

# AI for Astrophysics: Introduction to Machine Learning

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**Doctoral course - ED AAIF  
2024/2025**

# Provisional planning

**Day 1 :** Introduction to AI and Machine Learning, simple algorithms hands-on

**Day 2 and 3 :** Artificial Neural Networks presentation, simple guided implementation, Multi-Layer Perceptron principles and usage

**Day 3 and 4 :** Deep Learning and advanced neural networks architectures. Frameworks hands-on and application to image based dataset.

**Day 5 :** Advanced deep learning tasks and network structure.  
Application to object detection, image generation, etc.

- Programming language poll: C, Fortran, Python ?
- Programming proficiency poll

# Lessons materials

Slides, exercises, codes, corrections and datasets are **available on GitHub** and will be updated regularly:

[http://github.com/Deyht/AI\\_astro\\_ED\\_AAIF](http://github.com/Deyht/AI_astro_ED_AAIF)

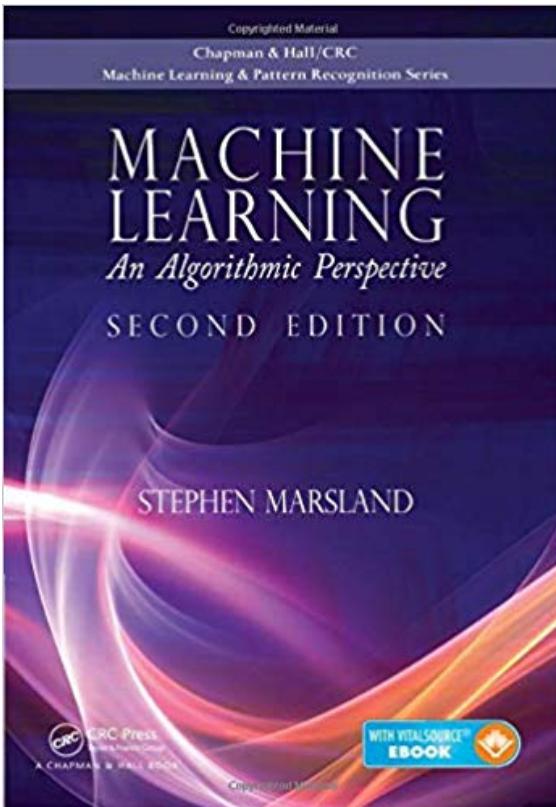
*git clone https://github.com/Deyht/AI\_astro\_ED\_AAIF  
git pull*

Or download the repository in zip file

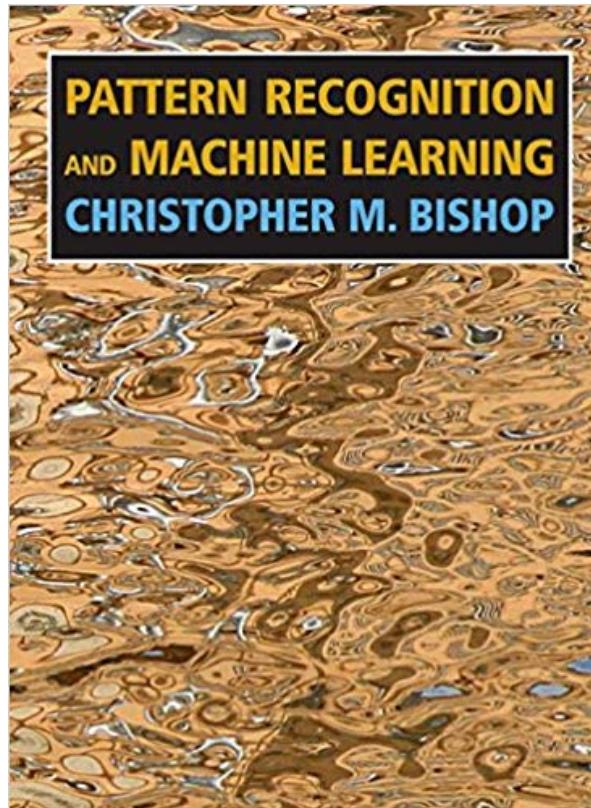
Avoid losing your work on forced pull updates by copying all files from the cloned repository into a working directory!

**Do not copy and past content from git-hub pages (lead to format errors and python scripts not running).**

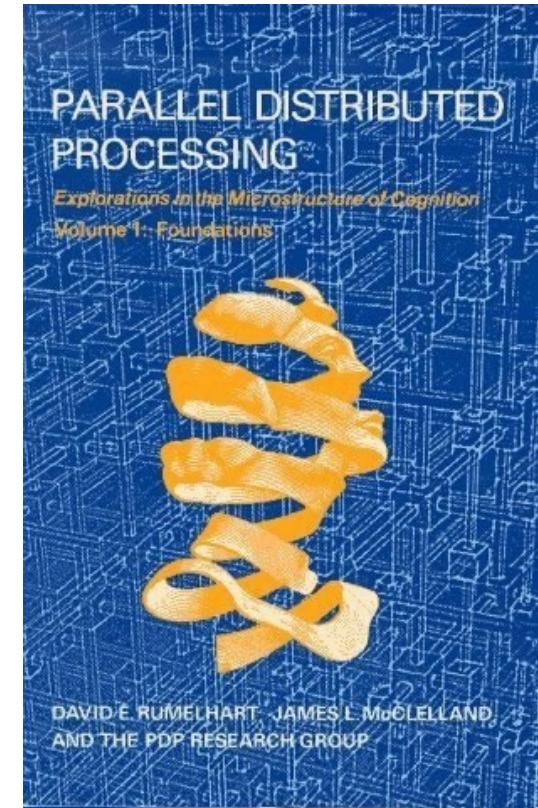
# Some learning materials and references



Stephen Marsland.  
**Machine Learning an  
Algorithmic Perspective.**  
Chapman and Hall/Crc,  
2015



Christopher M. Bishop.  
**Pattern Recognition and  
Machine Learning.**  
Springer, 2011



David E. Rumelhart et al.  
**Parallel Distributed  
Processing.** MIT press,  
1989

# Some learning materials and references

- My PhD Thesis: <https://arxiv.org/abs/2010.01431>  
or its updated version: <https://share.obspm.fr/s/X3xN6NxJbnZDBWX>  
**Chapters 2, 4 and 11 can be considered as a handout for this course**
- **The Fidle** (Formation Introduction au Deep Learning) **course from the CNRS:**  
<https://gricad-gitlab.univ-grenoble-alpes.fr/talks/fidle/>
- The Neural Network CS231n course from Stanford:  
<https://cs231n.github.io/>
- Some more references on a dedicated page on the MINERVA website  
<https://minerva-astro.obspm.fr/learning/>

*Take everything you read about ML and AI with a grain of salt! (This course included)*

*Lots of materials still contain practical or theoretical approximations and errors.  
Crossing references is most of the time necessary.*

# Attempt of learning definition

## The online Cambridge dictionary:

« *The process of getting an **understanding** of something by **experience*** »

## The *Tresor de la langue Française informatisé*:

« *Acquérir la **connaissance** d'une chose par l'**exercice** de l'**intelligence**, de la **mémoire**, des mécanismes gestuels, appropriés, etc.* »

« *Acquire the **knowledge** of something through the **practice** of **intelligence**, **memory**, appropriate gestures, etc.* »

But these definitions are biased toward a human definition of the learning process...

# Attempt of learning definition

In a more generic way, **animal learning** is usually summarized by these capabilities:

- Sensitivity

- Memory

- Adaptation

- Generalization

By adopting the proposed **statistical learning** definition, any algorithm that works using the following elements can be considered as **Machine Learning**:

- An adaptable input construction, which represents the **sensitivity** of the method.
- A form of **memory** to remember either the previous situations, or a reduced version of them.
- A way to estimate if its behavior (output prediction) is appropriate.
- A way to **adapt** its behavior during the learning process.
- A way to **generalize** its behavior to new outputs.

*Keywords to explore the notion of Artificial Intelligence from there (beyond the scope of this course) :*

- Symbolic and sub-symbolic representations
- Artificial General Intelligence
- Strong AI

# Types of Machine Learning

## Supervised

Learn from **labeled examples**. Try to find a **generalization** to get correct prediction most of the time.

