Machine Learning for Astrophysics

Supervised Learning strikes back

Outline

Introduction to ML & Supervised ML

- Introduction
- Regression, Regularization
- Classification, Logistic Regression
- Bias/Variance trade-off

Supervised ML strikes back

- Support Vector Machines
- Gaussian Processes
- Nearest Neighbors
- Ensemble Methods: random forests
- Gradient Boosting

You are here

Unsupervised ML

- Clustering: KMeans, DBScan, GMM, Agglomerative Clustering
- Anomaly Detection
- Dimensionality Reduction:
  - linear: PCA, NMF, ICA
  - manifold learning: LLE, IsoMap, t-SNE
- Self-Organizing Maps

Deep Learning

- A few notes on HPC and GPUs (*maybe*)
- Basics of NN: computation graphs
- Training a NN: *forth*- and *back*-propagation
- Optimization Algorithms
- Transfer Learning
- Autoencoders?
- Bayesian NN, Probabilistic BNN

Deep Learning, The Revenge

- (*hints on*) Reinforcement Learning
- Convolutional Neural Networks
- ResNet, Inception Module and MobileNet
- Generative Adversarial Networks
- (*hints on*) Recurrent Neural Networks
- Variational Autoencoders
- Transformers

The Holy Trinity of Machine Learning

Supervised Learning

Data: (x, y)
x is the data, with associated labels y

Goal:
learn a function that maps
$x \rightarrow y$

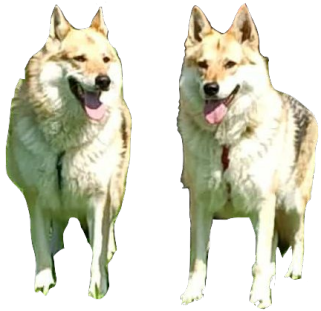
"This thing is a dog"

Unsupervised Learning

Data: x
there are no labels, only data x

Goal:

learn underlying structure of x



"These two things look alike"

Reinforcement Learning

Data: *state-action* pairs

Goal:
learn a policy π
maximizing future rewards

"Cuddling this thing will make you happy"

Supervised Learning

Data: (x, y)
x is the data, with associated labels y

Goal:
learn a function that maps
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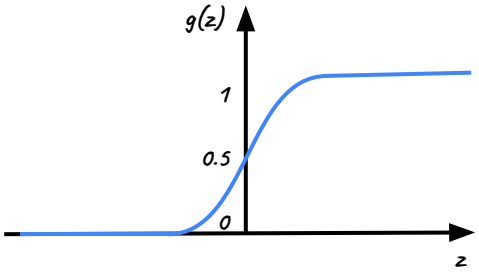
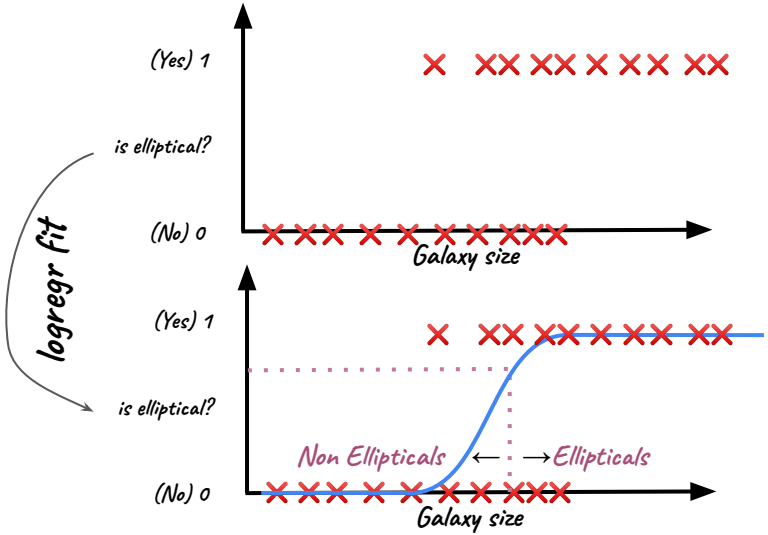
"This thing is a dog"

Build **models** that learn
how to ***combine*** **inputs**
to ***produce*** **predictions**
(even) on **never seen before data**

Logistic regression is the centerpiece of classification problems. It originates from the sigmoid (or logistic) function:

$$\boxed{g(z) = \frac{1}{1+e^{-z}}}$$





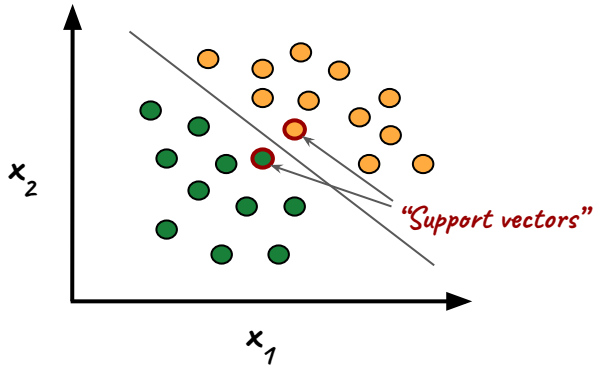
And with this function, define the logistic regression model:

$$f_{\vec{w},b} = g(\vec{w} \cdot \vec{x} + b) = \frac{1}{1+e^{-(\vec{w}\cdot\vec{x}+b)}}$$

where $f_{w,b}$ gives the probability that x belongs to a certain class (e.g. if the galaxy is elliptical once given a galaxy size in kpc).
With logistic regression you train on the training set, finding the optimal values for the weights w, b.
The logistic loss function (*logloss*) evaluated on a single training example is:

$$\mathcal{L}(f_{\vec{w},b}(x^{(i)}, y^{(i)})) = -y^{(i)} \log(f_{\vec{w},b}(x^{(i)})) - (1 - y^{(i)}) \log(1 - f_{\vec{w},b}(x^{(i)}))$$

A **Support Vector Machine** (SVM) is a supervised learning algorithm, mainly employed for classification tasks. SVMs are based on the idea of finding a hyperplane that best (and maximally) divides a dataset into two classes.



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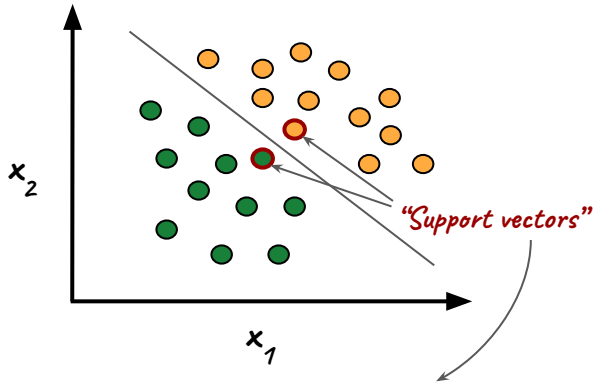

The data points nearest to the hyperplane. Their removal would alter the position of the dividing hyperplane.

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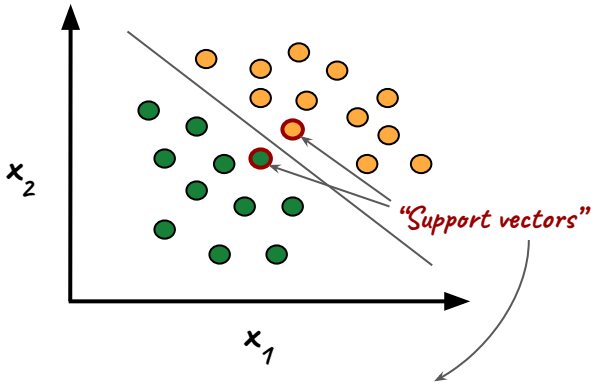

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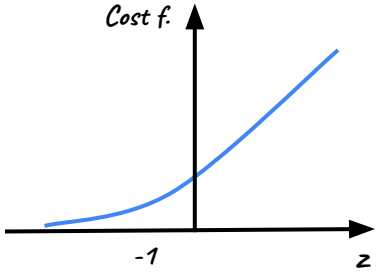
if $y = 0 \longrightarrow -\log(1-g(z))$



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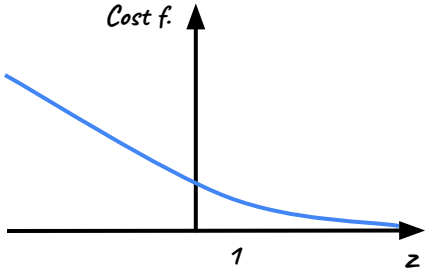

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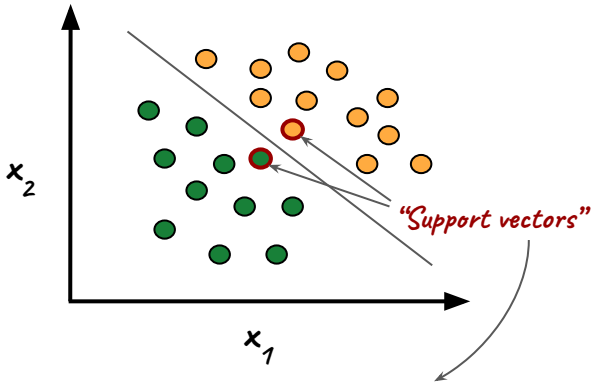

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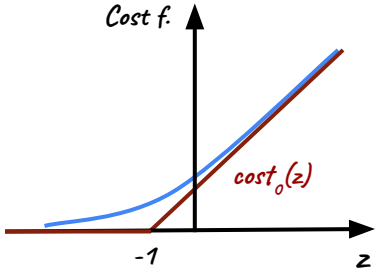

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if $y = 1$, $cost_1(z)$ is $\longrightarrow$
0 for $z > 1$
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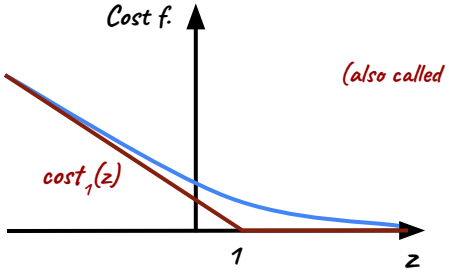

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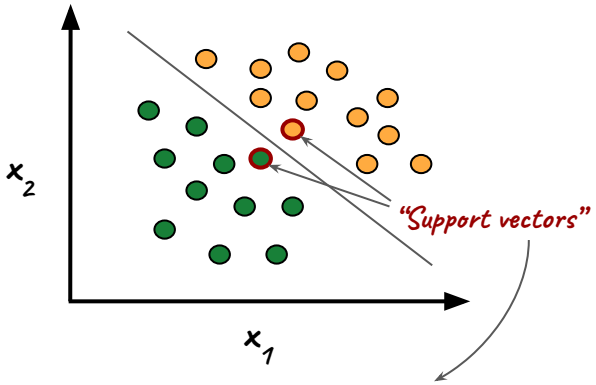

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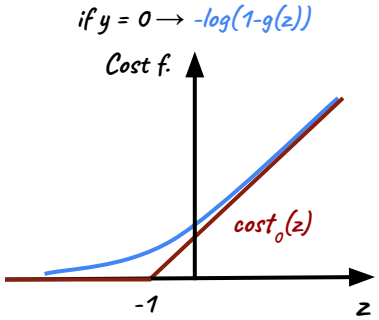

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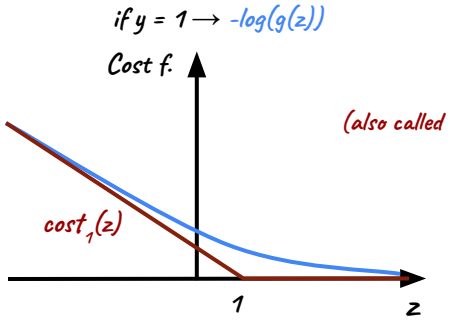

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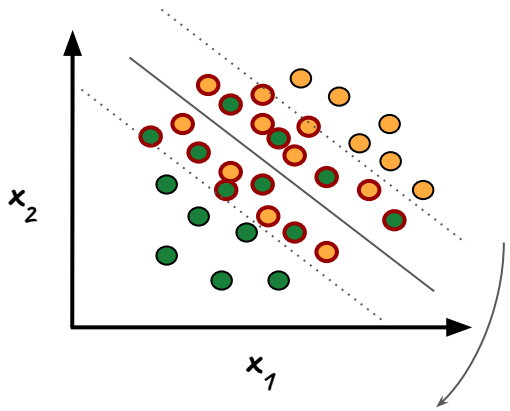

You can account for the presence of interlopers by adding a tolerance margin (soft margins)

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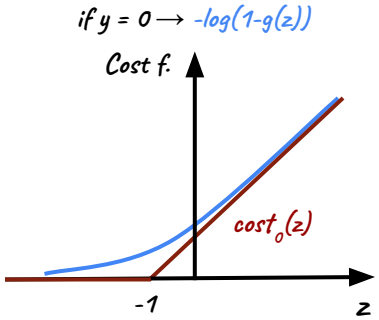

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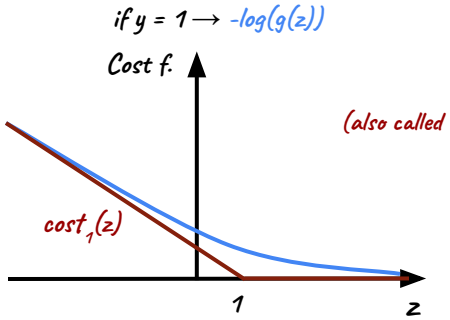

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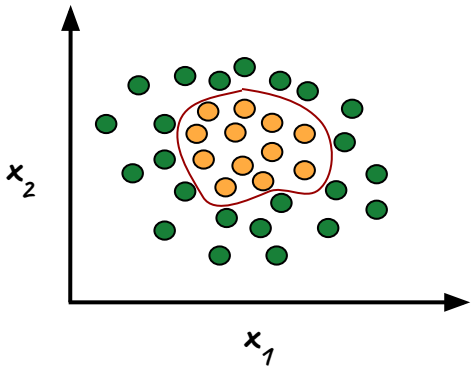

