphy, Machine Learning: a Probabilistic Perspective, MIT Press, 2012
  - ▶ Trevor Hastie, Robert Tibshirani and Martin Wainwright, Statistical Learning with Sparsity: The Lasso and Generalizations, CRC Press, 2015
  - ▶ R. O. Duda, P. E. Hart and D. G. Stork, Pattern Classification, 2nd ed., Wiley, New York, 2000
  - ▶ S. Theodoridis and K. Koutroumbas, Pattern Recognition, Academic Press, San Diego, 1999
  - ▶ K. Fukunaga, Introduction to Statistical Pattern Recognition, 2nd ed., Academic Press, New York, 1990
  - ▶ L. Devroye, L. Gyorfi and G. Lugosi, A probabilistic Theory of Pattern Recognition, Springer, 1996
  - ▶ I. Goodfellow, Y Bengio, and A. Courville, Deep Learning, MIT Press, 2016

# Academic ethics

- Your grade should reflect your own work
- Copying or paraphrasing someone's work (code included), or permitting your own work to be copied or paraphrased, even if only in part, is **strictly forbidden**, and will result in an automatic grade of **zero** for the entire assignment or exam in which the copying or paraphrasing was done.
- So, **ask yourself** before copying from others
- If you are going to have trouble completing an assignment, talk to the instructor and TA before due date