## Semi-Supervised

Usually a **mix of two algorithms**. A un-supervised one first that minimize the definition biases. A supervised one that remap to the expected groups.

## Un-Supervised

Dataset with examples is provided but with **no labels**. Try to find **similarities** in the input in order to **create groups**.

## Self-supervised

Dataset with **no external labels**. Use the data themselves to define labels and learn using a supervised formalism. (e.g., auto-encoders)

## Reinforced

Based on an **reward function**. Used when there is no easy error function. Corrections are applied based on an **external performance measurement**.

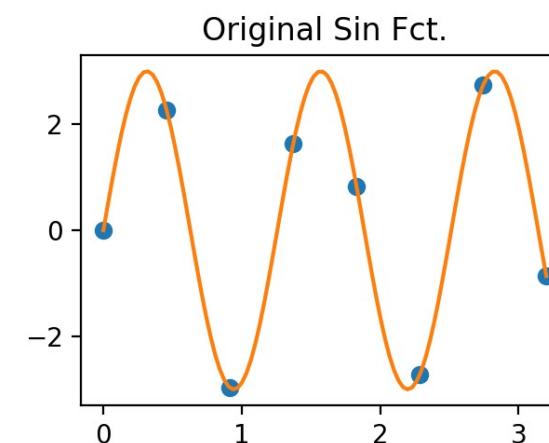
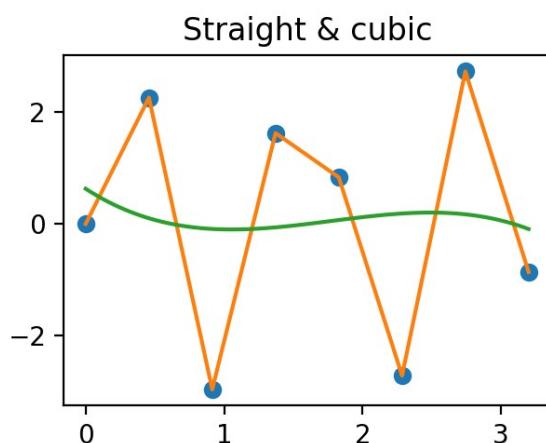
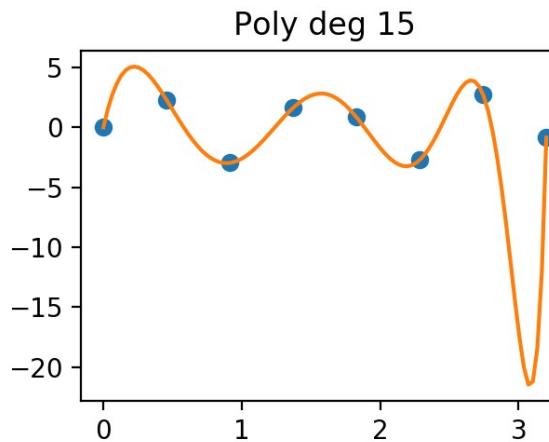
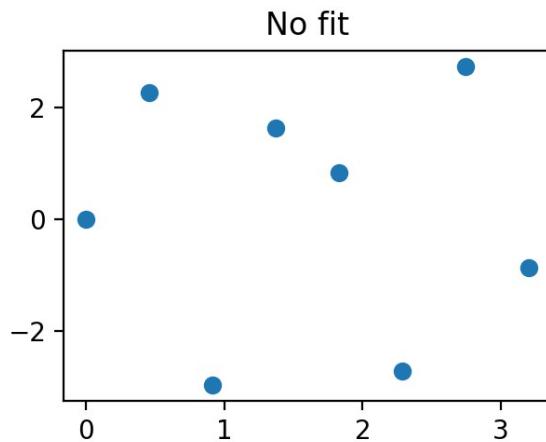
## Evolutionary

Similar to reinforced, explore the possibility space based on biological **evolution processes**. Selection effects, reproduction, mutation, etc.

# Use cases

## Simple example of regression

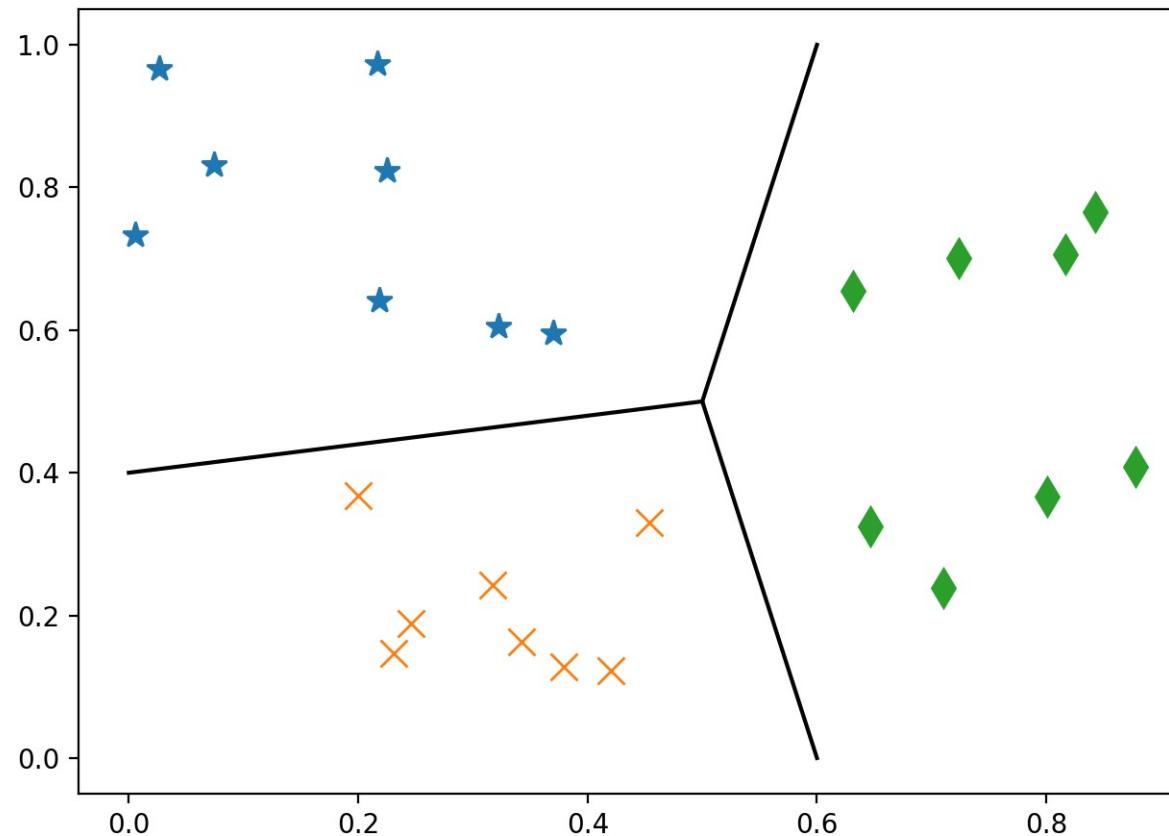
Reconstruct functions from a sample of data points (in any number of dimensions)