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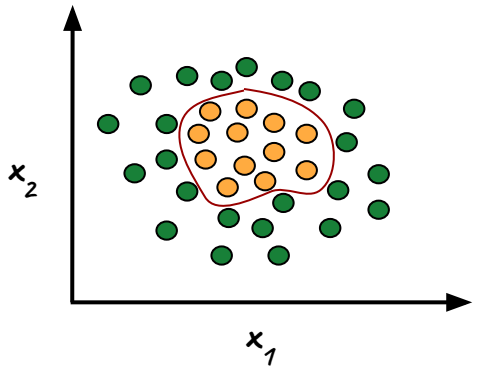

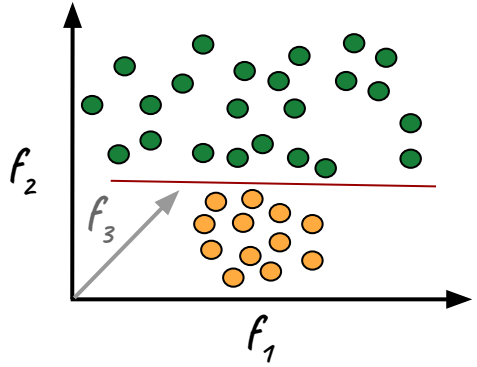

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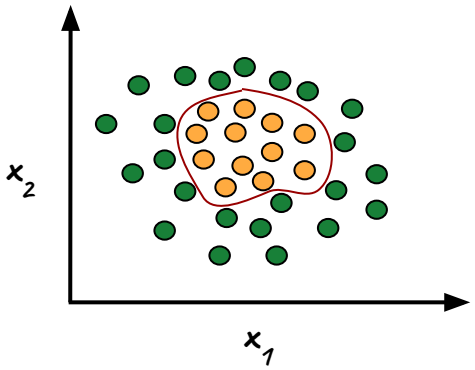

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$$w_0 + w_1 \underbrace{x_1^2}_{f_1} + w_2 \underbrace{x_2^2}_{f_2} + w_3 \underbrace{x_1 x_2}_{f_3}$$

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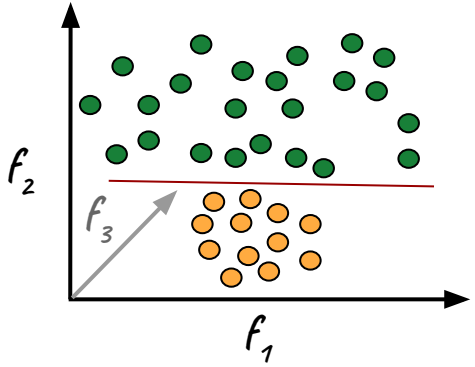

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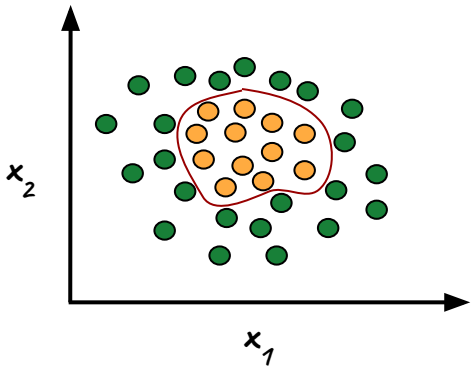

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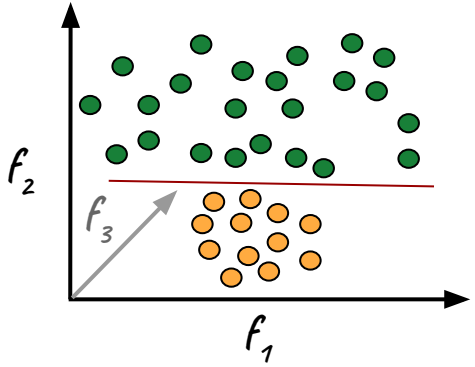

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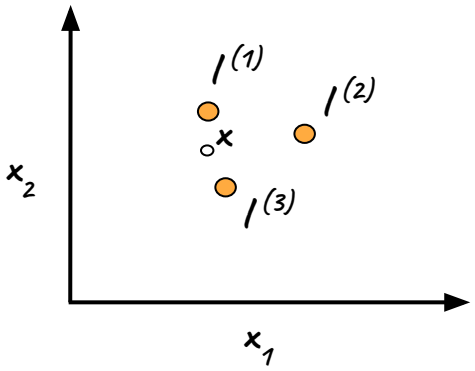

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Given x, compute new features depending on the proximity to landmarks points $l^{(1)}, l^{(2)}, l^{(3)}$

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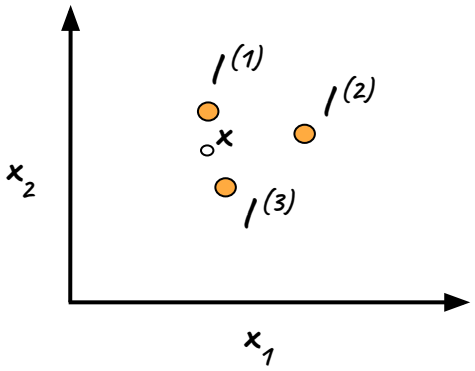

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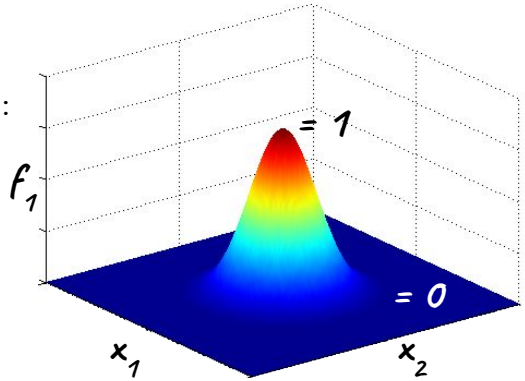
e.g. Gaussian kernel (or **radial basis function, RBF**):

$$K(x, l^{(i)}) = \exp\left(-\frac{||x - l^{(i)}||^2}{2\sigma^2}\right)$$



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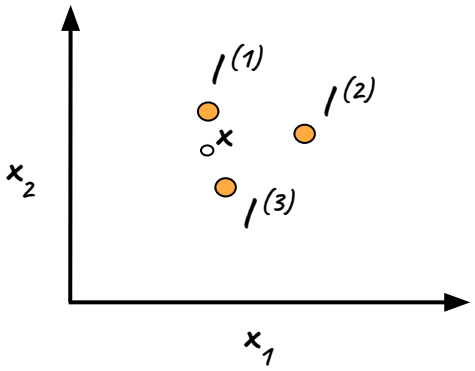
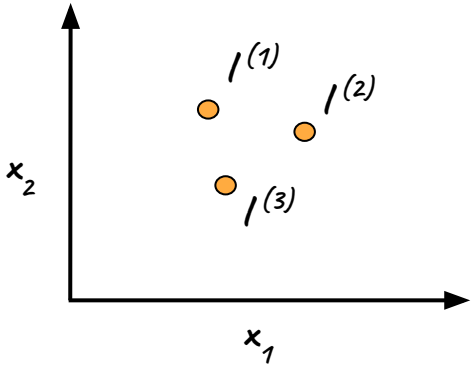


Let's assume e.g. a model with:

$w_0 = -.5,\ w_1 = +1,\ w_2 = +1\ w_3 = 0$



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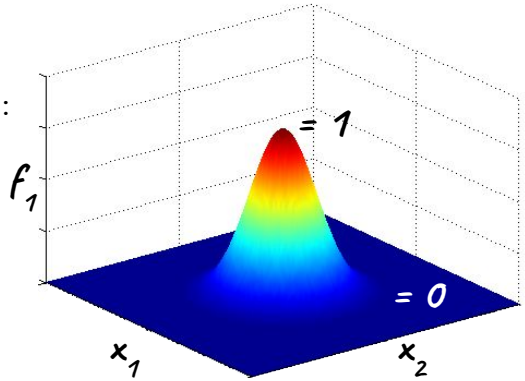

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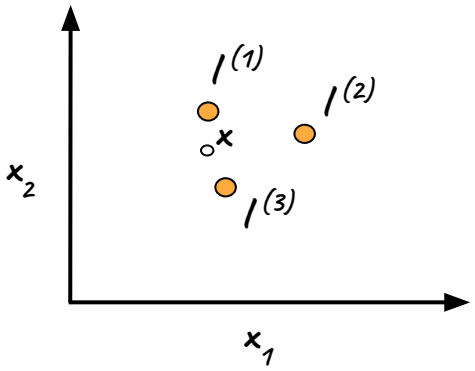

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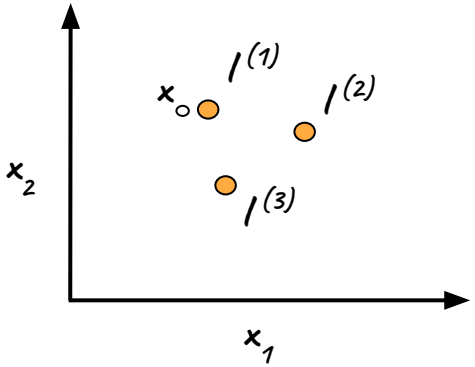

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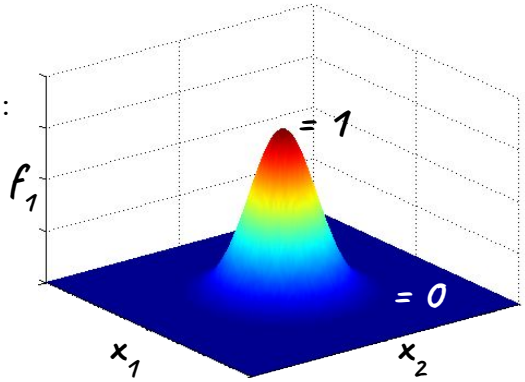

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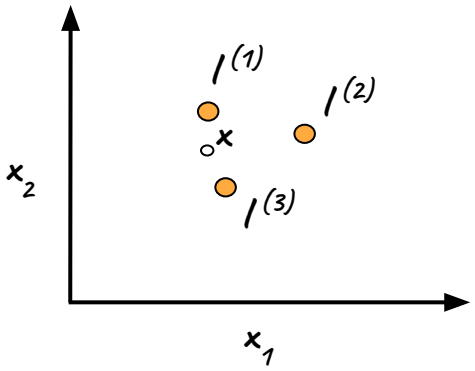

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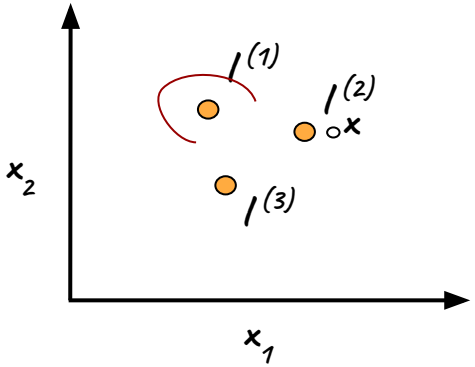

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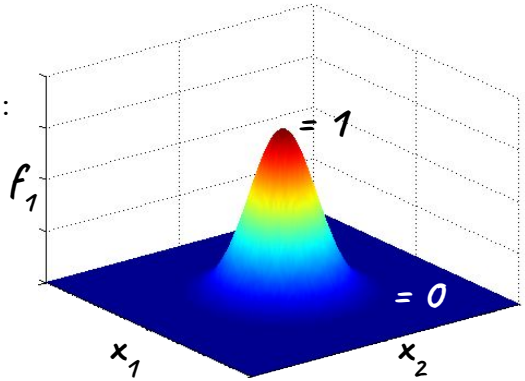

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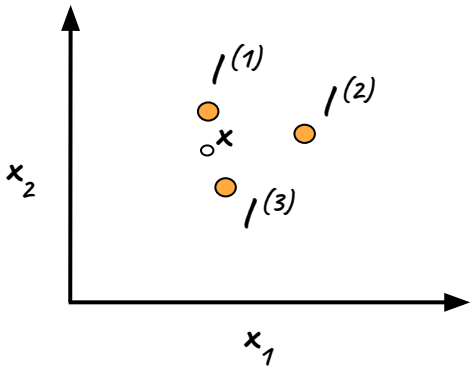

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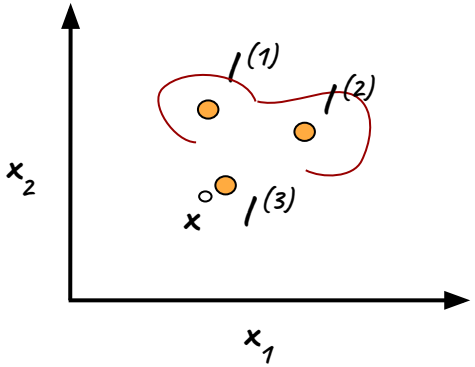

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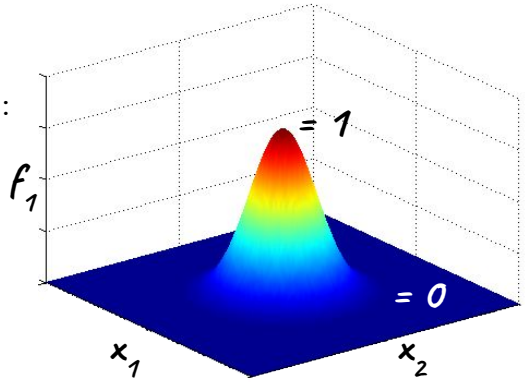

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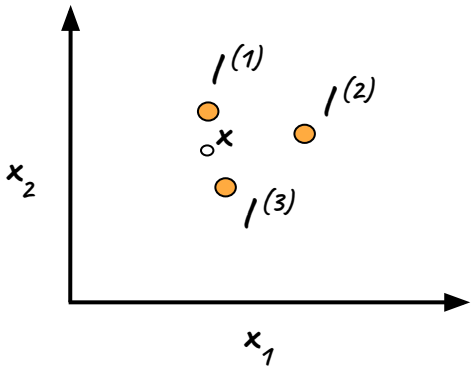

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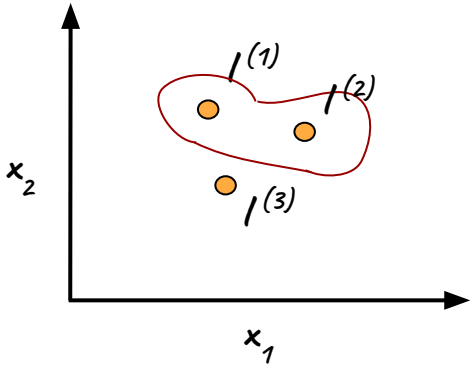