# Data

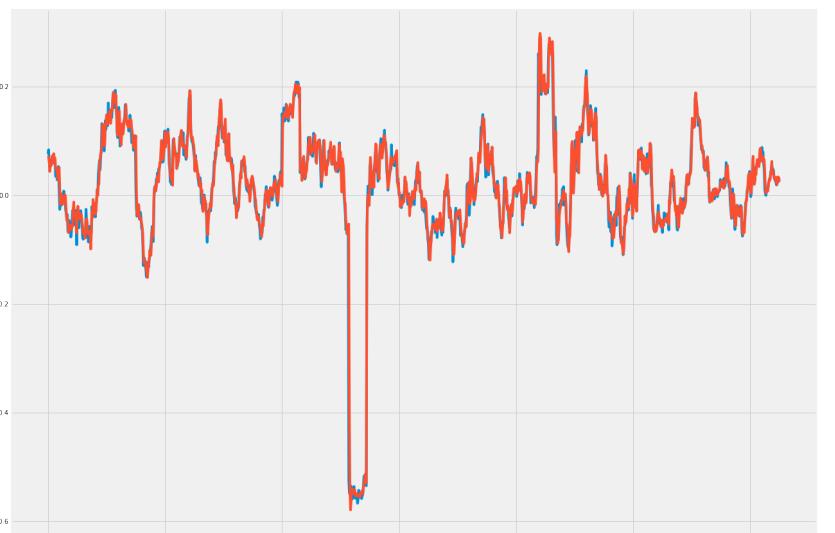
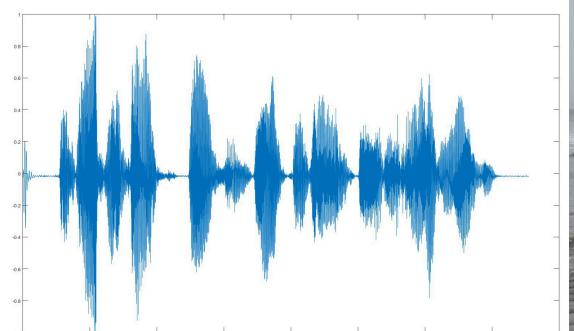
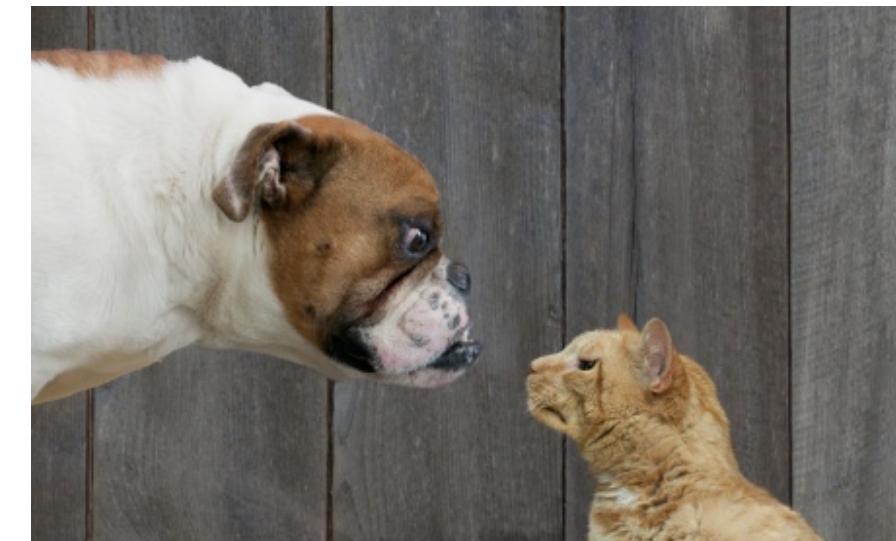
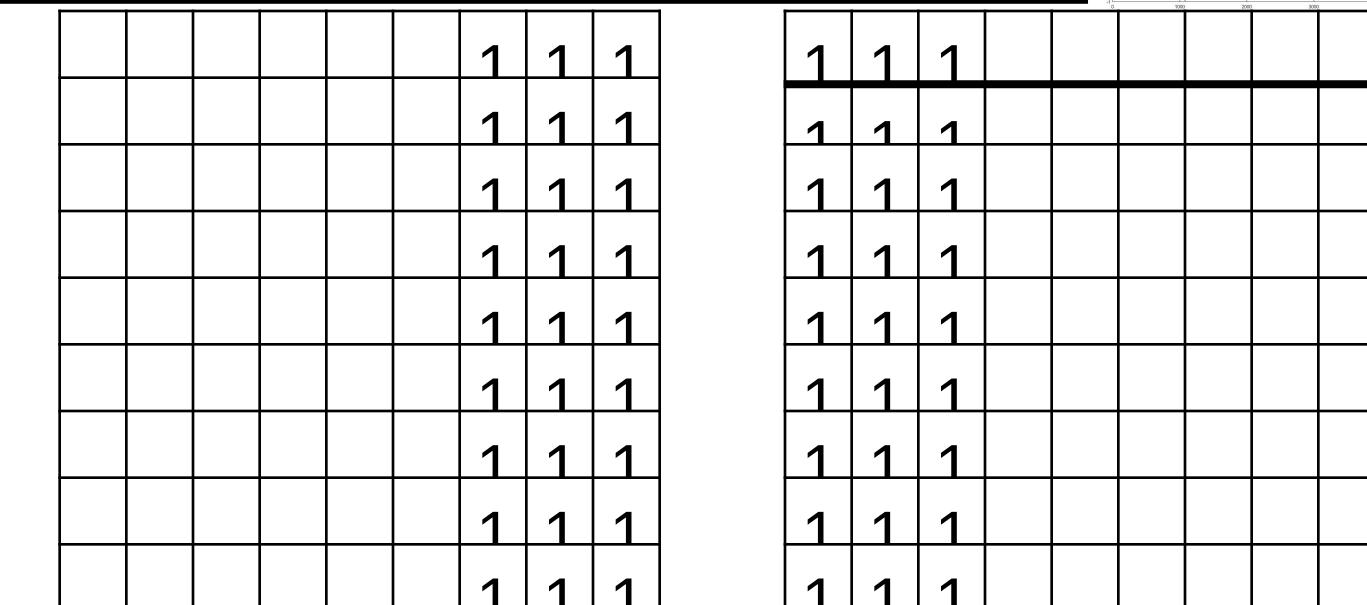
# Recap

- What is ML?
- Some applications of ML
- Deductive vs Inductive inference

# Data

- Different types of data
  - ▶ Text, Audio, Images, Videos, etc.
- Representation
  - ▶ Example:
    - Hand-written digit recognition
    - Cat vs Dog
    - Stock (particular) price prediction
  - ▶ Feature
    - Any distinct aspect, quality or characteristic
      - Ex. numeric (height)
      - Combination of  $d$  features is  $d$ -dims column vector, we will call it as **feature vector**
      - $d$ -dims space defined by the feature vectors is called **feature space**
      - Data are represented as a **point** in the feature space

Hello everyone, today is our second ML class and we will start from a motivating example.