# Use cases

## Simple example of classification

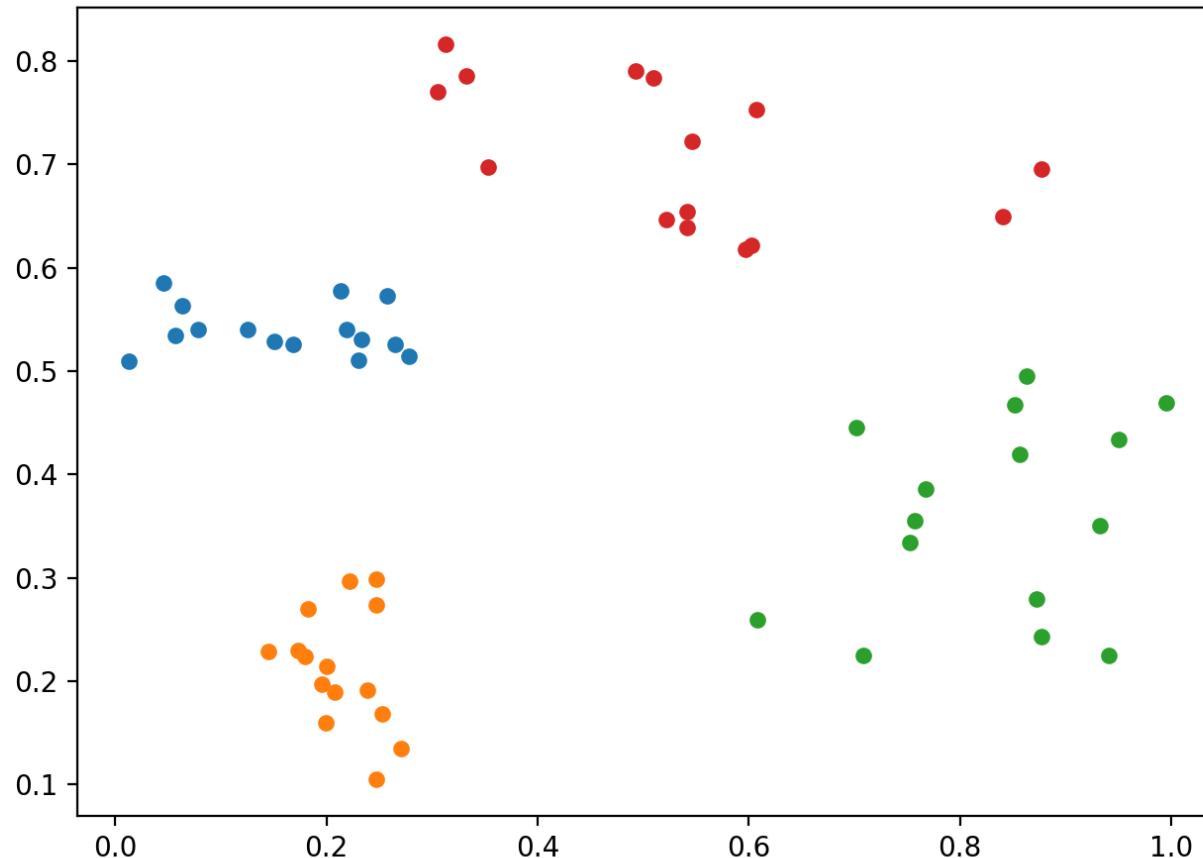
Decide from an input vector with several dimensions to which class it should be associated.

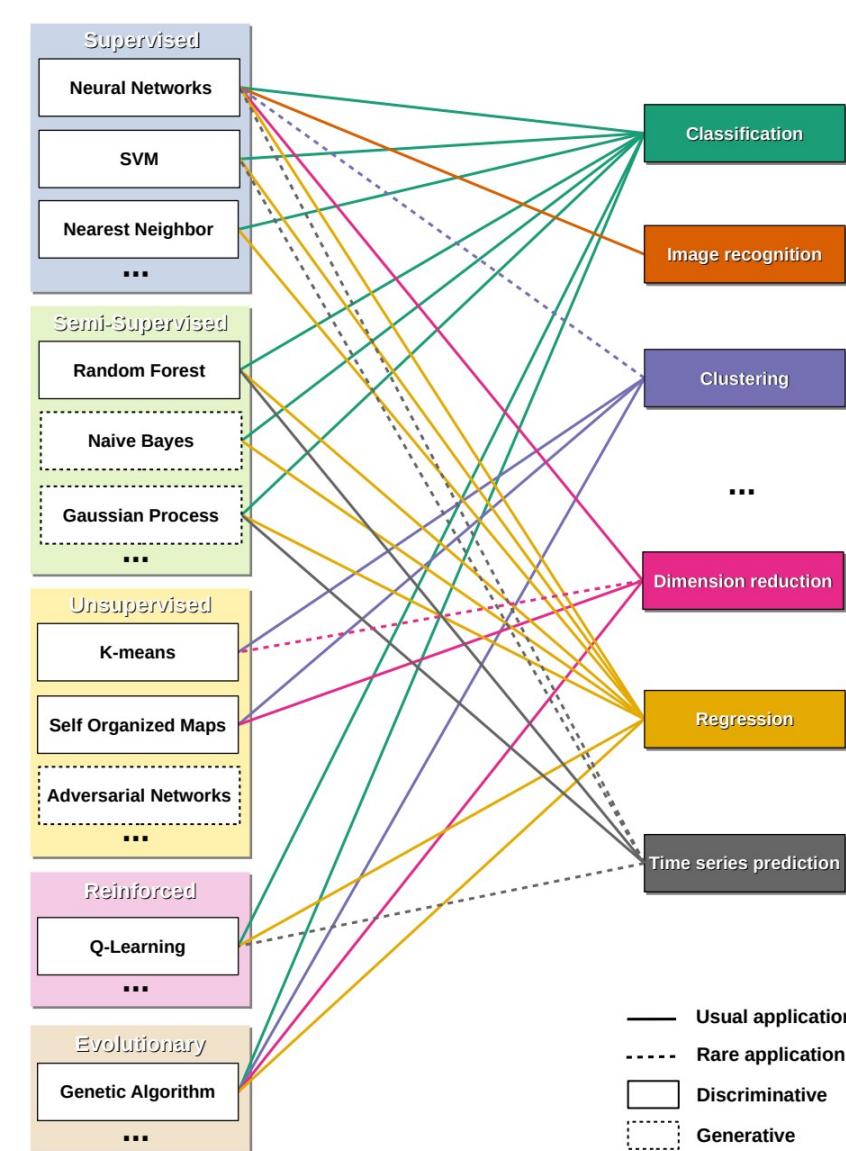


# Use cases

## Simple example of clustering

Find groups in data based on a predefined strategy (e.g geometric distance) without prior knowledge on the number of groups, nor the solution for any example.





# A wide variety of applications ...

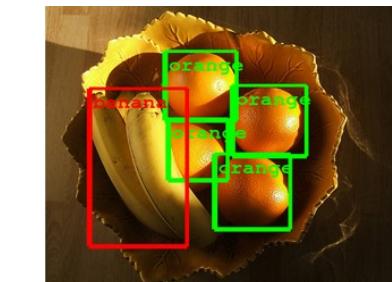
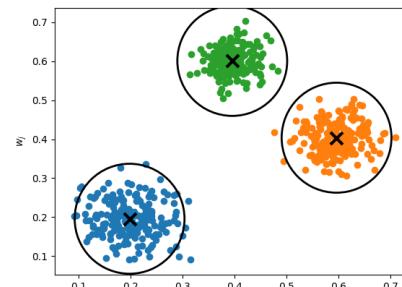
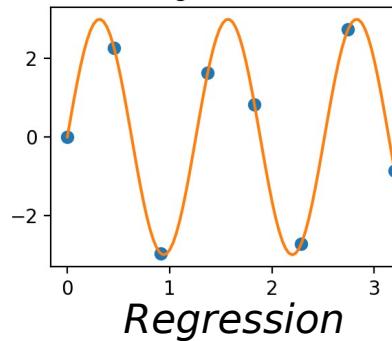
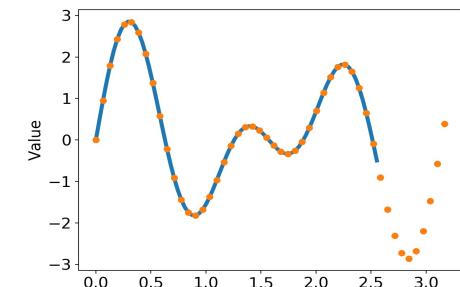
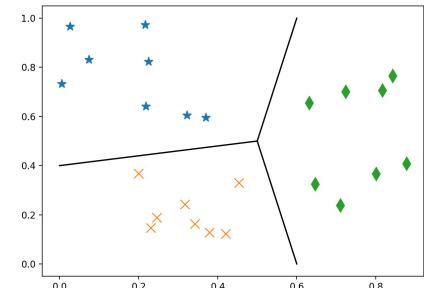
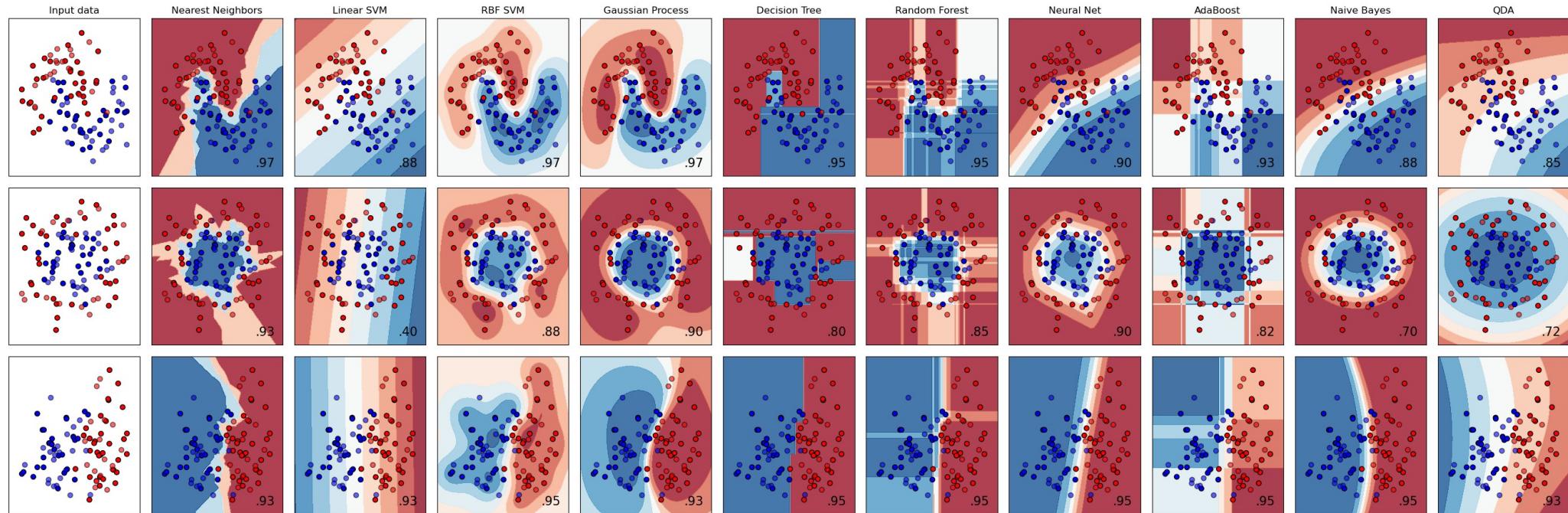