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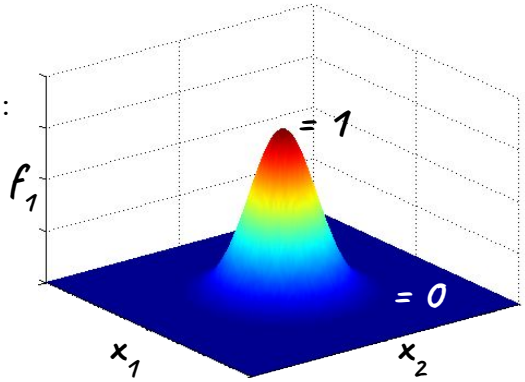

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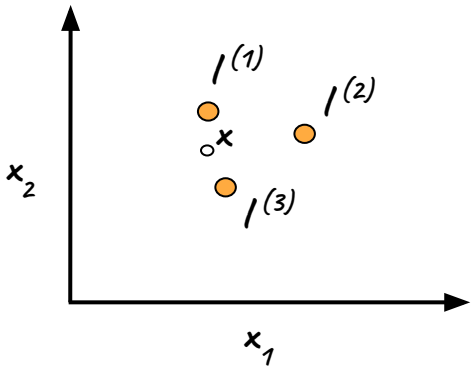

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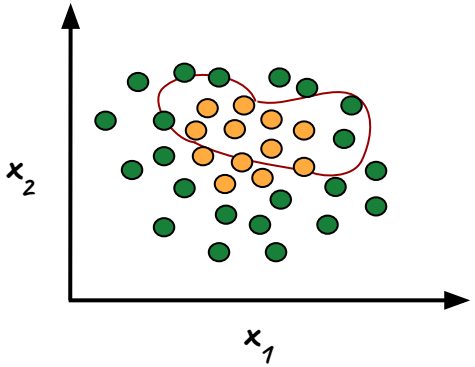

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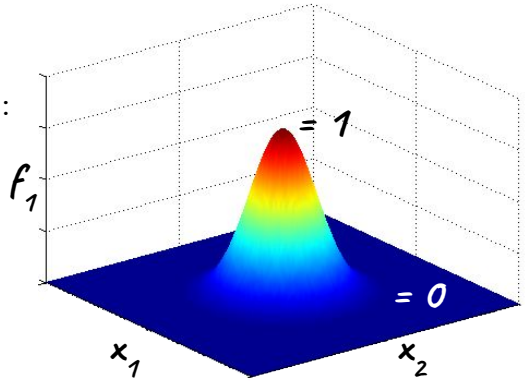

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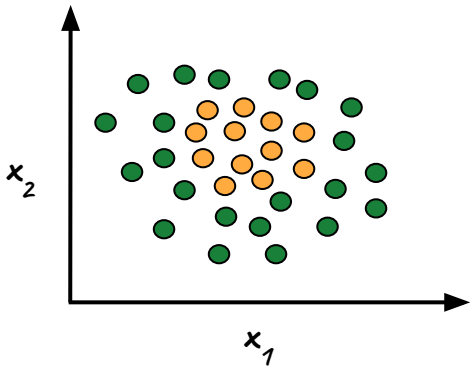
How do we choose the landmarks $l^{(i)}$? And what other kernels are available?



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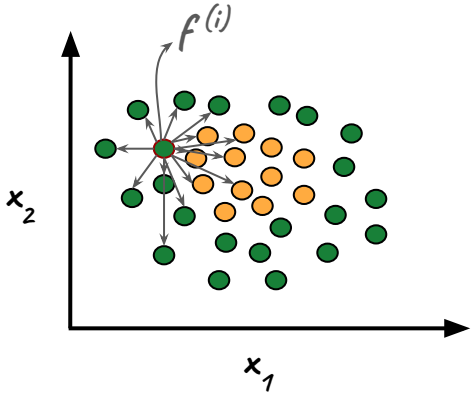

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$$f^{(i)} = [f_0^{(i)}, f_1^{(i)} \dots, f_i^{(i)}, \dots, f_m^{(i)}]$$

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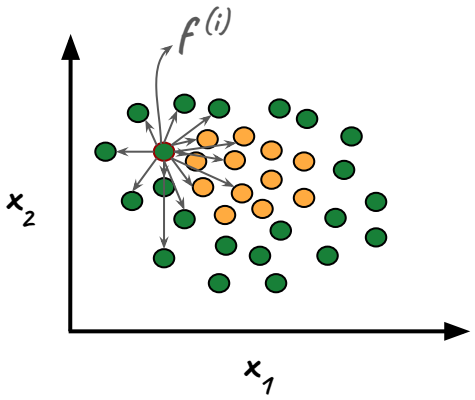

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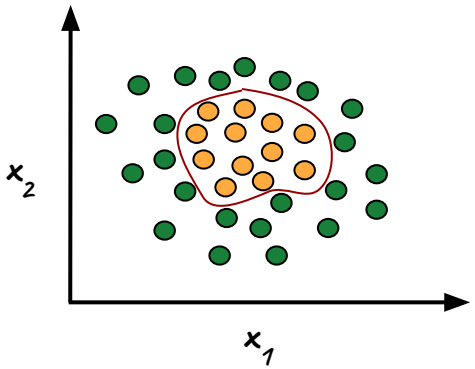
So, we have a feature vector $f^{(i)}$, a weight vector $W = [w_0, w_1, \dots, w_m]$, and a model:

$$w_0 + w_1 f_1^{(i)} + w_2 f_2^{(i)} + \dots + w_m f_m^{(i)} = W^T f^{(i)} \begin{cases} \text{if } W^T f^{(i)} \geq 0 \rightarrow \text{predict } y = 1 \\ \text{if } W^T f^{(i)} < 0 \rightarrow \text{predict } y = 0 \end{cases}$$



trained by minimizing the SVM cost as a function of $W^T f^{(i)}$

$$J(w_i) = C \sum_{i=1}^{m} \left(y^{(i)} \text{cost}_1(W^T f^{(i)}) + (1 - y^{(i)}) \text{cost}_0(W^T f^{(i)}) \right) + \frac{1}{2} \sum_{j=1}^{m} w_j^2$$

In this case (RBF Kernel) the model hyperparameters are:

- C (the inverse of the regularization term)
- $\gamma = 1/\sigma^2$

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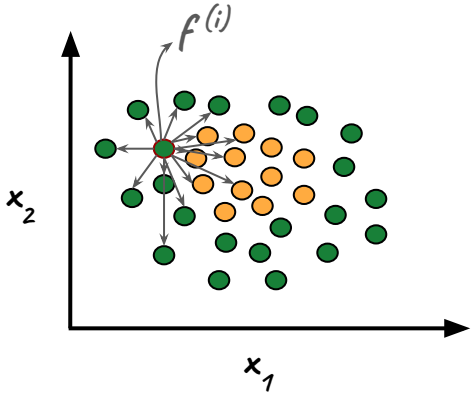
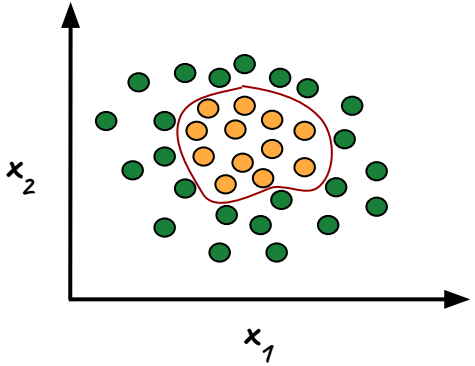
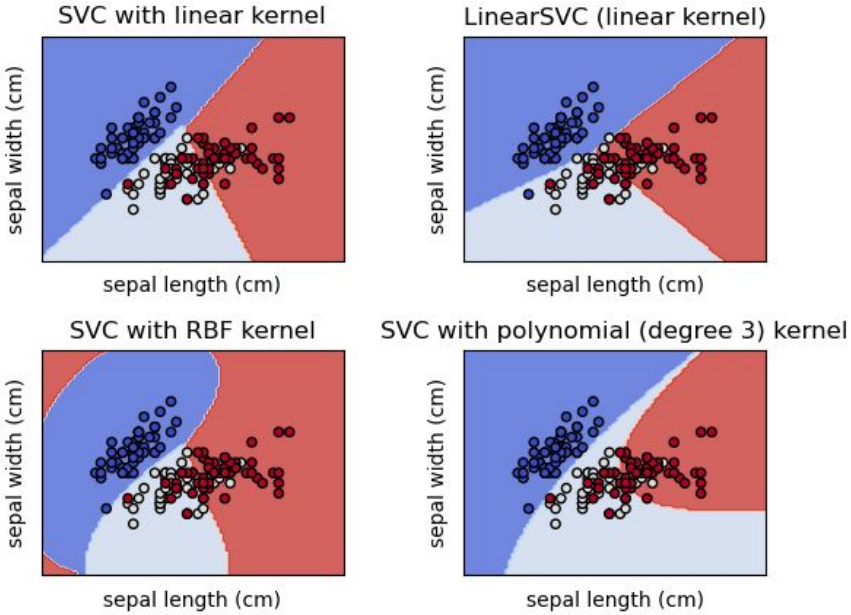




The most commonly used kernels are:

- linear kernel (that is, no kernel altogether)
- radial basis function: $K(x, l^{(i)}) = \exp\{-\gamma \, ||x - l^{(i)}||^2\}$
- polynomial kernel: $K(x, l^{(i)}) = (x^T l^{(i)} + const)^d$
- chi-square kernel: $K(x, l^{(i)}) = \exp\{-\gamma \, \Sigma_i \, [(x - l^{(i)})^2 / (x + l^{(i)})]\}$
- … and more esoteric ones (https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics.pairwise)



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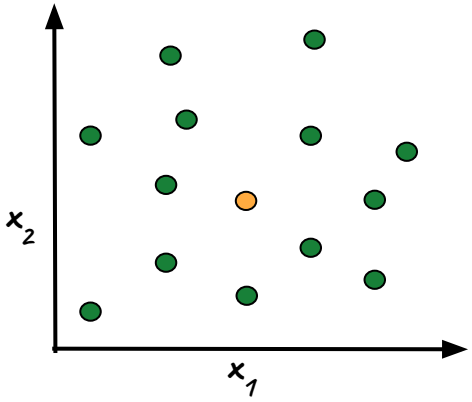
You have a **training** (or ***reference***) sample, $x^{(i)}$, $y^{(i)}$, and a **target** example. The principle is to find a number of **reference** examples closest to the **target** example in the features space, and predict the **target** label y from these.



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The distance can, in general, be **any** metric measure: standard Euclidean distance is the most common choice, but also χ^2 distance, Cosine Distance, Manhattan Distance…

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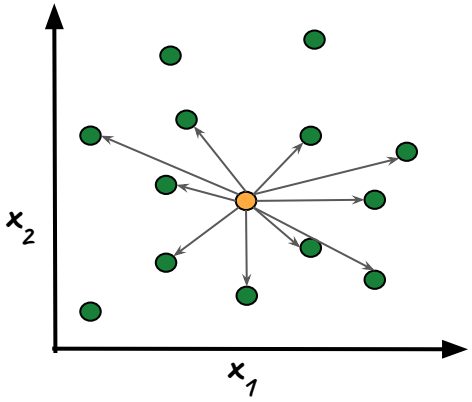

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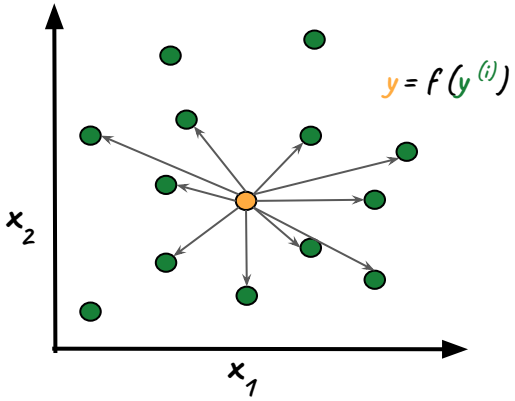

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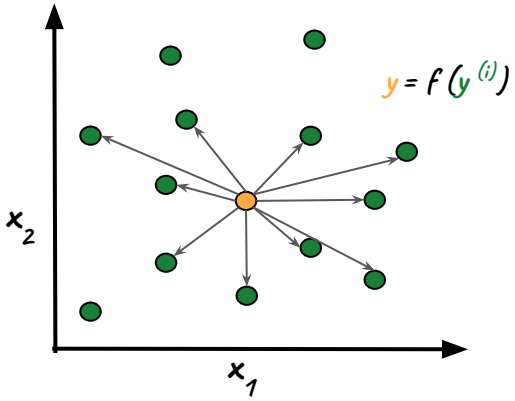

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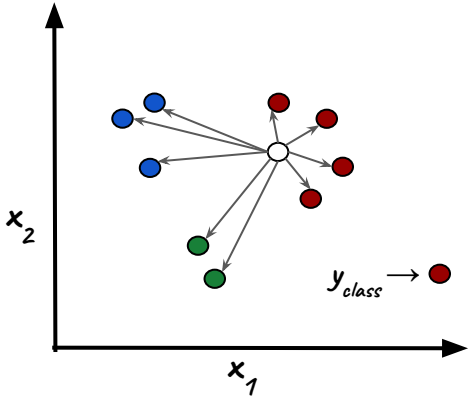

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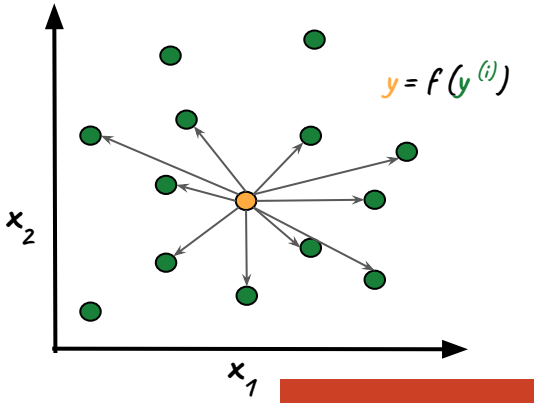

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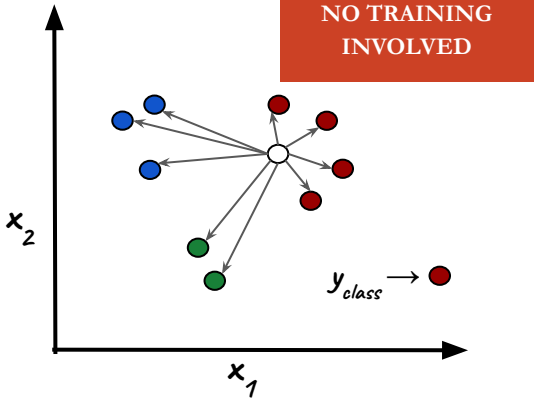

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Finding the nearest neighbors can be achieved in three different ways, depending on the size of your samples.