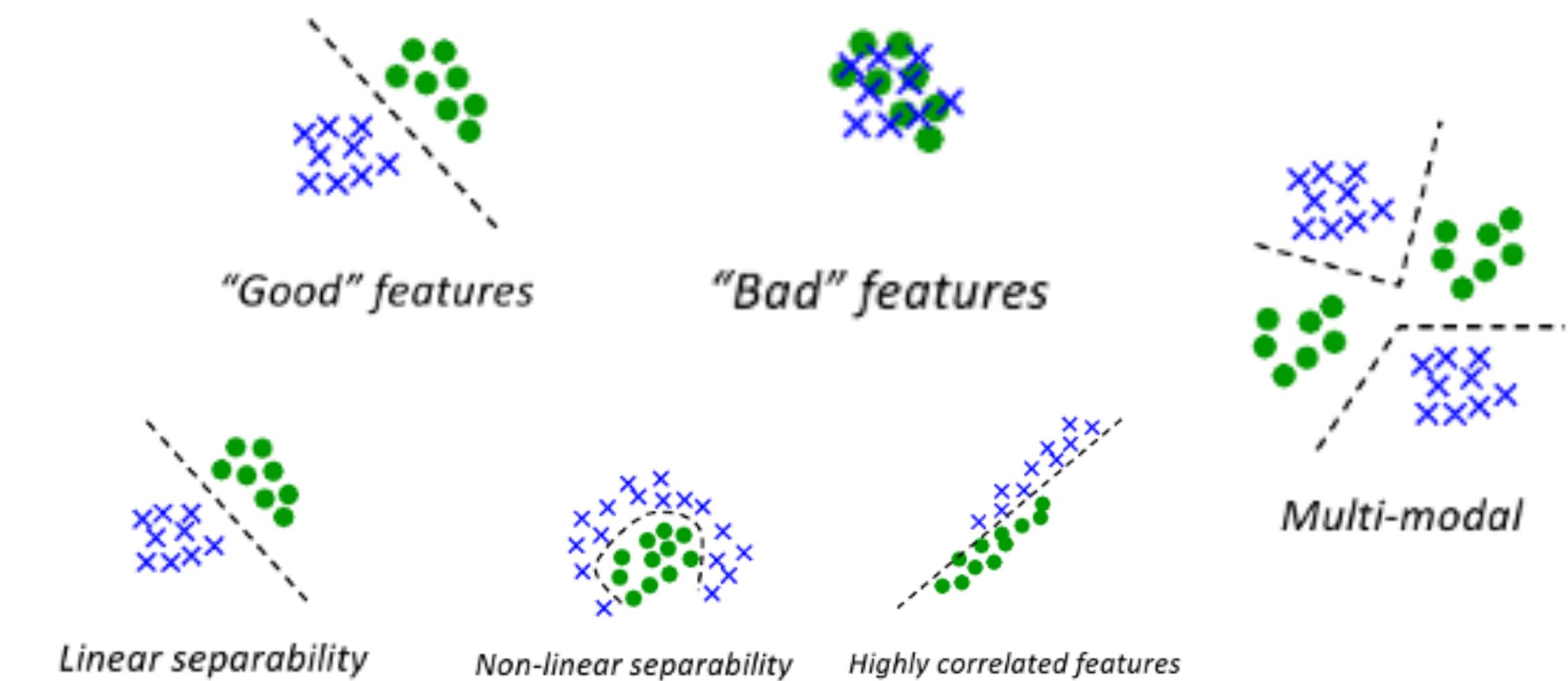