Image recognition



And much more ...

# Methods comparison regarding data distribution



Some methods are **more suited for specific data distributions**, while others work well enough for most data distributions you might encounter.

In any case, **every method has its weaknesses** that you must identify and understand.

**Choosing a method is selecting a balance between:**

- The method capability on your data
- The computational efficiency of the method
- The required time of development / integration
- Your own proficiency with the various methods
- ...

# How to use Machine Learning ?

## Software



Nowadays, there are dedicated ML frameworks for almost **every programming language**.

They all have specific advantages, but any of them is enough to start learning and using ML.

## Hardware

ML methods require a **lot of data** and **computing power** during the **training phase**.

However, these methods are very **compute efficient** when making **predictions**, meaning that it is often possible to deploy already trained models on light hardware (laptops or even modern smartphones)

Still, light resources are usually enough to **explore relatively simple ML methods**, and many complex problems can be expressed in a simple form, allowing preliminary studies on low-end hardware resources to be conducted.

When training powerful models that work on images, it is helpful to **use GPU hardware** that is very efficient for most modern ML approaches.



Note that **hardware dedicated to ML methods** are more and more present and accessible.

(*Tensor Cores in CPUs and GPUs, Neural Processing Units (NPU), etc ...*)

# Framework examples: TensorFlow

[Install](#)[Learn](#) ▾[API](#) ▾[Resources](#) ▾[Community](#) ▾[Why TensorFlow](#) ▾ Search

## Overview

[TensorFlow](#)  
[TensorFlow JavaScript](#)  
[TensorFlow Lite](#)  
[TensorFlow Extended](#)  
[Swift for TensorFlow](#)

## Versions

[Overview](#)  
[2.7 \(stable\)](#)  
[1.15](#)  
▶ [More...](#)

## Community supported languages

[Haskell](#) ↗  
[C#](#) ↗  
[Julia](#) ↗  
[R](#) ↗  
[Ruby](#) ↗  
[Rust](#) ↗  
[Scala](#) ↗  
▶ [Unsupported](#)

## Resources

[Addons](#)  
[Datasets](#)  
[Federated](#)  
[Graphics](#)  
[Hub](#)  
[Model Optimization](#)  
[Neural Structured Learning](#)  
[Probability](#)

TensorFlow > API > TensorFlow Core v2.7.0

Was this helpful? [Up](#) [Down](#)

## API Documentation

TensorFlow has APIs available in several languages both for constructing and executing a TensorFlow graph. The Python API is at present the most complete and the easiest to use, but other language APIs may be easier to integrate into projects and may offer some performance advantages in graph execution.

A word of caution: the APIs in languages other than Python are not yet covered by the [API stability promises](#).

- [Python](#)
- [JavaScript](#)
- [C++](#)
- [Java](#)

We encourage the community to develop and maintain support for other languages with the [approach recommended by the TensorFlow maintainers](#). For example, see the bindings for:

- C#: [TensorFlowSharp](#) ↗ and [TensorFlow.NET](#) ↗,
- [Haskell](#) ↗,
- [Julia](#) ↗,
- [MATLAB](#) ↗,
- [R](#) ↗,
- [Ruby](#) ↗,
- [Rust](#) ↗, and
- [Scala](#) ↗.

We also provide the C++ API reference for TensorFlow Serving:

- [TensorFlow Serving](#) ↗

There are also some archived or unsupported language bindings:

- [Go](#) ↗
- [Swift](#)

# Framework examples: TensorFlow in Python

## Set up TensorFlow

Import TensorFlow into your program to get started:

```
import tensorflow as tf
print("TensorFlow version:", tf.__version__)
```

If you are following along in your own development environment, rather than [Colab](#), see the [install guide](#) for setting up TensorFlow for development.

Note: Make sure you have upgraded to the latest `pip` to install the TensorFlow 2 package if you are using your own development environment. See the [install guide](#) for details.

## Load a dataset

Load and prepare the [MNIST dataset](#). Convert the sample data from integers to floating-point numbers:

```
mnist = tf.keras.datasets.mnist
(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0
```

## Build a machine learning model

Build a `tf.keras.Sequential` model by stacking layers.

```
model = tf.keras.models.Sequential([
    tf.keras.layers.Flatten(input_shape=(28, 28)),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.Dropout(0.2),
    tf.keras.layers.Dense(10)
])
```

For each example, the model returns a vector of `logits` or `log-odds` scores, one for each class.

```
predictions = model(x_train[:1]).numpy()
predictions
```

The `tf.nn.softmax` function converts these logits to *probabilities* for each class:

```
tf.nn.softmax(predictions).numpy()
```

Note: It is possible to bake the `tf.nn.softmax` function into the activation function for the last layer of the network. While this can make the model output more directly interpretable, this approach is discouraged as it's impossible to provide an exact and numerically stable loss calculation for all models when using a softmax output.

Define a loss function for training using `losses.SparseCategoricalCrossentropy`, which takes a vector of logits and a `True` index and returns a scalar loss for each example.

```
loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
```

This loss is equal to the negative log probability of the true class: The loss is zero if the model is sure of the correct class.

This untrained model gives probabilities close to random (1/10 for each class), so the initial loss should be close to `-tf.math.log(1/10) ~= 2.3`.

```
loss_fn(y_train[:1], predictions).numpy()
```

Before you start training, configure and compile the model using Keras `Model.compile`. Set the `optimizer` class to `adam`, set the `loss` to the `loss_fn` function you defined earlier, and specify a metric to be evaluated for the model by setting the `metrics` parameter to `accuracy`.

```
model.compile(optimizer='adam',
              loss=loss_fn,
              metrics=['accuracy'])
```

## Train and evaluate your model

Use the `Model.fit` method to adjust your model parameters and minimize the loss:

```
model.fit(x_train, y_train, epochs=5)
```

The `Model.evaluate` method checks the models performance, usually on a "Validation-set" or "Test-set".

```
model.evaluate(x_test, y_test, verbose=2)
```

The image classifier is now trained to ~98% accuracy on this dataset. To learn more, read the [TensorFlow tutorials](#).