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With brute force computation, you just measure the distance metric between the target example and **every** reference example. For N samples in D dimensions, this approach scales as O[DN^2]. Works fine for small dataset, quickly explodes as the number of samples N grows.

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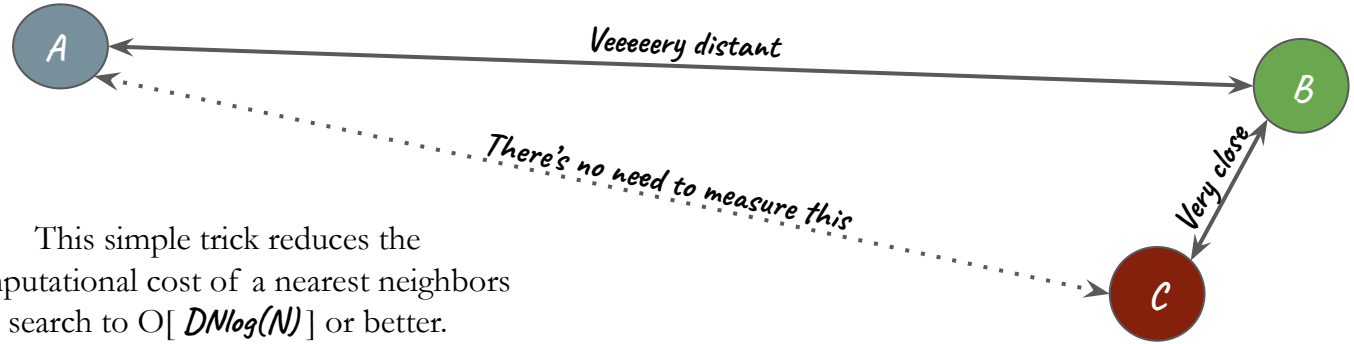
To address the computational inefficiencies of the brute-force approach, a variety of *tree-based data structures* have been invented. These structures attempt to reduce the required number of distance calculations by efficiently encoding aggregate distance information.



This simple trick reduces the computational cost of a nearest neighbors search to O[$DN\log(N)$] or better.

A very distant from B
C very close to B

→A very distant from C without the need to actually compute the distance

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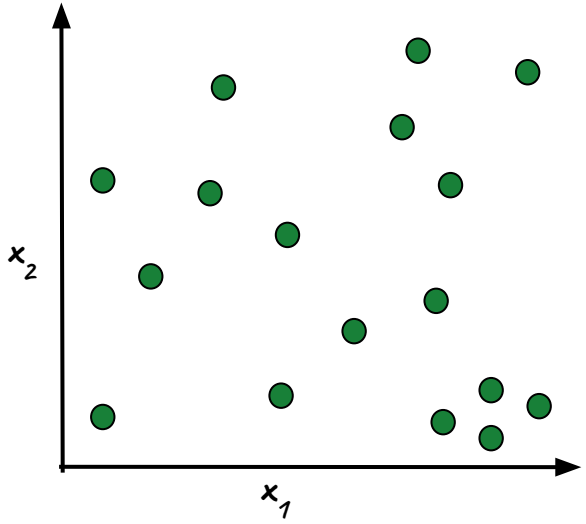

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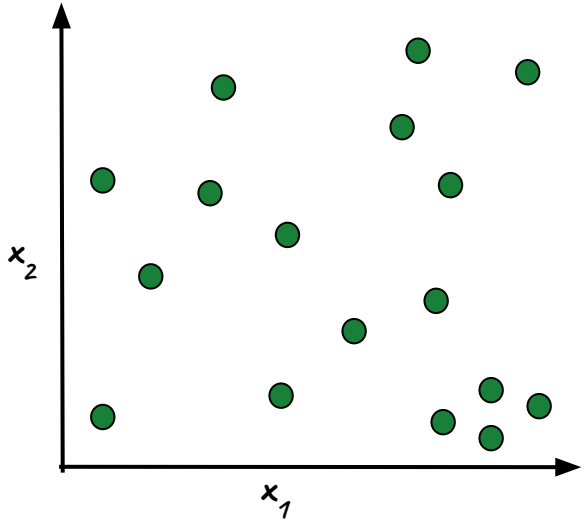

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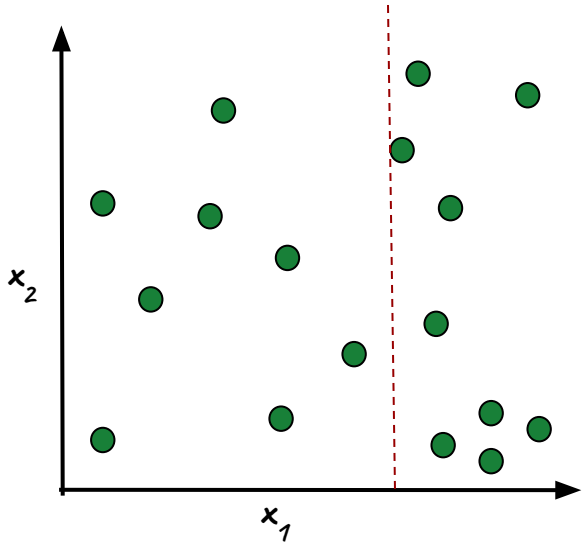

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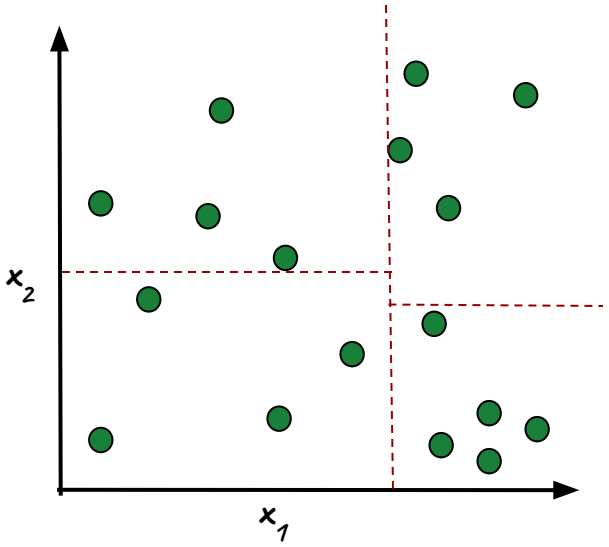

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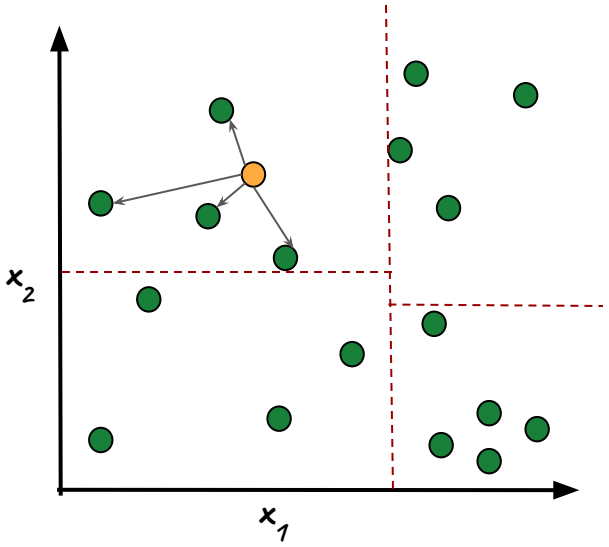

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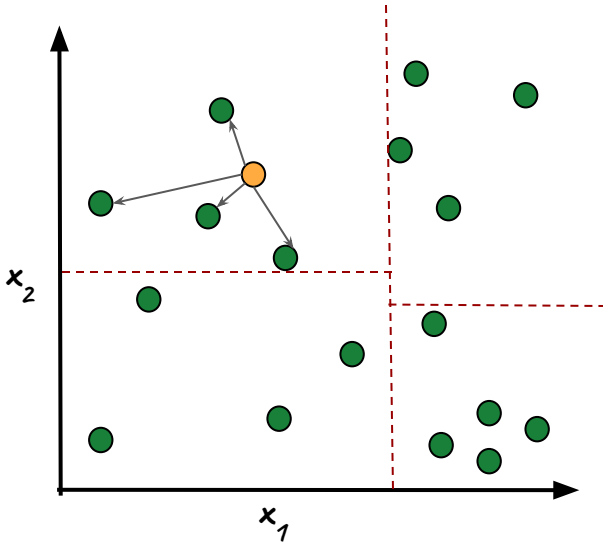

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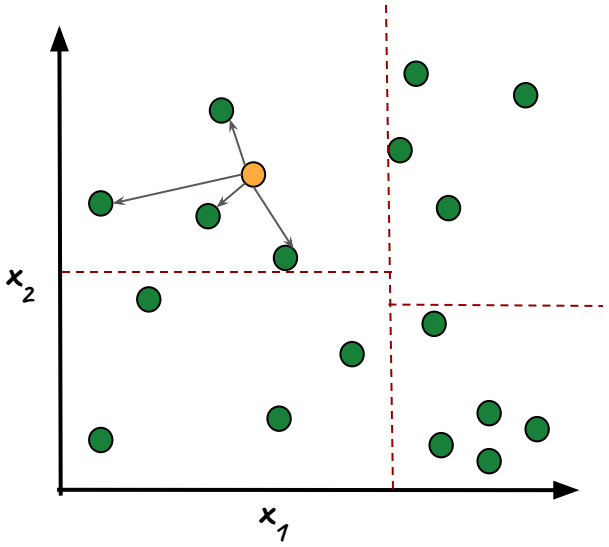

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Building a a KD tree is very fast: partitioning is performed only along the data axes, so no dimensional distances need to be computed.
Once built, the nearest neighbor of a query point can be determined with only O[$\log(N)$] distance computations.
Though the KD tree approach is very fast for low-dimensional ($D<20$) neighbors searches, it becomes inefficient as D grows very large: this is one manifestation of the so-called "*curse of dimensionality*" (more on that next week in Unsupervised Learning)

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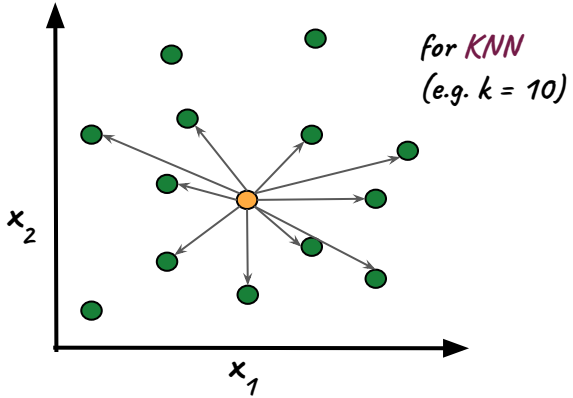

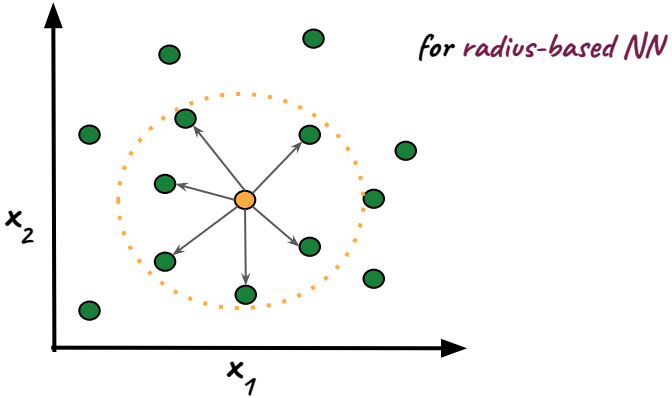

Consider the following example: measuring galaxies' distances based on their observed photometry (photometric redshift).
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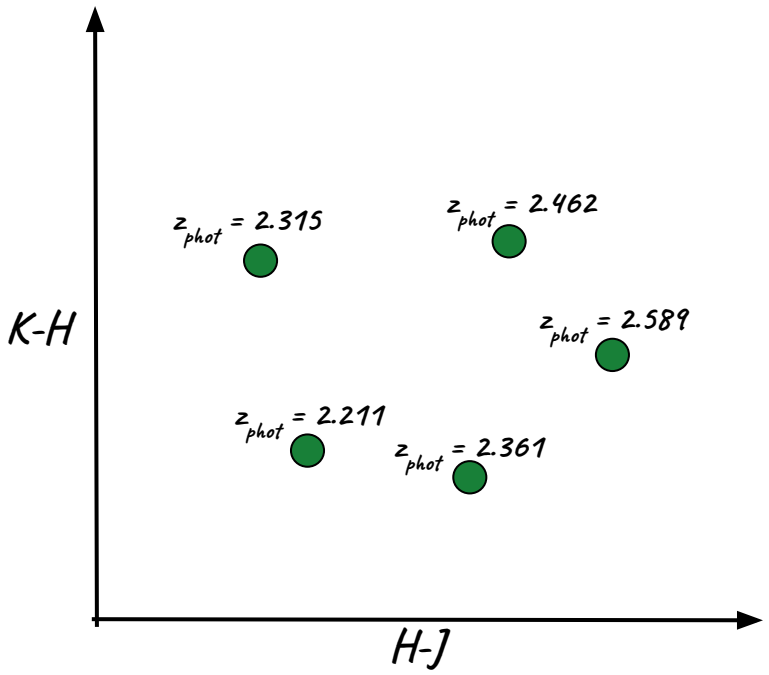