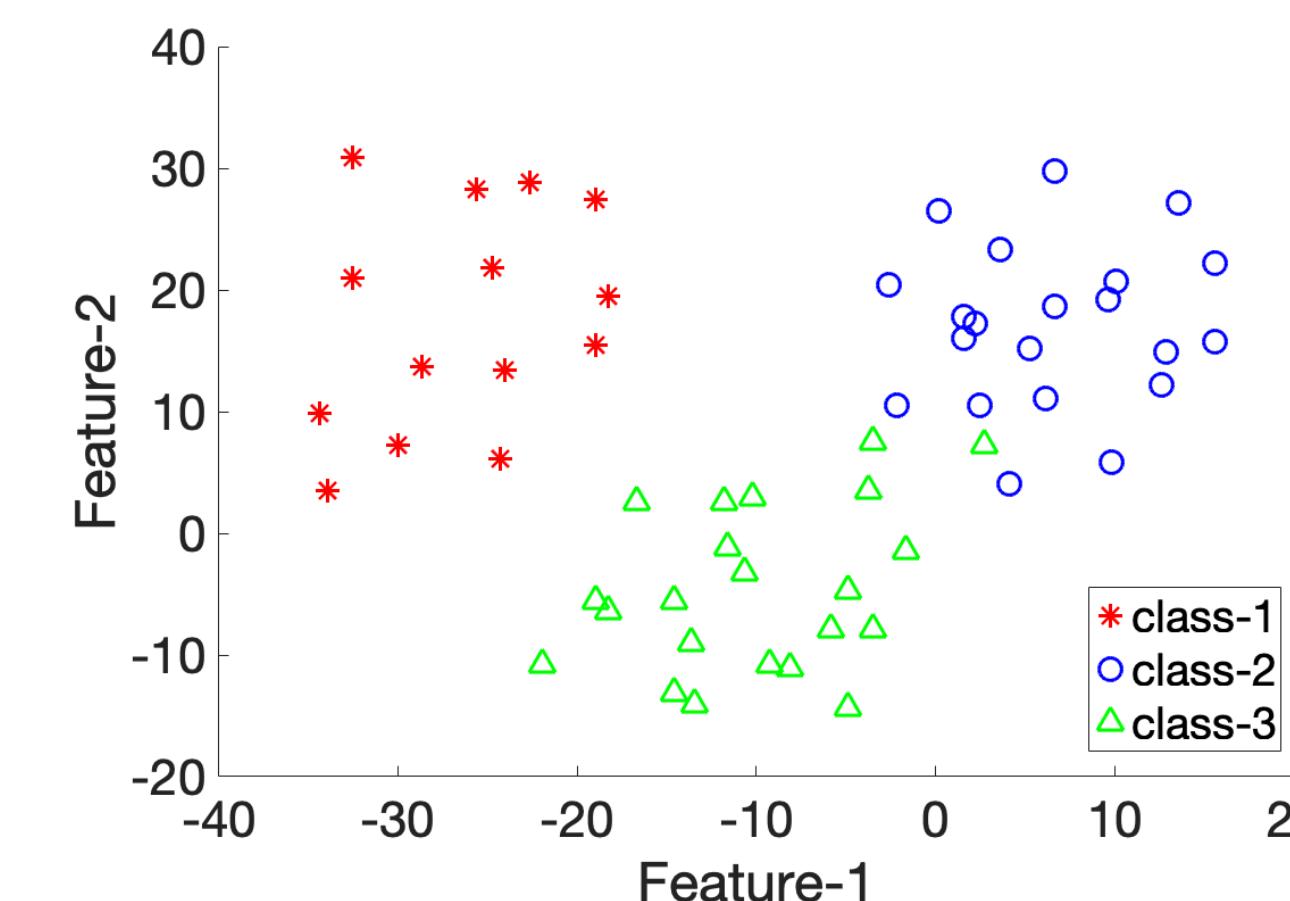