If you want your model to return a probability, you can wrap the trained model, and attach the softmax to it:

```
probability_model = tf.keras.Sequential([
    model,
    tf.keras.layers.Softmax()
])
```

```
probability_model(x_test[:5])
```

## Conclusion

Congratulations! You have trained a machine learning model using a prebuilt dataset using the [Keras API](#).

# Framework examples: TensorFlow in R

```
library(keras)

# Data Preparation ----

batch_size <- 128
num_classes <- 10
epochs <- 12

# Input image dimensions
img_rows <- 28
img_cols <- 28

# The data, shuffled and split between train and test sets
mnist <- dataset_mnist()
x_train <- mnist$train$x
y_train <- mnist$train$y
x_test <- mnist$test$x
y_test <- mnist$test$y

# Redefine dimension of train/test inputs
x_train <- array_reshape(x_train, c(nrow(x_train), img_rows, img_cols, 1))
x_test <- array_reshape(x_test, c(nrow(x_test), img_rows, img_cols, 1))
input_shape <- c(img_rows, img_cols, 1)

# Transform RGB values into [0,1] range
x_train <- x_train / 255
x_test <- x_test / 255

cat('x_train_shape:', dim(x_train), '\n')
cat(nrow(x_train), 'train samples\n')
cat(nrow(x_test), 'test samples\n')

# Convert class vectors to binary class matrices
y_train <- to_categorical(y_train, num_classes)
y_test <- to_categorical(y_test, num_classes)

# Define Model -----
```



```
# Define Model ----

# Define model
model <- keras_model_sequential() %>%
  layer_conv_2d(filters = 32, kernel_size = c(3,3), activation = 'relu',
                 input_shape = input_shape) %>%
  layer_conv_2d(filters = 64, kernel_size = c(3,3), activation = 'relu') %>%
  layer_max_pooling_2d(pool_size = c(2, 2)) %>%
  layer_dropout(rate = 0.25) %>%
  layer_flatten() %>%
  layer_dense(units = 128, activation = 'relu') %>%
  layer_dropout(rate = 0.5) %>%
  layer_dense(units = num_classes, activation = 'softmax')

# Compile model
model %>% compile(
  loss = loss_categorical_crossentropy,
  optimizer = optimizer_adadelta(),
  metrics = c('accuracy')
)

# Train model
model %>% fit(
  x_train, y_train,
  batch_size = batch_size,
  epochs = epochs,
  validation_split = 0.2
)

scores <- model %>% evaluate(
  x_test, y_test, verbose = 0
)

# Output metrics
cat('Test loss:', scores[[1]], '\n')
cat('Test accuracy:', scores[[2]], '\n')
```

# What about from scratch programming ?

## « Opening the box »

	Frameworks	Custom
Pros	<ul style="list-style-type: none"><li>• Lots of learning material and support</li><li>• Often already parallel and optimized</li><li>• Low effort for good results</li><li>• Updated regularly (performance improvement without changes in your own code)</li></ul>	<ul style="list-style-type: none"><li>• May grant a deeper understanding</li><li>• Allow finer control and optimization for specific tasks or hardware</li><li>• Independent of library lifespan</li><li>• Grant non-framework-specific capabilities</li><li>• Can create new methods/paradigms</li></ul>
Cons	<ul style="list-style-type: none"><li>• Binned to the supported methods, hardware, and programming paradigm</li><li>• No control over the supported features and update schedule</li><li>• If the library dies, all of your code and practical experience dies with it</li></ul>	<ul style="list-style-type: none"><li>• LOTS OF SUPPLEMENTARY WORK!</li><li>• More prone to programming errors</li><li>• Requires a lot of programming and hardware knowledge to be efficient</li><li>• Necessity to constantly demonstrate the proper working of your tool</li></ul>

In this course, we will implement simple algorithms AND learn to use widely adopted frameworks.

We will also look at the custom framework [CIANNA](#) for specific tasks.

# Use cases

## Examples of modern applications

The screenshot shows the DeepL translation interface. At the top, there's a navigation bar with links for DeepL Traducteur, DeepL Pro, Services, API, Forfaits et tarifs, Applications (with a GRATUIT button), Nous contacter, Commencer l'essai gratuit, Connexion, and a menu icon. Below the navigation bar are two input fields: "Traduire du texte" (26 langues) and "Traduire des fichiers" (.pdf, .docx, .pptx). The main area shows a translation from English to French. The English text is:

I believe that in about fifty years' time it will be possible to programme computers, with a storage capacity of about  $10^9$ , to make them play the imitation game so well that an average interrogator will not have more than 70 per cent. chance of mating the right identification after five minutes of questioning.

The French translation is:

Je pense que d'ici une cinquantaine d'années, il sera possible de programmer des ordinateurs, avec une capacité de stockage d'environ  $10^9$ , pour qu'ils jouent si bien le jeu de l'imitation qu'un interrogateur moyen n'aura pas plus de 70 % de chances de faire la bonne identification après cinq minutes d'interrogatoire.

At the bottom of the interface, there are icons for volume, like, dislike, and sharing, along with the text "311 / 5000".

# Use cases

## Examples of modern applications

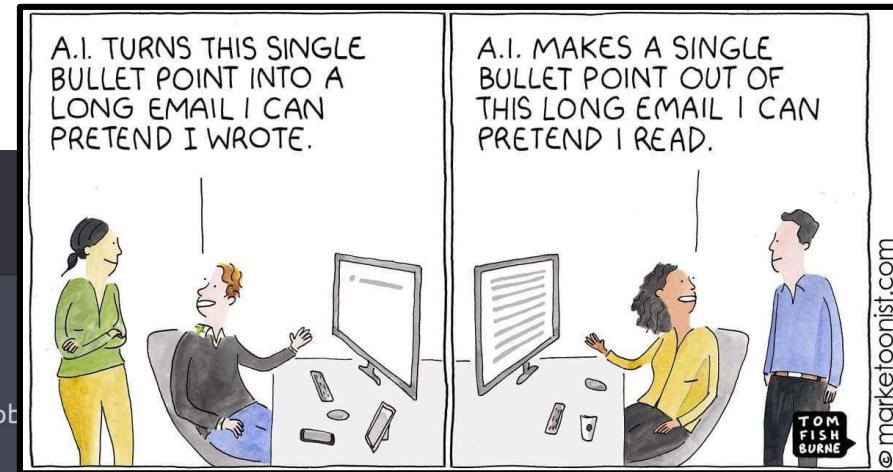
TH

Got any creative ideas for a 10 year old's birthday?



Sure! Here are some creative birthday ideas for a 10-year-old:

1. A themed birthday party such as a movie or video game character or a favorite hobby
2. A scavenger hunt with friends, either indoors or outdoors
3. A craft or DIY project, like creating tie-dye shirts or friendship bracelets
4. An outing to an amusement park, trampoline park, or laser tag center
5. A baking or cooking class, where the birthday child and friends can make and enjoy treats together
6. A sleepover with friends, complete with games, movies, and a special breakfast
7. A science or art experiment-themed party, where children can participate in hands-on activities
8. A sporty day with a visit to a rock climbing gym, batting cage, or mini golf course
9. A virtual escape room or game experience, played together with friends over video chat
10. A wildlife or nature exploration outing, such as a hike or a trip to a local zoo or aquarium.



© marketoonist.com

*Modern AI LLMs generated text is now quite convincing for human reader, but it remains detectable with automated tools based on ... AI LLMs (adversarial attack)!*

# Use cases

## Examples of modern applications



Use cases Pricing FAQ API ⚙

### Use cases

Photographers

Creative Agencies

Real Estate

E-commerce

Remove text, logo or watermark

Developers API



Photographers use Cleanup.pictures to remove time stamps or remove tourists from holiday pictures before printing them for their customers.

They clean portrait photos to create the perfect profile pictures.

Cleanup.pictures is the perfect app to remove cracks on photographs. You can clean any images, removing any unwanted things. It is a must-have for professional studios.

\*Based on the LaMa: Resolution-robust Large Mask Inpainting with Fourier Convolutions method  
→ <https://arxiv.org/abs/2109.07161> and for fun <https://cleanup.pictures>

# Use cases

## Examples of modern applications

These persons do not exist !