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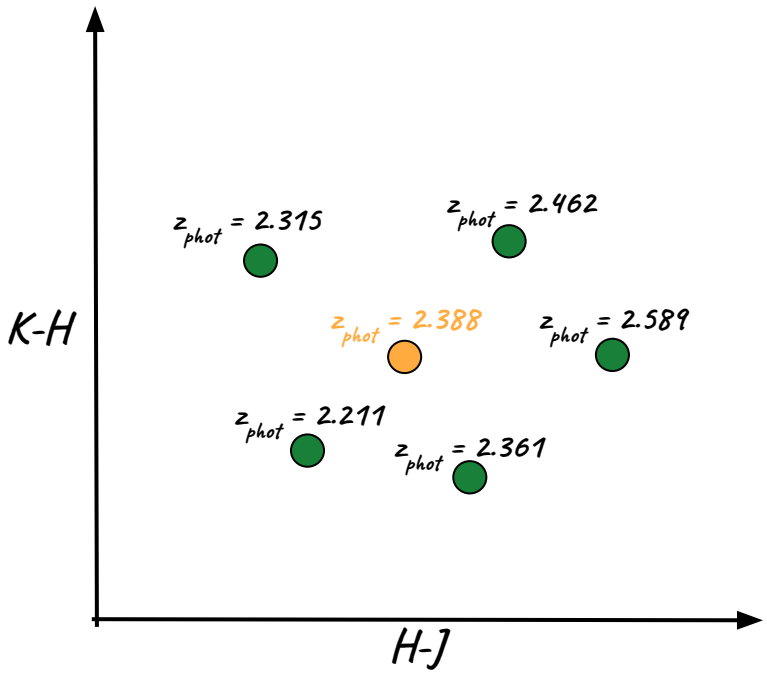

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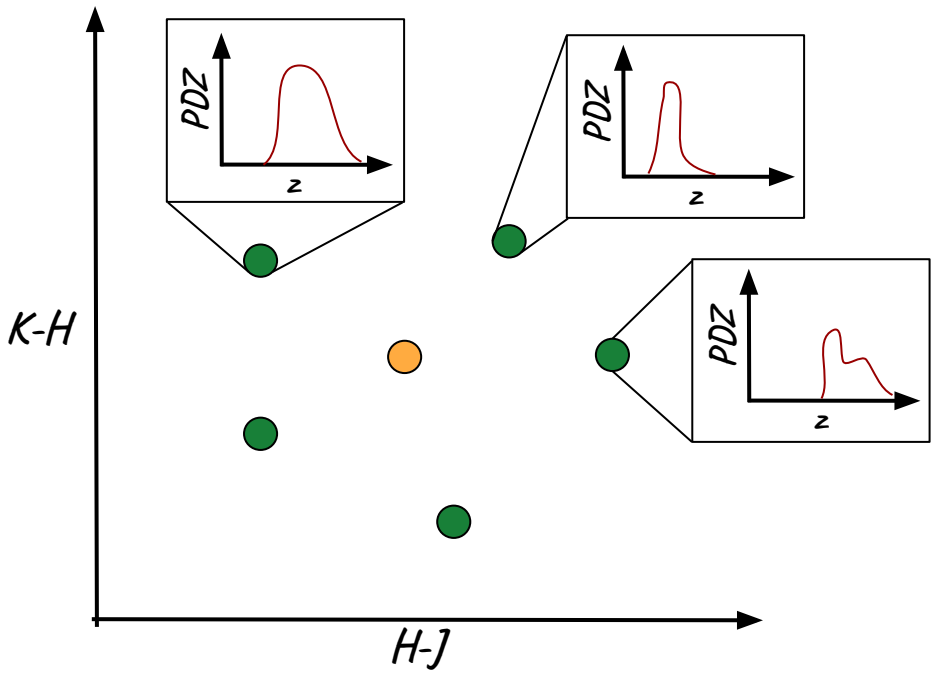

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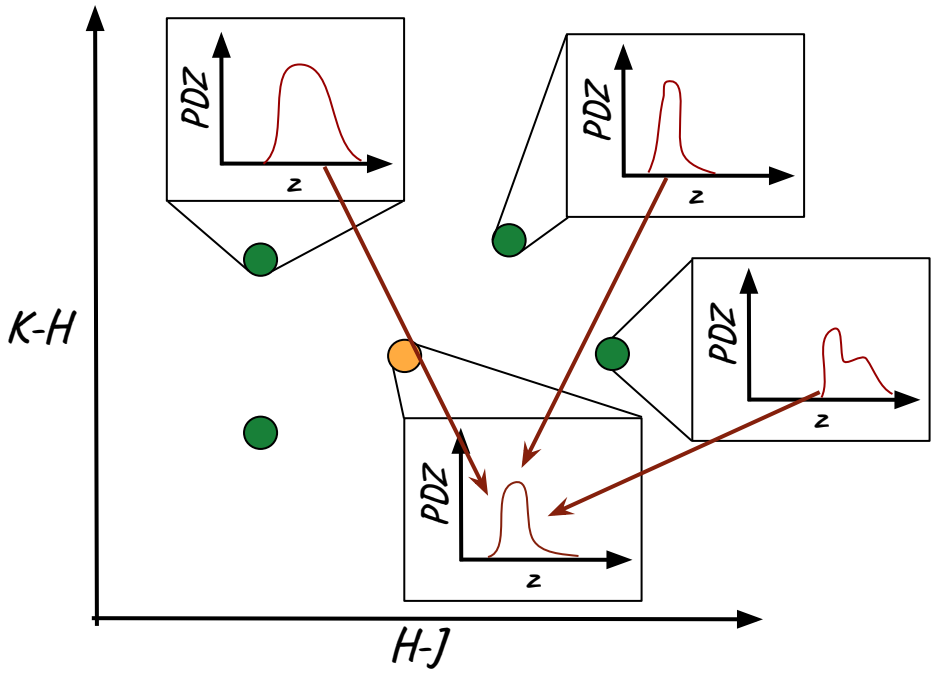

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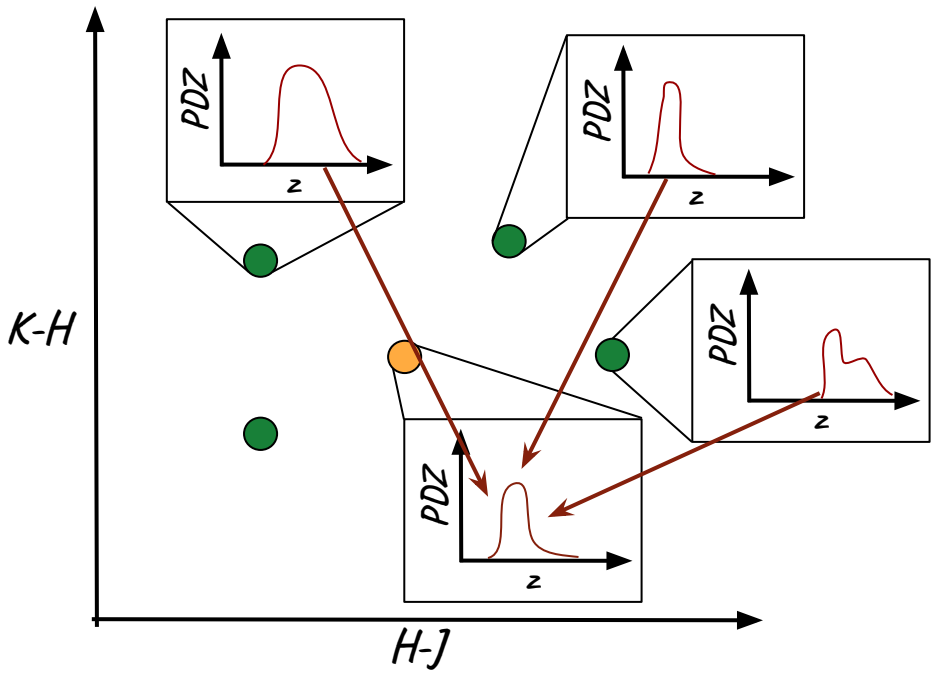

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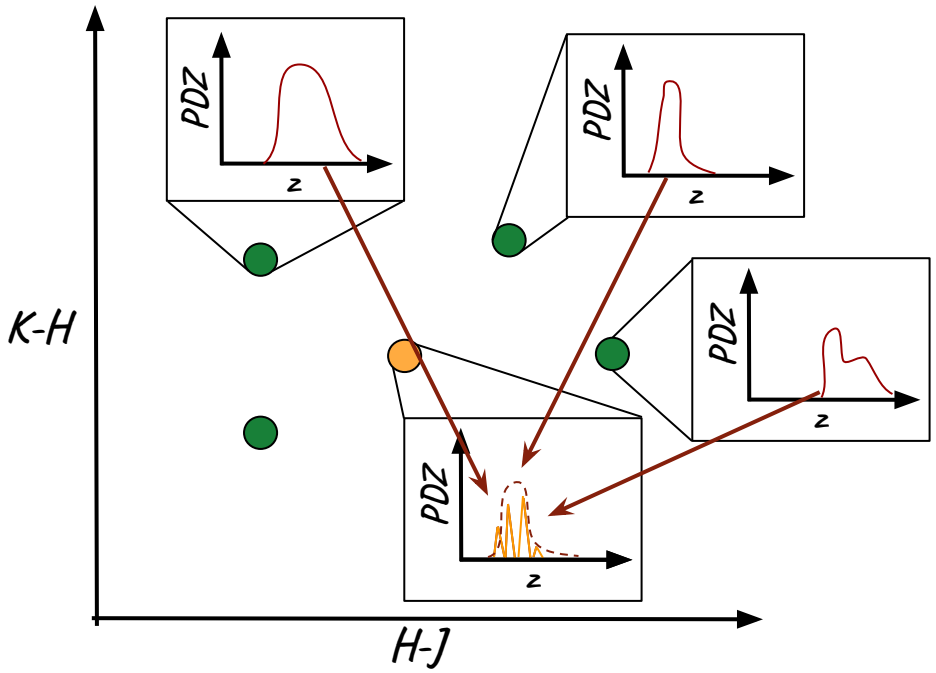

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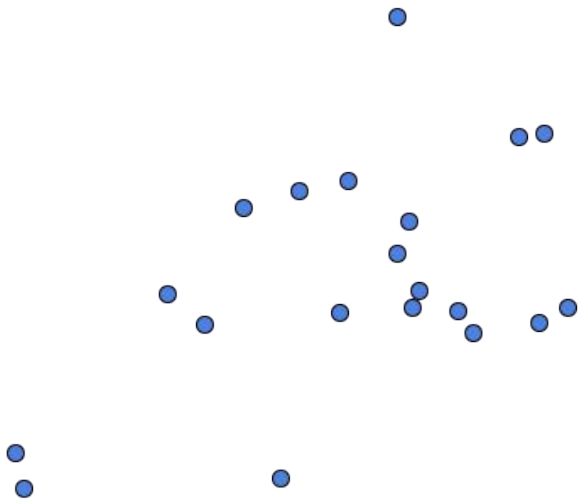

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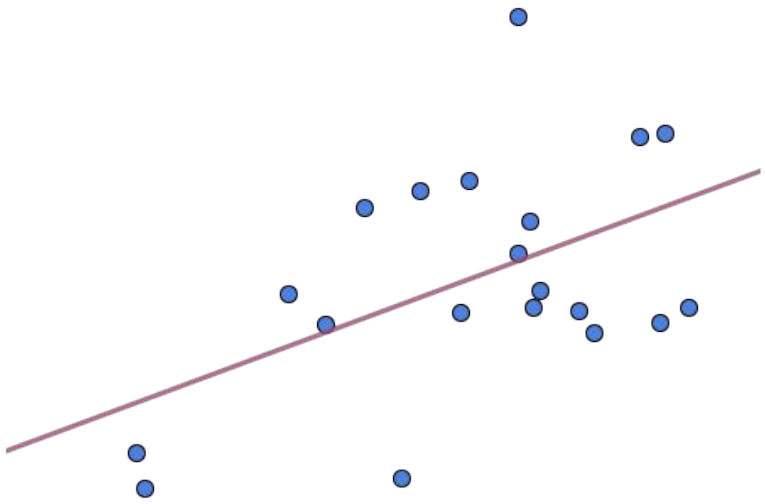

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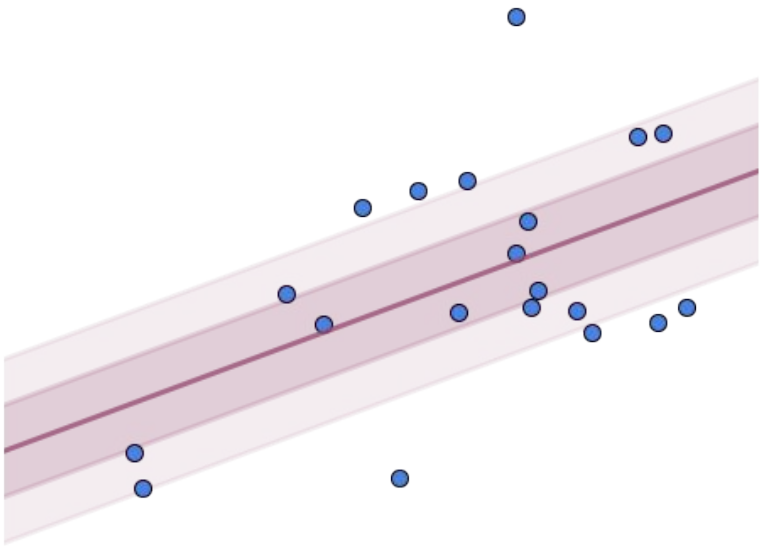

This is the typical linear regression algorithm showed yesterday, which gives back informative results once coupled with the variance of the observed (training) data, but misses completely the uncertainty on the model itself.
How to capture it?

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Let's forget for the data for a second, and consider the model we're trying to fit. Without data, the model is a set of all the possible linear solutions that are in the parameter space. We'll call it the ***prior samples*** (on the left, 70 possible linear solutions with some priors on the weight $\boldsymbol{w}$ and bias $\boldsymbol{b}$) *.