Images: Kaggle, Stackexchange  
Video: LuCiD

# Data (cont.)

- Feature
  - ▶ Any distinct aspect, quality or characteristic  
Ex. numeric (height)
  - ▶ Combination of  $d$  features is  $d$ -dims column vector, we will call it as **feature vector**
  - ▶  $d$ -dims space defined by the feature vectors is called **feature space**
  - ▶ Data are represented as a **point** in the feature space ( $\mathcal{X}$ )

$$X = \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^d \end{bmatrix}$$



# Data (cont.)

- Syntax:
  - ▶ Data:  $(X_i, Y_i); i = 1, \dots, n$ 
    - Where  $X_i$  is the  $i^{th}$  data representation (**features**) and  $X_i \in R^d$
    - $Y_i$  is the  $i^{th}$  data label (class) and  $Y_i \in R$
  - ▶ Let  $f$  be a model/algorithm for a particular task
  - ▶  $\bar{Y}_i$  is the model/algorithm output:  $\bar{Y}_i := f(X_i)$
  - ▶ How do you evaluate your model/algorithm?
    - Loss:  $\ell(X_i, Y_i, \bar{Y}_i)$

# Data similarity

- How do we compare two objects?



-



=

?

1

-

5

=

?

# Data similarity (cont.)

- Why we need comparison?

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5
6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7	7
8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8	8
9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9	9

1  
?  
5  
0  
?

# Similarity measure

- Distance between two points  $X_1 \in R^d$  and  $X_2 \in R^d$ :  $\mathcal{D}(X_1, X_2)$ ?
  - ▶  $\mathcal{D}(X_1, X_2)$  considered a metric if it satisfies the following properties:
    - $\mathcal{D}(X_1, X_2) \geq 0$ ,  $\mathcal{D}(X_1, X_2) = 0$  iff  $X_1 = X_2$
    - $\mathcal{D}(X_1, X_2) = \mathcal{D}(X_2, X_1)$
    - $\mathcal{D}(X_1, X_3) \leq \mathcal{D}(X_1, X_2) + \mathcal{D}(X_2, X_3)$
- Commonly used metrics are:
  - ▶ **Minkowski** distance/metric of order  $p$ :

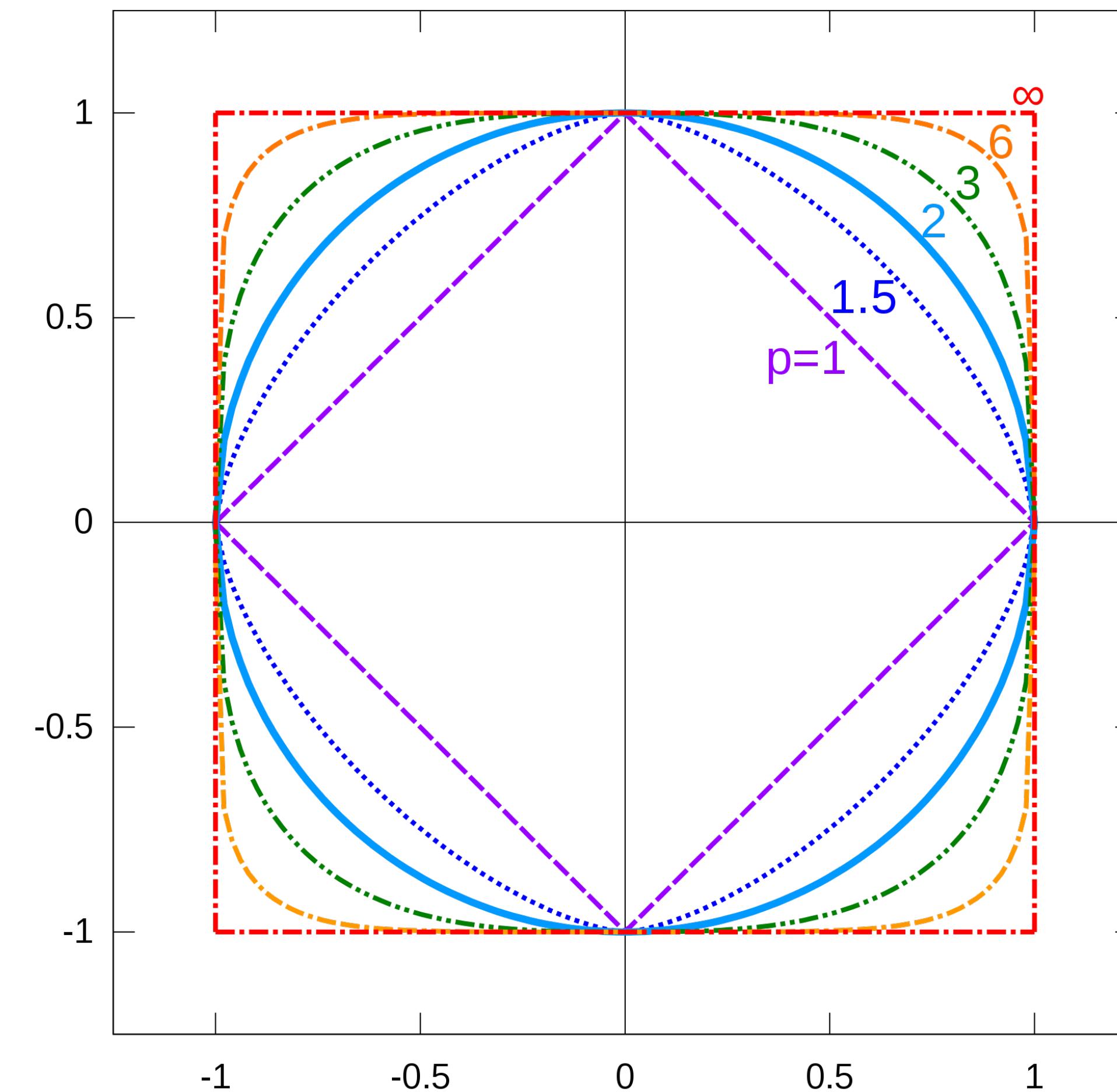
- $$- \mathcal{D}^p(X_1, X_2) = \left\{ \sum_{i=1}^d |x_1^i - x_2^i|^p \right\}^{\frac{1}{p}}$$