\*Based on the Style Generative Adversarial Network model

→ <https://arxiv.org/abs/1812.04948> and for fun <https://thispersondoesnotexist.com/>

# Use cases

## Examples of modern applications

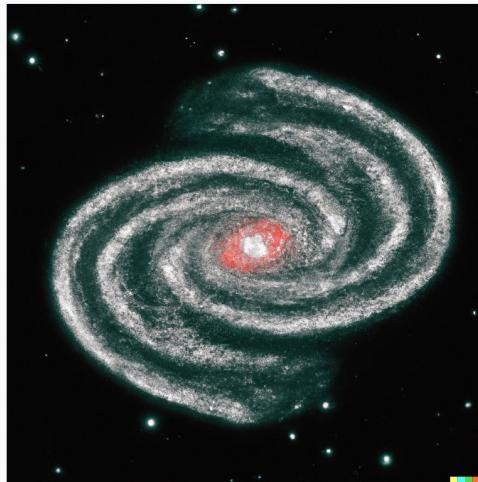
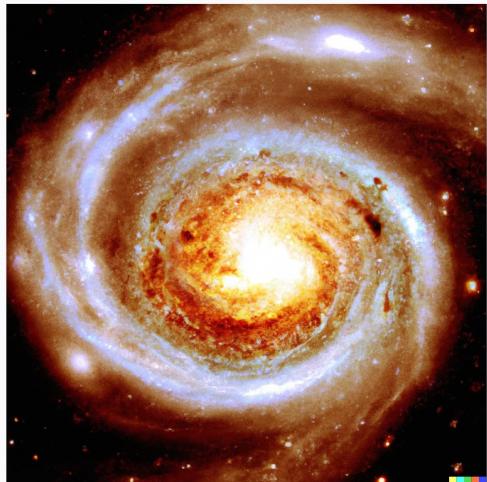
Edit the detailed description

Surprise me

Upload →

An artistic view of a barred spiral galaxy observed in the infrared

Generate



\*Dall-E, based on CLIP word embedding and diffusion decodeur => <https://arxiv.org/abs/2204.06125>

# Use cases

## Examples of modern applications

Generate an image of "An artistic view of a barred spiral galaxy observed in the infrared"



Here are the artistic views of a barred spiral galaxy observed in the infrared. The images highlight the central bar structure, swirling spiral arms, and vibrant infrared colors with distant stars and cosmic dust in the background.

Generate a more realistic image that would resemble an astronomical observation



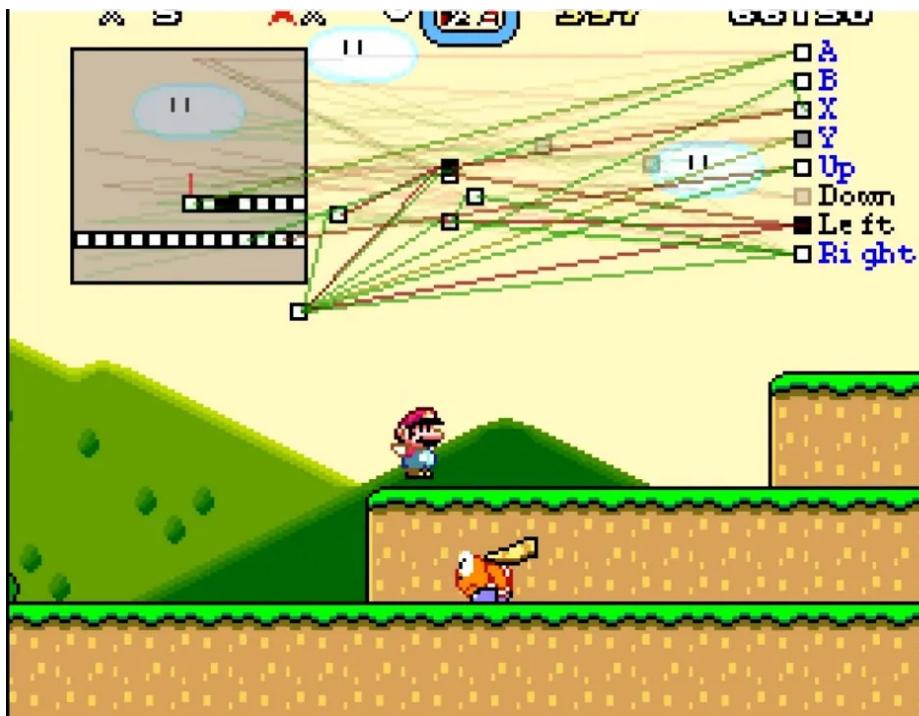
Here are the more realistic images of a barred spiral galaxy observed in the infrared, resembling actual astronomical observations.

*With DALL-E 3 through ChatGPT 4 interface*

# Use cases

## Examples of modern applications

The same processes are used to train robots to walk. But can also be used to infer any function from which you can only define a global posterior fitness score.



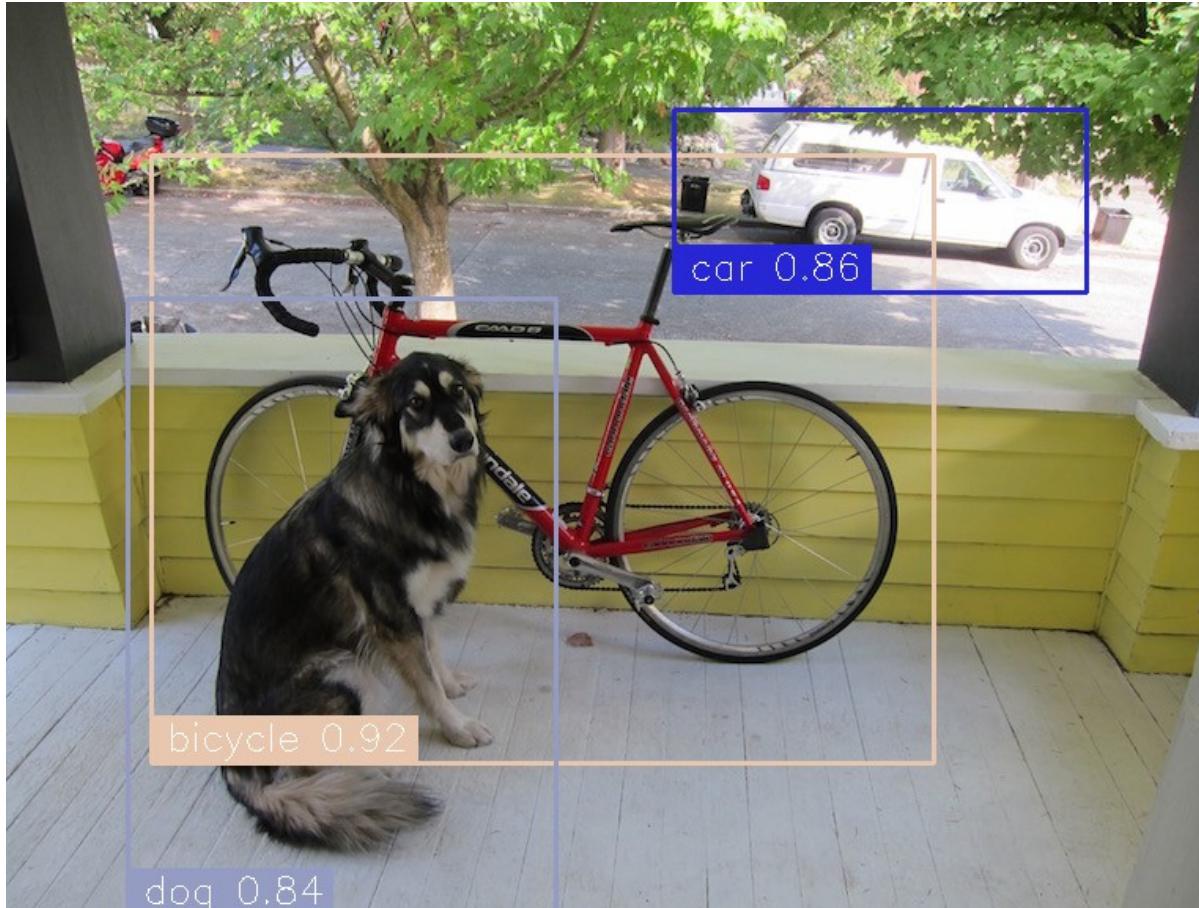
\*Based on Genetic Neural Evolution  
→ <https://www.youtube.com/watch?v=qv6UVQ0F44>