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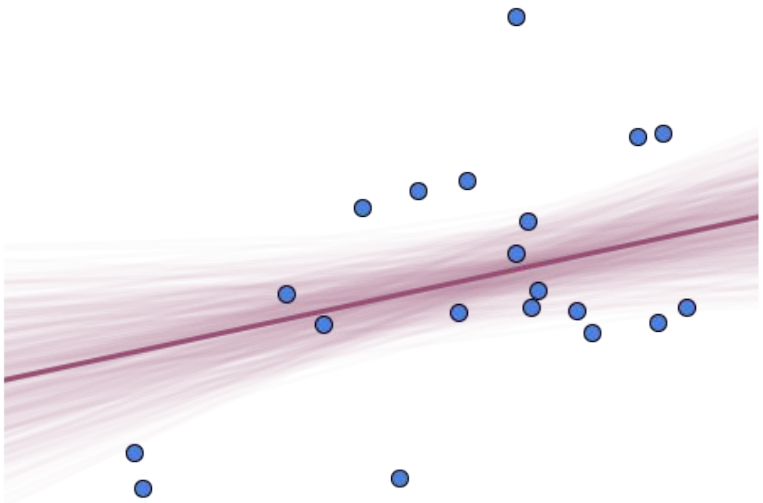

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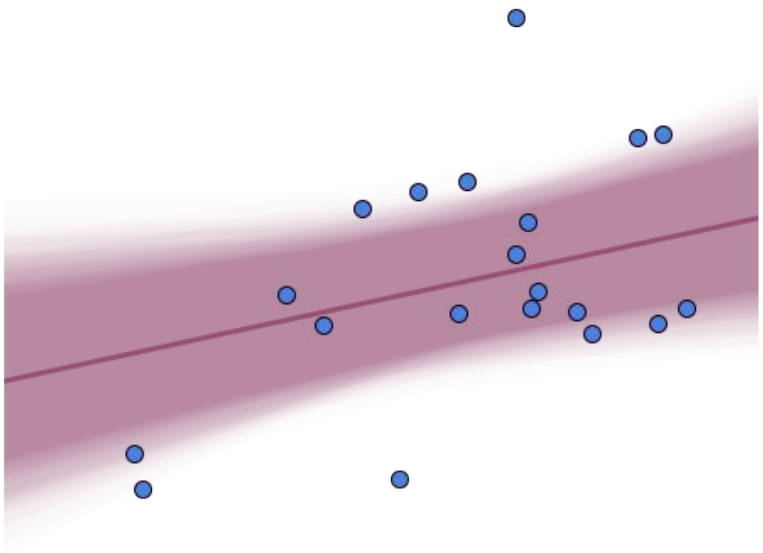

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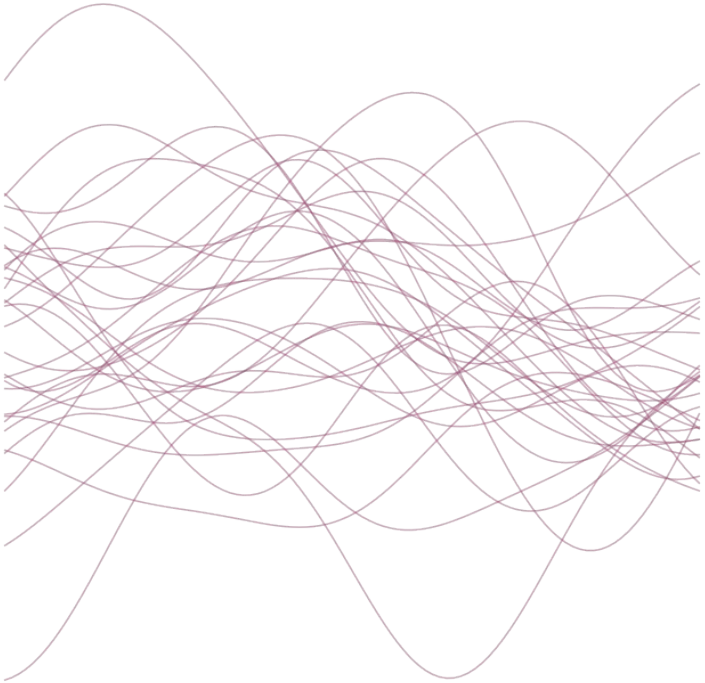

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The mechanics of GPs is exactly the same, but instead of dealing with lines, we deal with samples over general functions.

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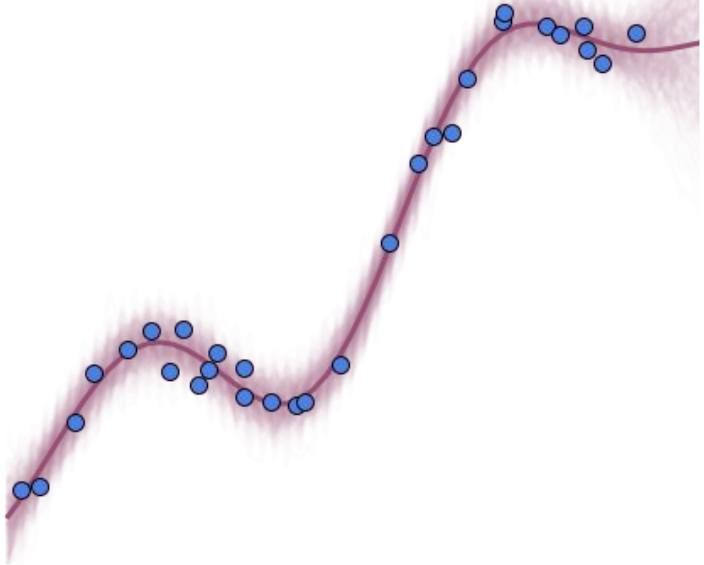

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Let's forget for the data for a second, and consider the model we're trying to fit. Without data, the model is a set of all the possible linear solutions that are in the parameter space. We'll call it the *prior samples* (on the left, 70 possible linear solutions with some priors on the weight w and bias b).
Now, we use Bayes' theorem to update the model such that it produces samples that agree with our data.
In this way we get the *posterior samples*:

$$\text{Prior samples (Model)} + \text{Data} \xrightarrow[\text{theorem}]{\text{Bayes'}} \text{Posterior samples}$$

Applying a noise variance to each sample will lead to a predictive distribution, that we can average over many (in principle infinite) samples.
As you can see, the intervals become a bit wider far away from the bulk of data, which is a big improvement with respect to the fixed intervals we had with simple linear regression.
The mechanics of GPs is exactly the same, but instead of dealing with lines, we deal with samples over general functions.

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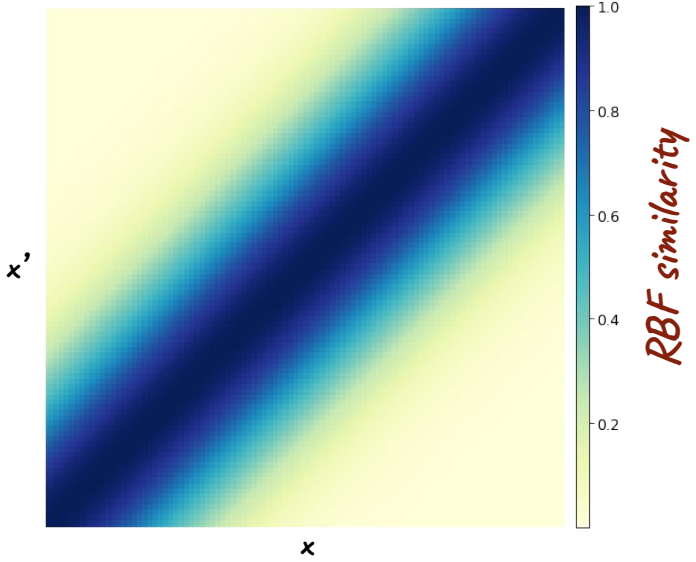

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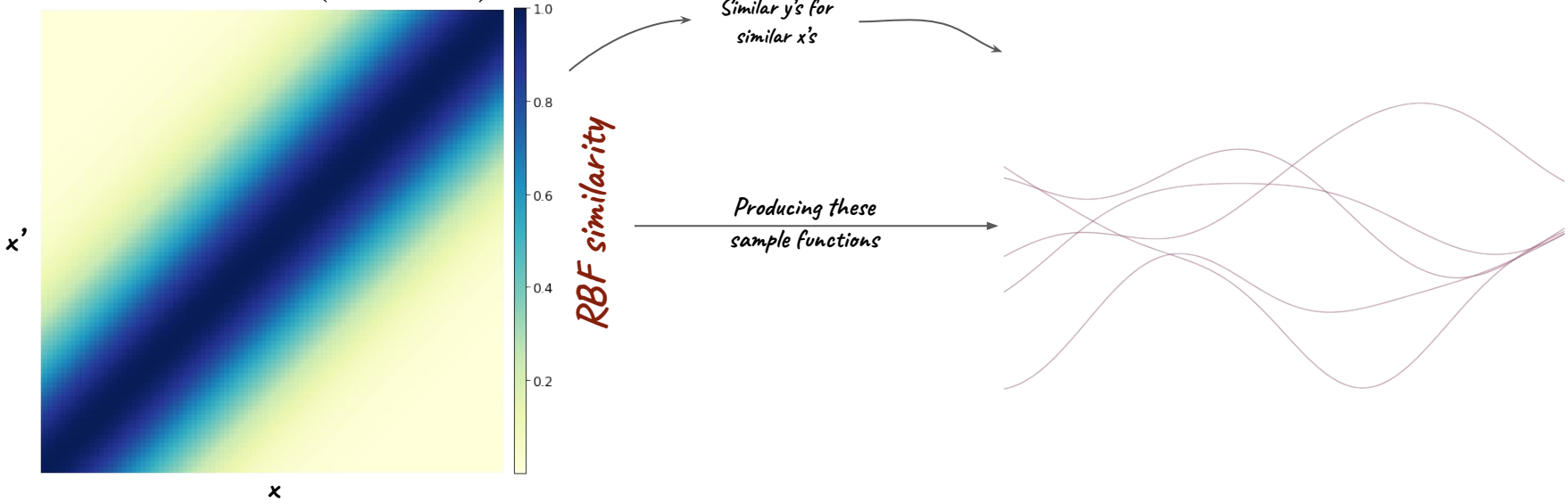

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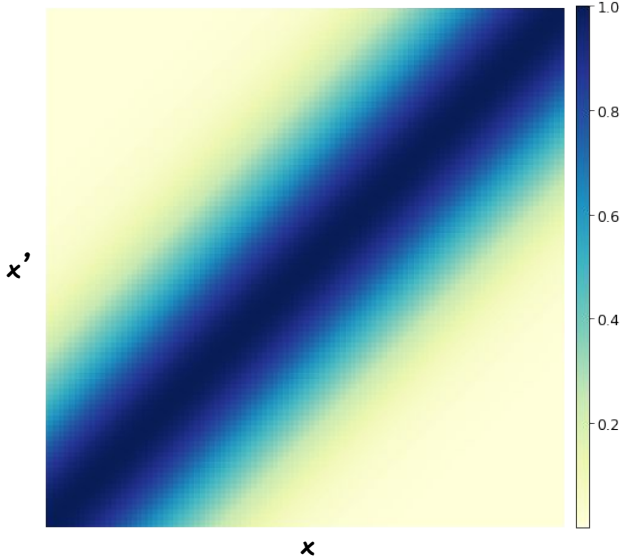
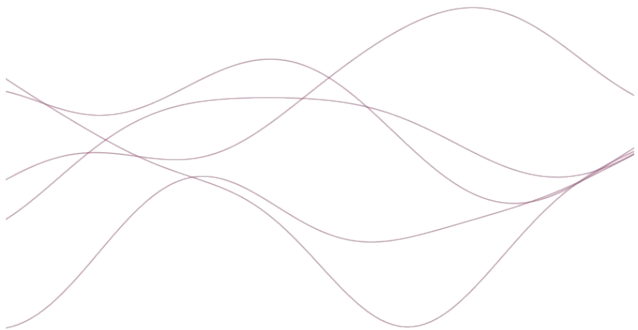
"length scale".



Producing these sample functions



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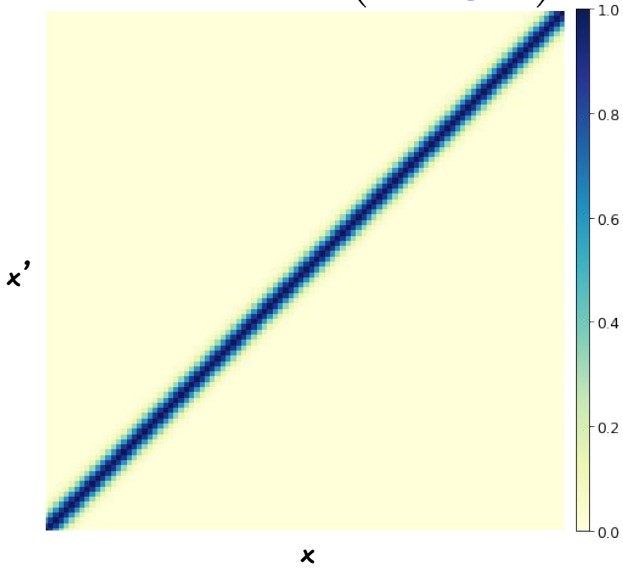
"length scale": *for smaller values, most input pairs are considered different, therefore the samples wiggle more rapidly*



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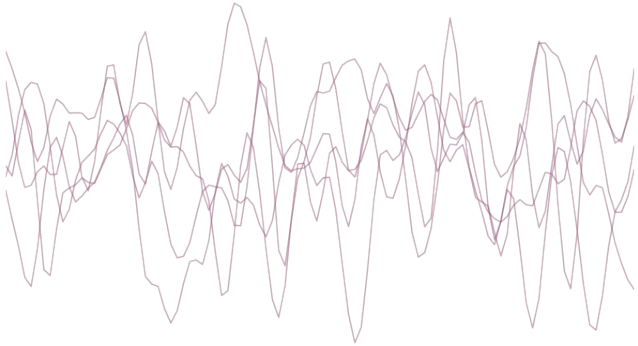