- ▶ **Manhattan** or city-block distance

- $$- \mathcal{D}(X_1, X_2) = \sum_{i=1}^d |x_1^i - x_2^i|$$

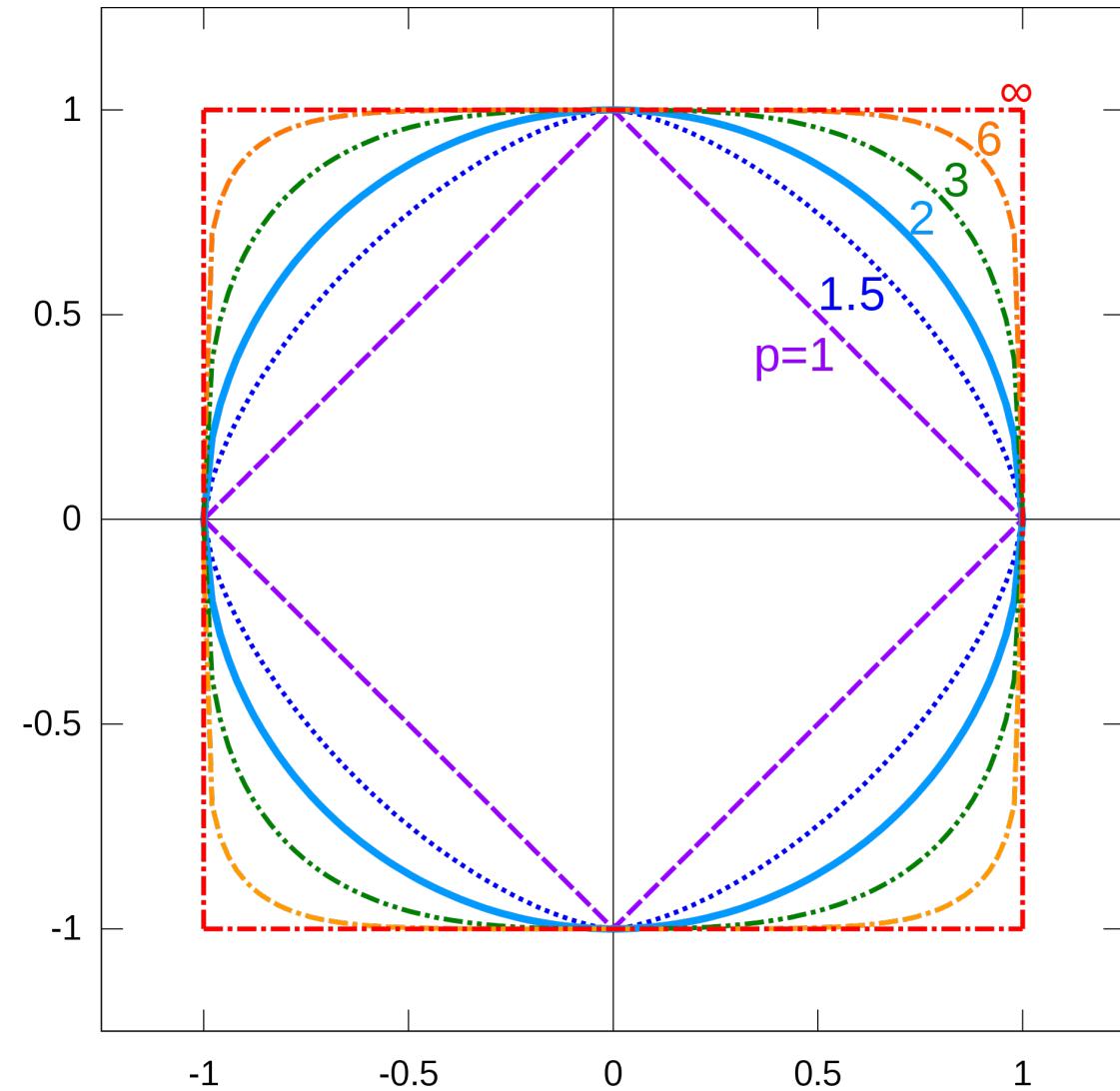
# Similarity measure (cont.)