\*Based on Deep Reinforced Learning method AC3  
→ <https://arxiv.org/abs/1602.01783v2>  
→ <https://youtu.be/nMR5mjCFZCw>

# Use cases

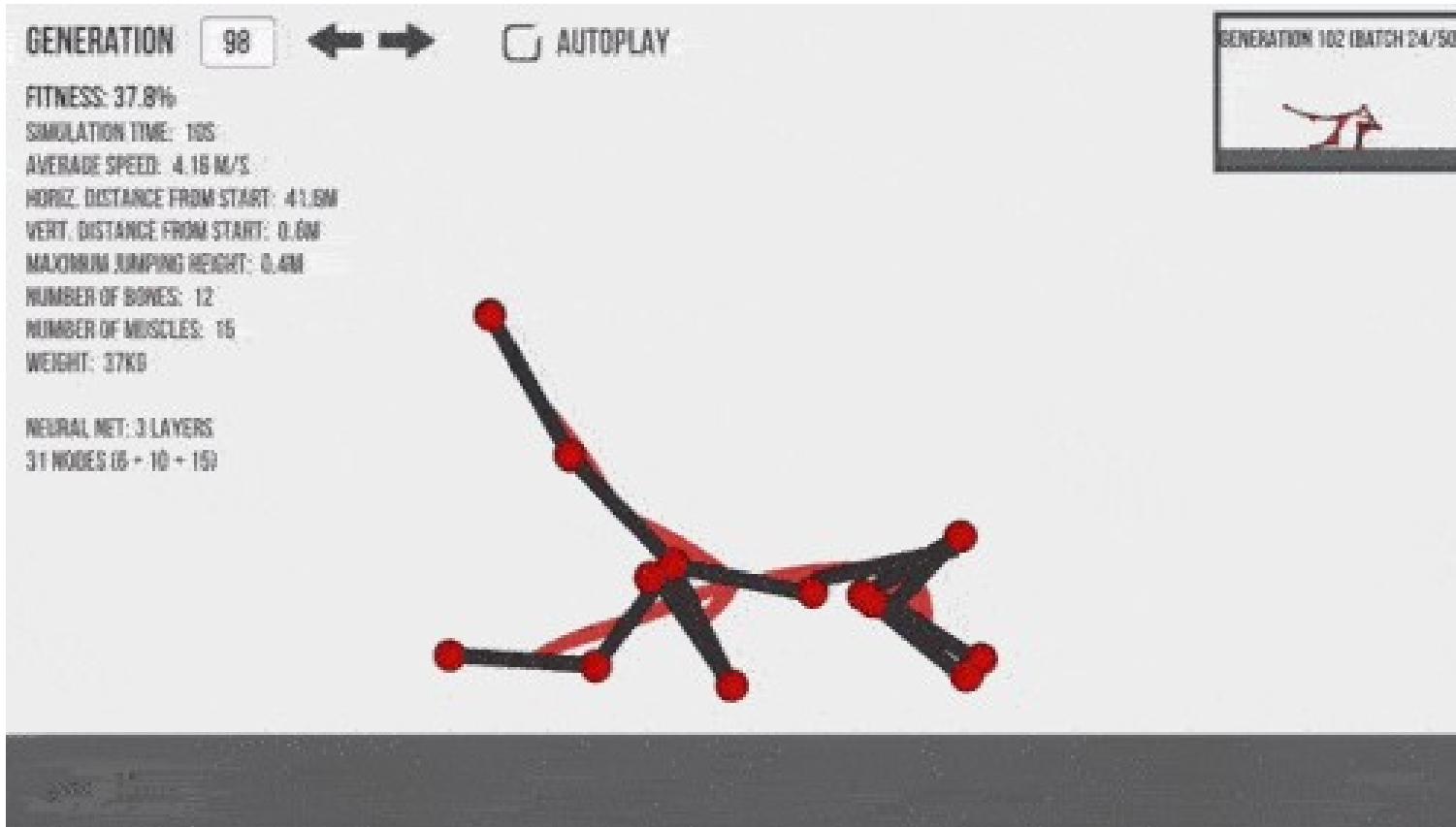
## Examples of modern applications



\*Based on the YOLO Convolutional Neural Network architecture for object detection  
→ <https://www.youtube.com/watch?v=MPU2HistivI> and <https://arxiv.org/abs/1804.02767>

# Use cases

## Examples of modern applications

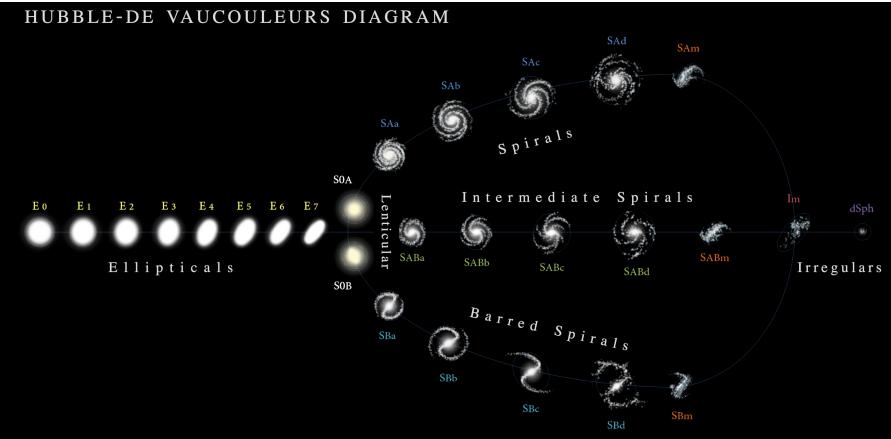


\*Based on Genetic Neural Evolution

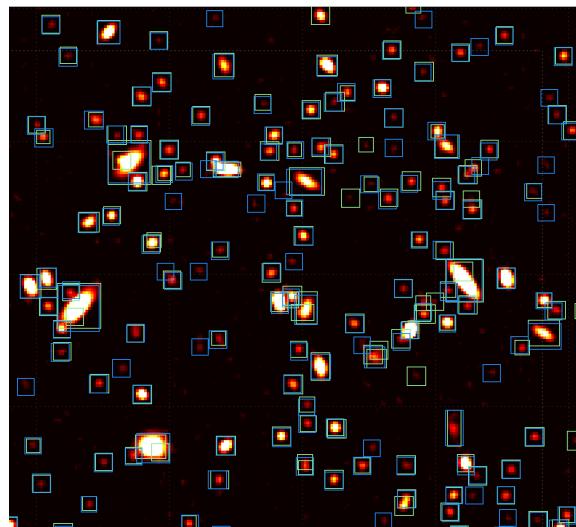
→ Interactive creature creation at <https://keiwan.itch.io/evolution>

# What about astronomical applications ?

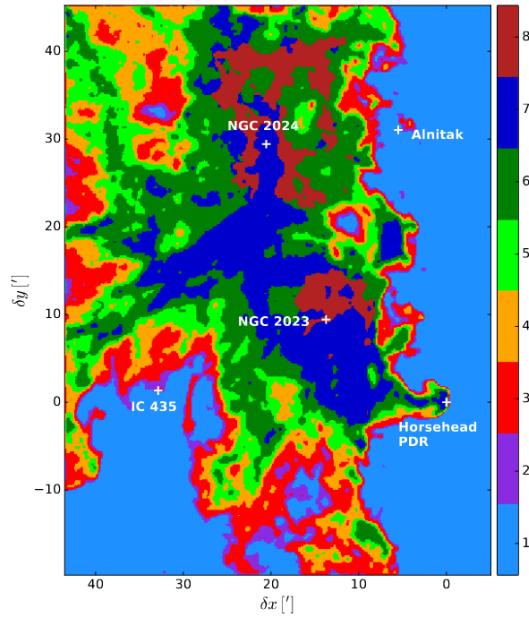
HUBBLE-DE VAUCOULEURS DIAGRAM



Morphological classification of galaxies



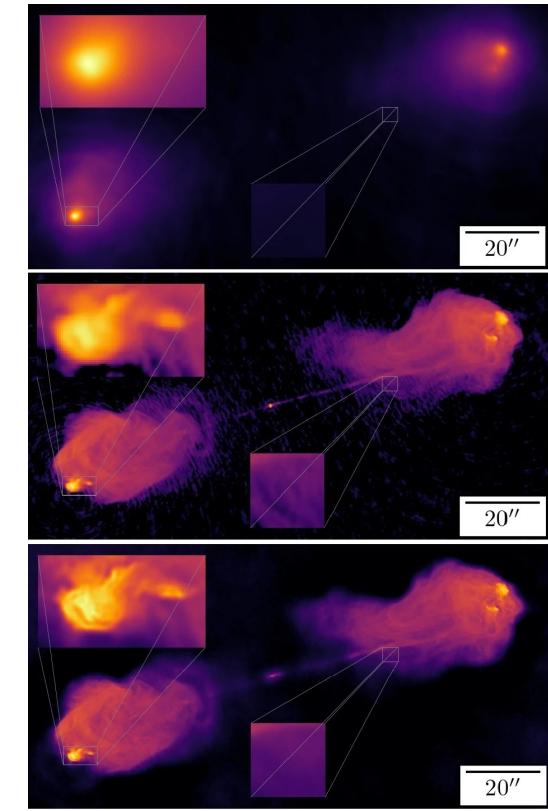
Detection and characterization of galaxies