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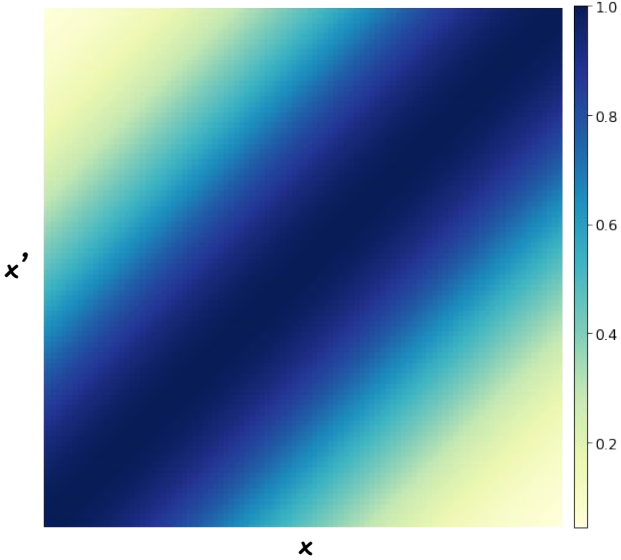

RBF similarity

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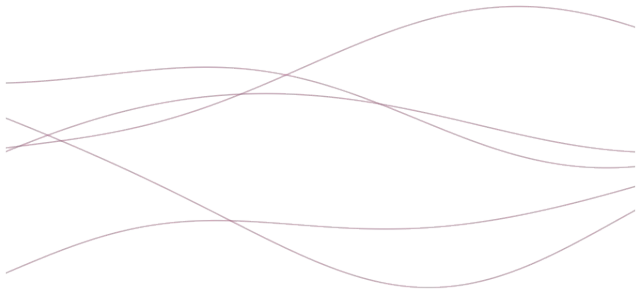

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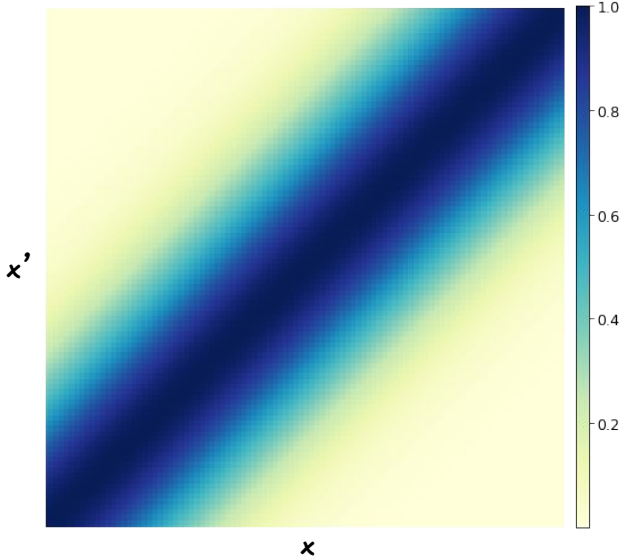
"output scale": determines the scale of the y axis.



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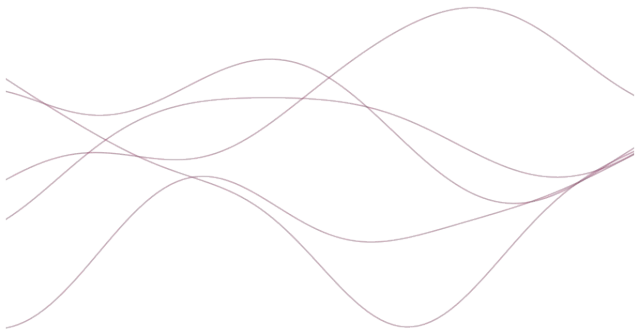

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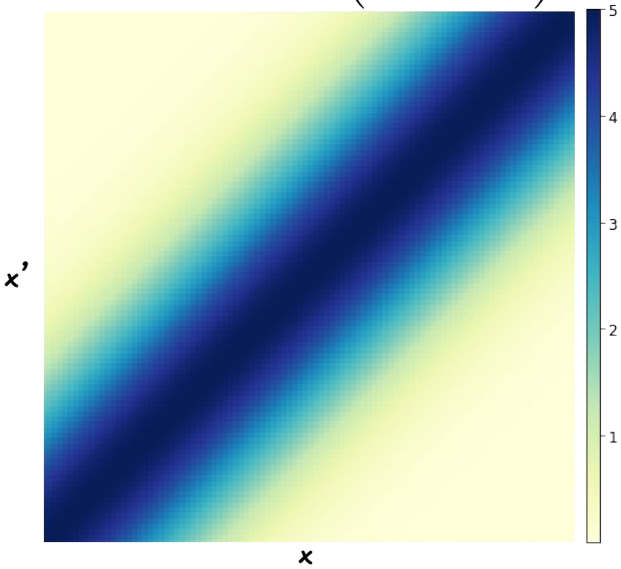
"output scale": *determines the scale of the y axis. Increase it and the functions will span more of the vertical axes (notice the color limits on the left)*



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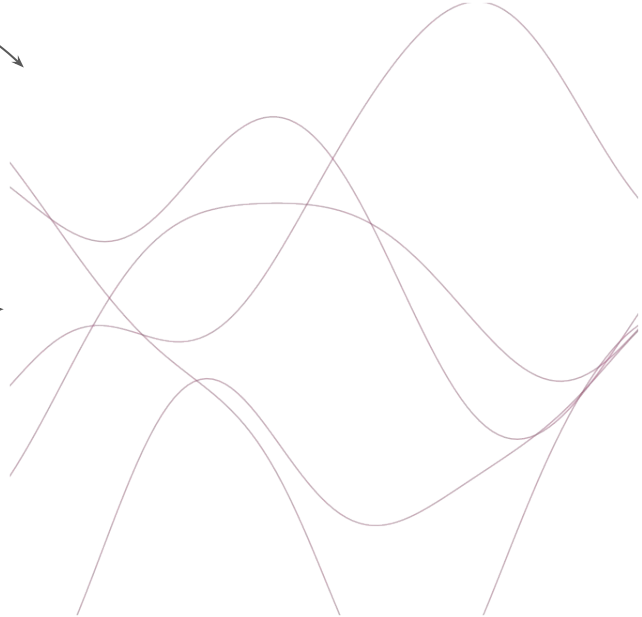

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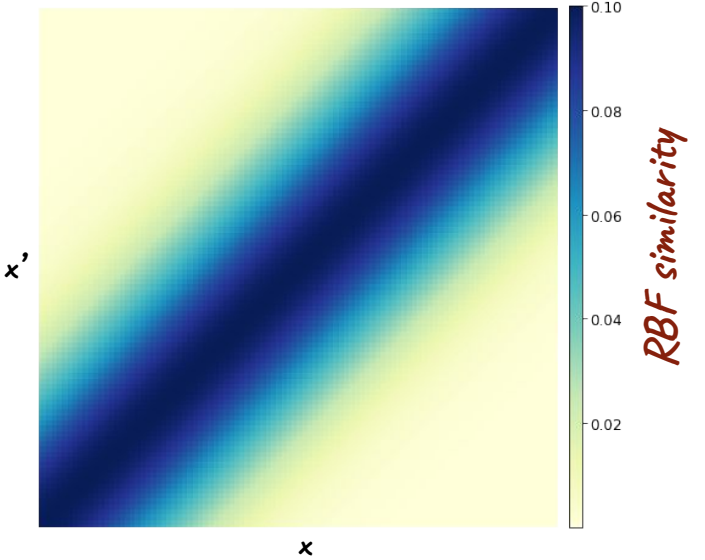

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$$K_c(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}_c) = K_a(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}_a) + K_b(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}_b)$$

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$$K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}) = cK(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau})$$

$$K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}) = g(\mathbf{x})K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau})g(\mathbf{x}') \text{ for any function } g$$

$$K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}) = q(K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau})) \text{ for positive coefficient polynomial } q$$

$$K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}) = \exp(K(\mathbf{x}, \mathbf{x}' / \boldsymbol{\tau}))$$

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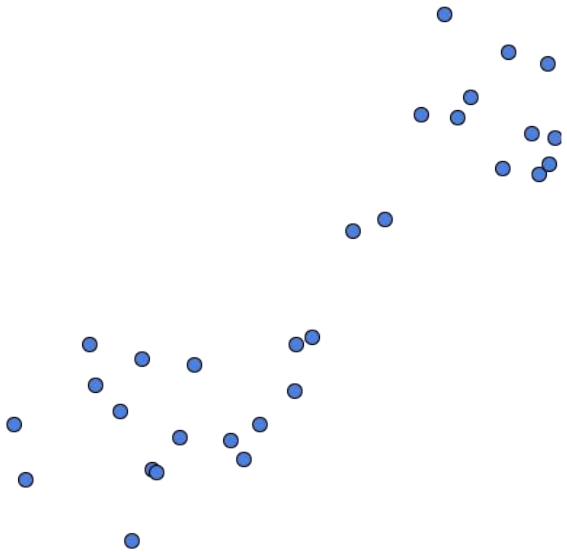

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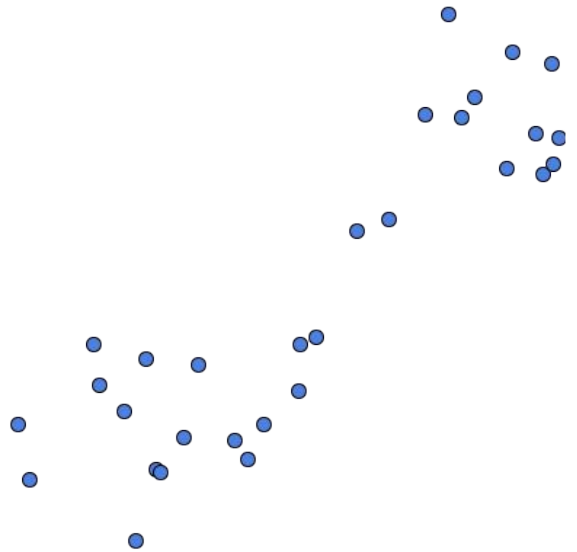

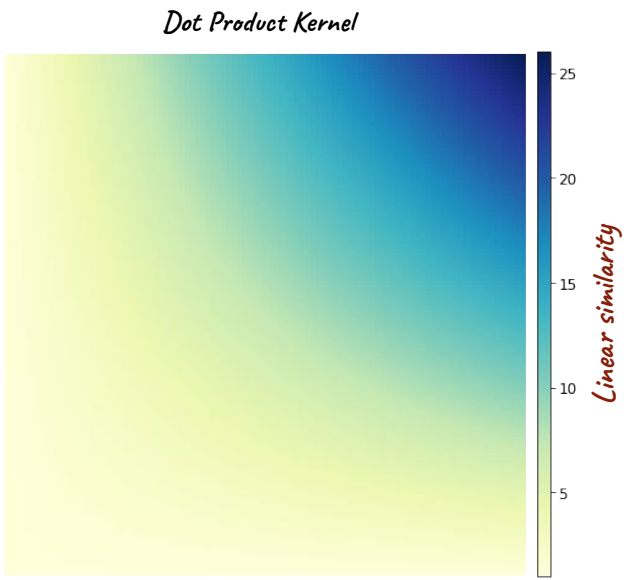

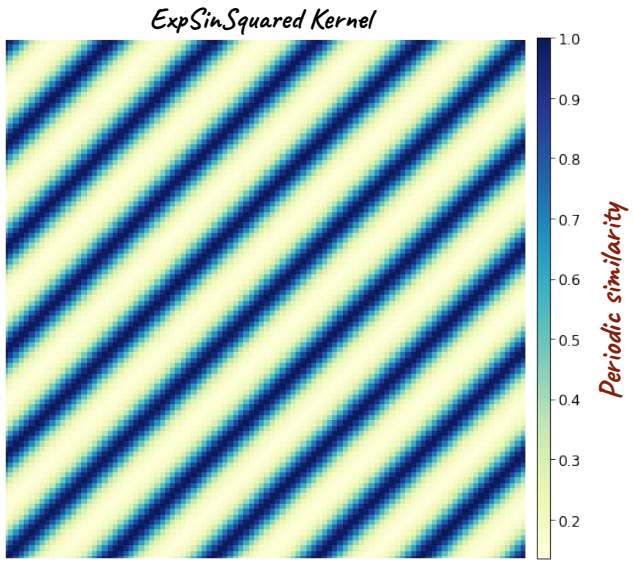

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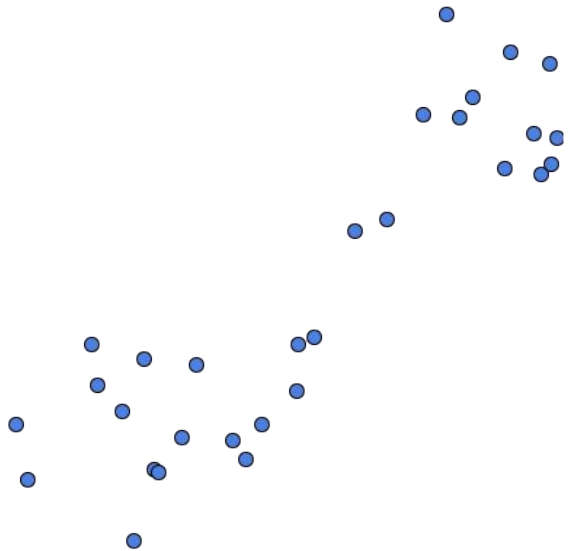