- Commonly used metrics are:
  - Minkowski distance/metric of order  $p$ :
    - $\mathcal{D}^p(X_1, X_2) = \left\{ \sum_{i=1}^d |x_1^i - x_2^i|^p \right\}^{\frac{1}{p}}$
  - Manhattan or city-block distance:
    - $\mathcal{D}(X_1, X_2) = \sum_{i=1}^d |x_1^i - x_2^i|$
  - Euclidean distance:
    - $\mathcal{D}(X_1, X_2) = \left\{ \sum_{i=1}^d |x_1^i - x_2^i|^2 \right\}^{\frac{1}{2}}$
  - Chebyshev distance:
    - $\mathcal{D}(X_1, X_2) = \max_i \{ |x_1^i - x_2^i| \}$



# Homework-1

- Can you draw this type of figure in 2D & 3D?
  - ▶ Use **Minkowski** distance for  $p = -2, -1, 0, 1, 1.5, 2, 3, 6, \infty$
  - ▶ Draw all the points within the the intervals has unit distance from the origin for all  $p$ 's:
    - 2D:  $x \in [-1, 1]$  and  $y \in [-1, 1]$
    - 3D:  $x \in [-1, 1]; y \in [-1, 1]$  and  $z \in [-1, 1]$



# Which data to evaluate the model?

- Data partition/division:
  - ▶ Training, Validation and Testing
    - Training- 50%
    - Validation - 20%
    - Testing - 30%

# Which data to evaluate the model?

- Model:
  - ▶ Let  $f$  be a model/algorithm for a particular task
    - Example: Regression  $f: X \rightarrow \mathbf{R}$
    - $f(X) = w^0 + w^T X$

Model parameters:  $w^0, w = \begin{bmatrix} w^1 \\ w^2 \\ \vdots \\ w^d \end{bmatrix}$

# Which data to evaluate the model?

- Data partition/division:
  - ▶ Training, Validation and Testing
    - Training- 50%
    - Validation - 20%
    - Testing - 30%

# Homework-2

- Create a random dataset in  $\mathbf{R}^{100}$  of size 50000 with random class labels from {1,2,3,4}. Now partition the data into the following subsets:
  - ▶ Training- 50%
  - ▶ Validation - 20%
  - ▶ Testing - 30%
  - ▶ Plot (bar) the frequency of each class label for each subset.

# How do you evaluate your model/algorithm?

- How do you evaluate your model/algorithm?
  - ▶ Accuracy (%) - classification
  - ▶ Mean square error (MSE) - regression
  - ▶ ...