Molecular cloud emission clustering

And much more :

- Cosmological simulation acceleration
- Inverse modeling for cosmological models
- Stellar classification based on spectra
- ISM turbulence regime classification
- Transient events time series prediction
- ...



Radio-astronomical image enhancing

Wide diversity of objects, methods, scales, data representation, etc...

# Supervised algorithm example : SVM

## Description

The Support Vector Machine algorithm is a supervised ML method used for classification.

## Objective

Find the best separation between predefined classes in a multi-dimensional parameter space.

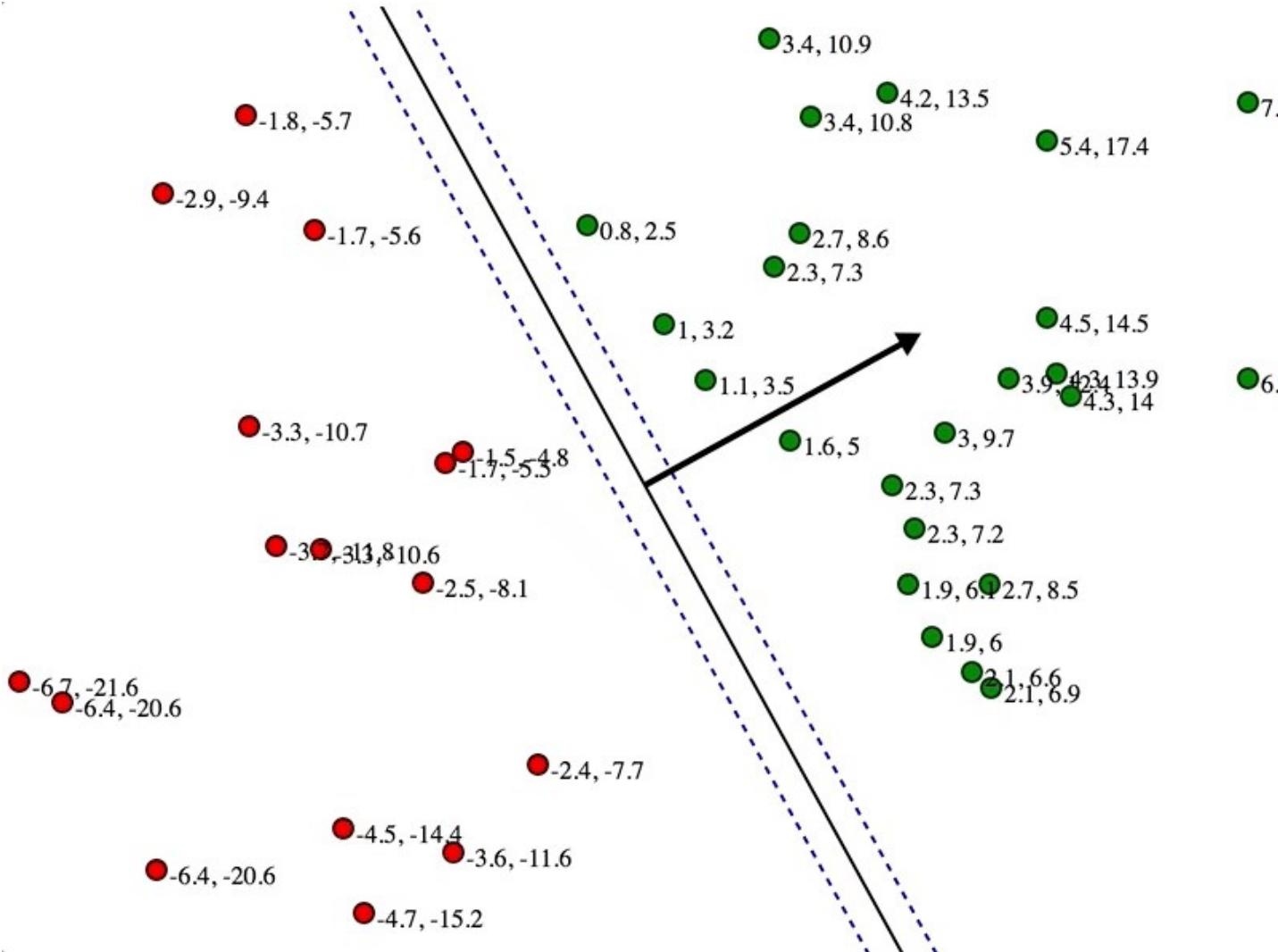
## Method (simplified)

Define **anchor points** representing the closest to the separation between the two classes. The algorithm then searches for the optimal **linear separation**. For this, it will iteratively try to **maximize the orthogonal distance around the separation** that does not contain any anchor point.

## Why is it ML?

This algorithm respects our definition of ML. It aims to **generalize** knowledge from specific data points into a continuous **parameter space**. It is equipped with a metric that evaluates the quality of the splitting and an **iterative adaptation** scheme based on the orthogonal distance to the anchor. The **memory** is characterized by the changing value of the linear separation parameters and of the maximum orthogonal distance.

# Supervised algorithm example : SVM



# **Unsupervised algorithm example : k-means clustering**

## **Description**

The k-means algorithm is an unsupervised ML method that is used for clustering.

*\*Not to be confused with the k-nearest Neighbors (kNN) algorithm*

## **Objective**

Find groups in a dataset based on a geometrical distance in a multi-dimensional parameter space.

## **Method**

Define a **number “k”** of centers (define the maximum number of groups/clusters). For each point, it **searches the closest « cluster center »** based on a geometrical distance. The cluster centers are moved toward the **gravity center** of their associated data points. This operation is repeated until the cluster centers stop moving.

## **Why is it ML ?**

This algorithm respects our definition of ML. It aims to **generalize** knowledge from specific data points into a continuous **parameter space**. It is equipped with a metric that evaluates the convergence of the method and an **iterative adaptation** scheme based on the averaged geometrical distance to a list of data points. The **memory** is characterized by the changing value of the cluster center positions in the parameter space.

# **Unsupervised algorithm example : k-means clustering**



# Hands-on : k-means algorithm

**Main Loop:** until the cluster centers stop moving

- **Identification phase:** loop over the data points
  - Compute the current point distance to all the cluster centers ( $k$ )
  - Associate the current point to the closest center
- **Update phase:** loop over the cluster centers
  - Compute the centroid of the data point list for the current cluster
  - Move the cluster center to the obtained centroid position

# Hands-on : k-means algorithm

**Data:** a data file ***kmeans\_input\_file.dat*** is provided (in 2D and 3D), along with the Python code that was used to generate it.

**Code:** incomplete codes are provided in Python, C, and Fortran. It includes the reading of the data file and distance compute function. Some useful variables are declared, but some necessary ones are still missing.

**Objective:** Complete a working k-means program based on the given algorithm.

**Key points of the exercise:**

- Identify the additional variables that are required for the algorithm.
- Identify the algorithm loops and phases and code them.
- Take the time to think of the best way to find the minimum distance in a list.
- Find how to end the main loop properly.
- While the first version can be specific to 2D data, try to have a non-dimension-specific implementation at the end.

**Results:** A visualization tool is provided with the script ***kmeans\_visual.py***