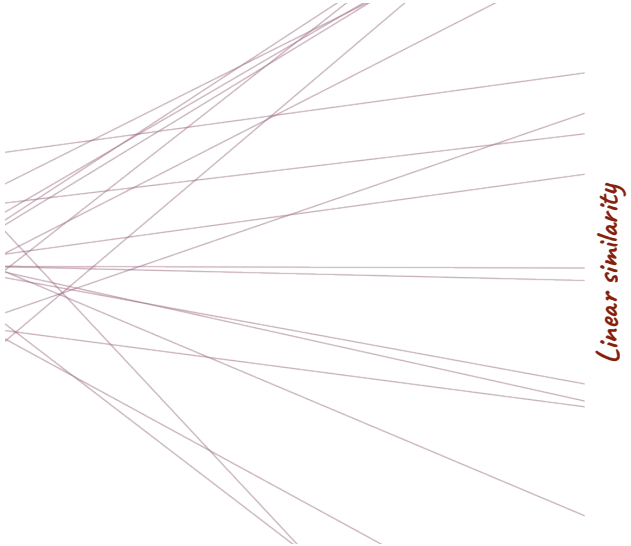

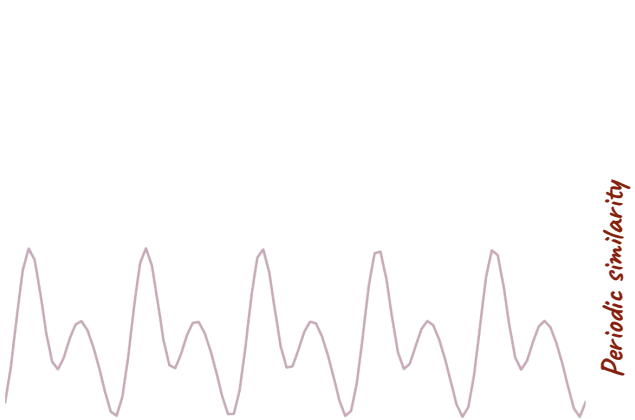

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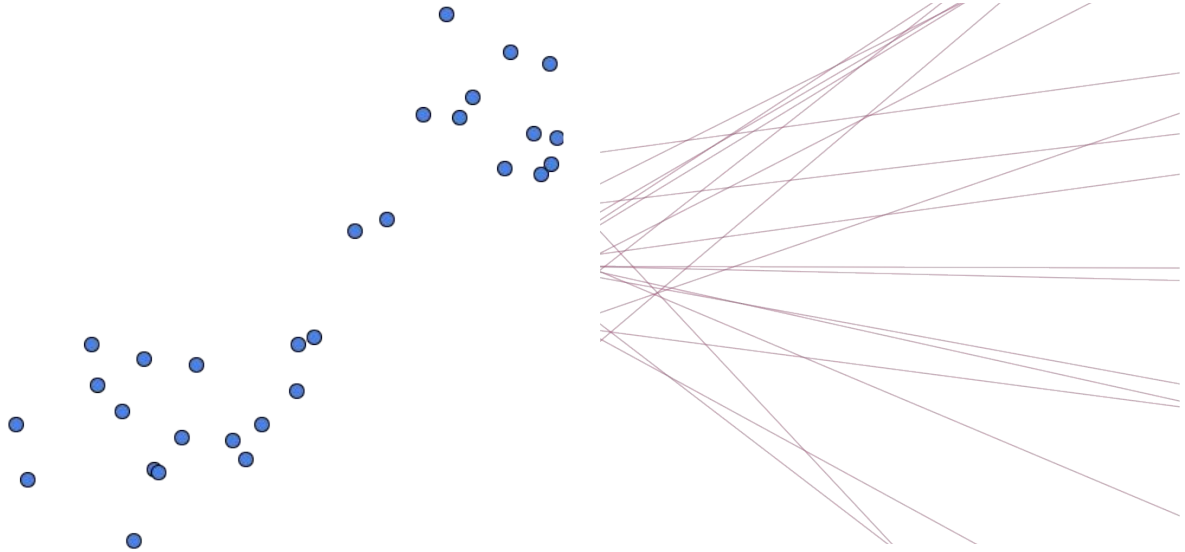

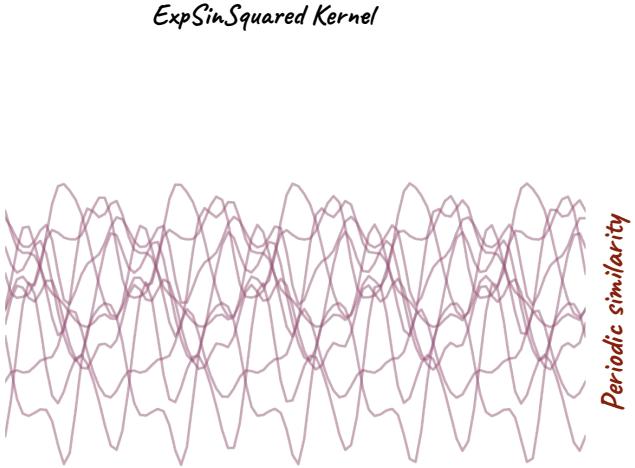

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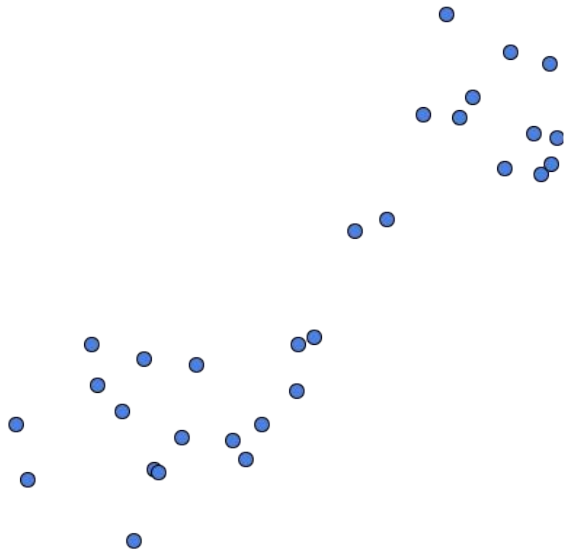

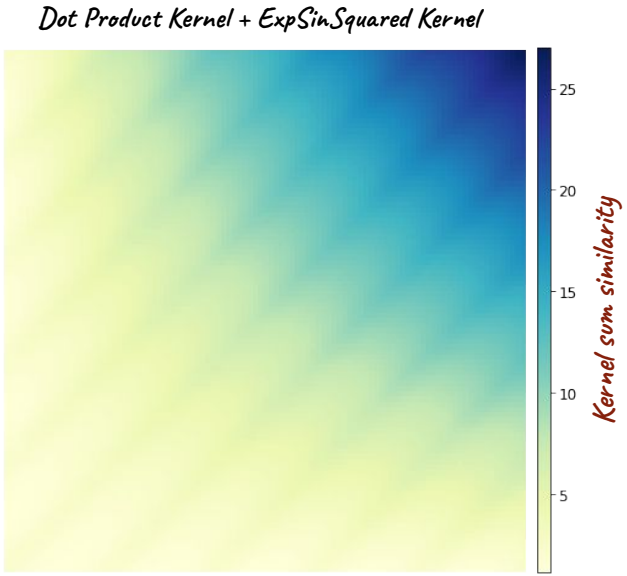

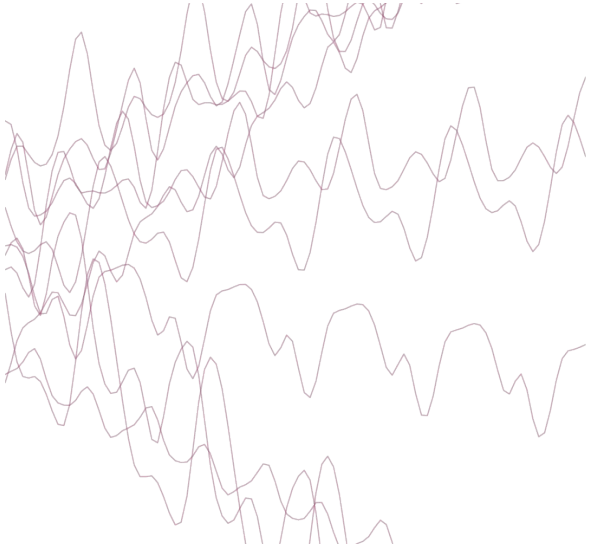

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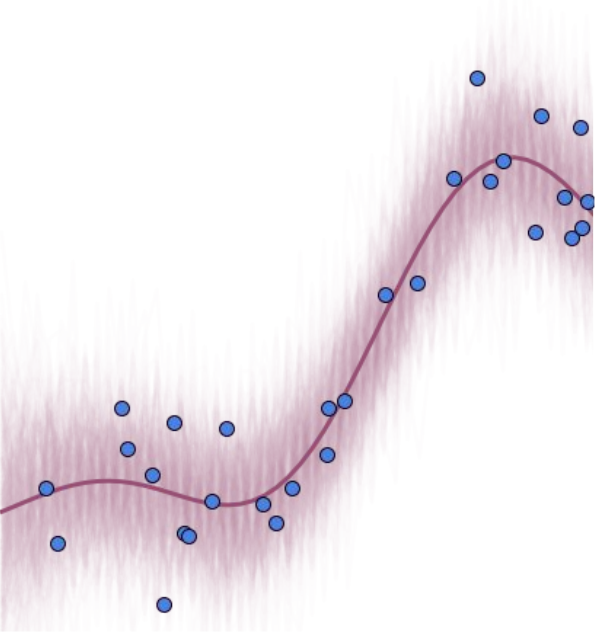

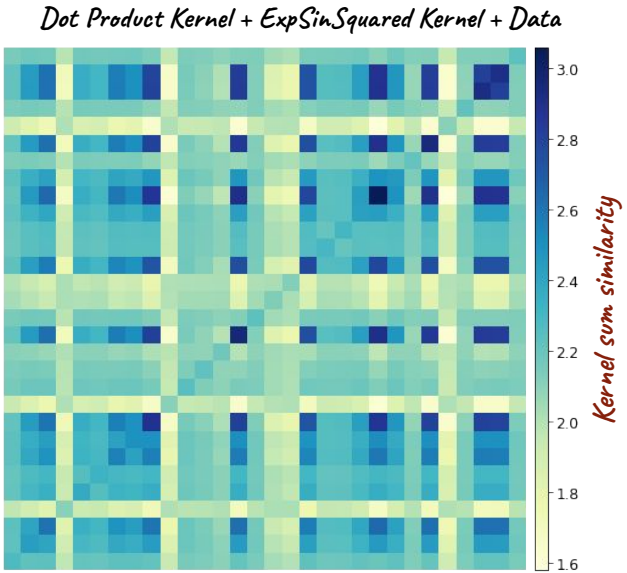

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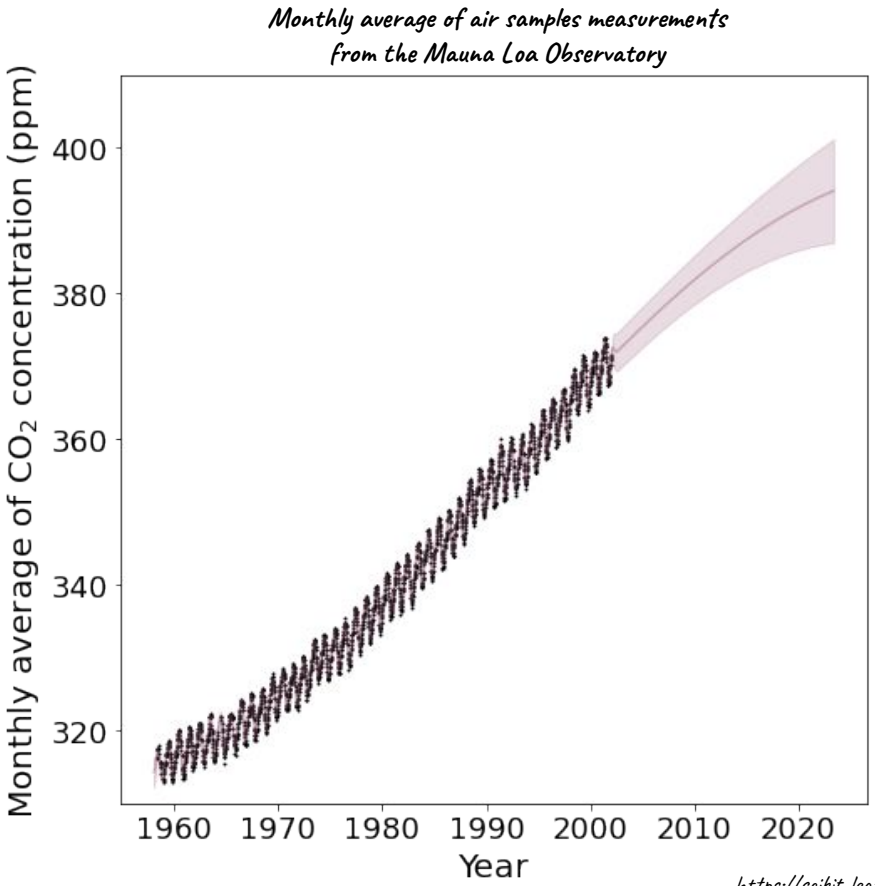

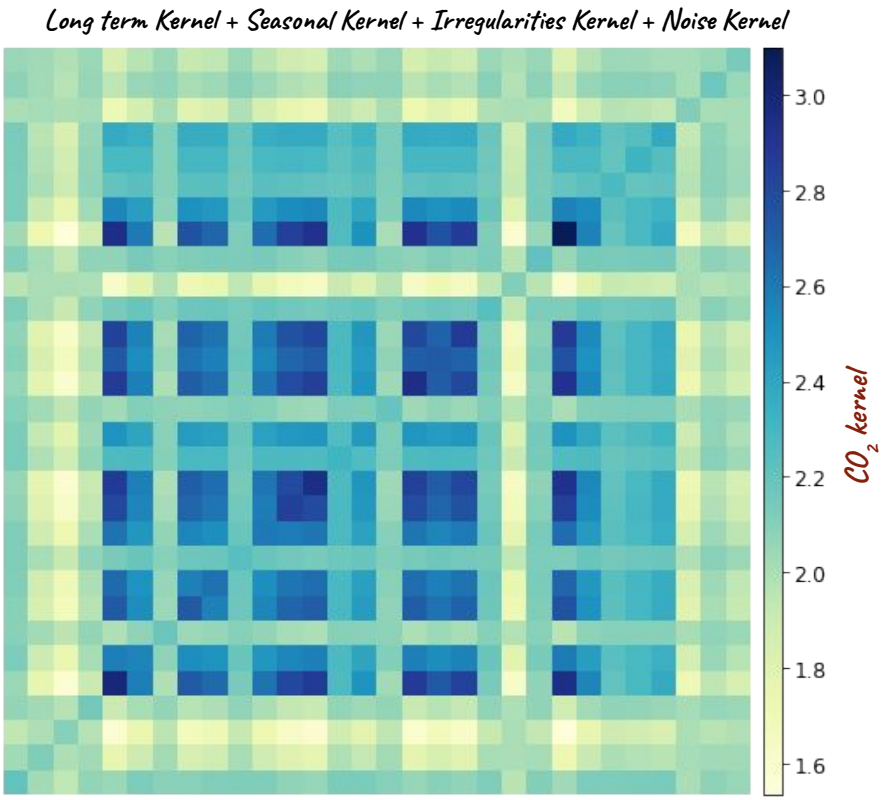

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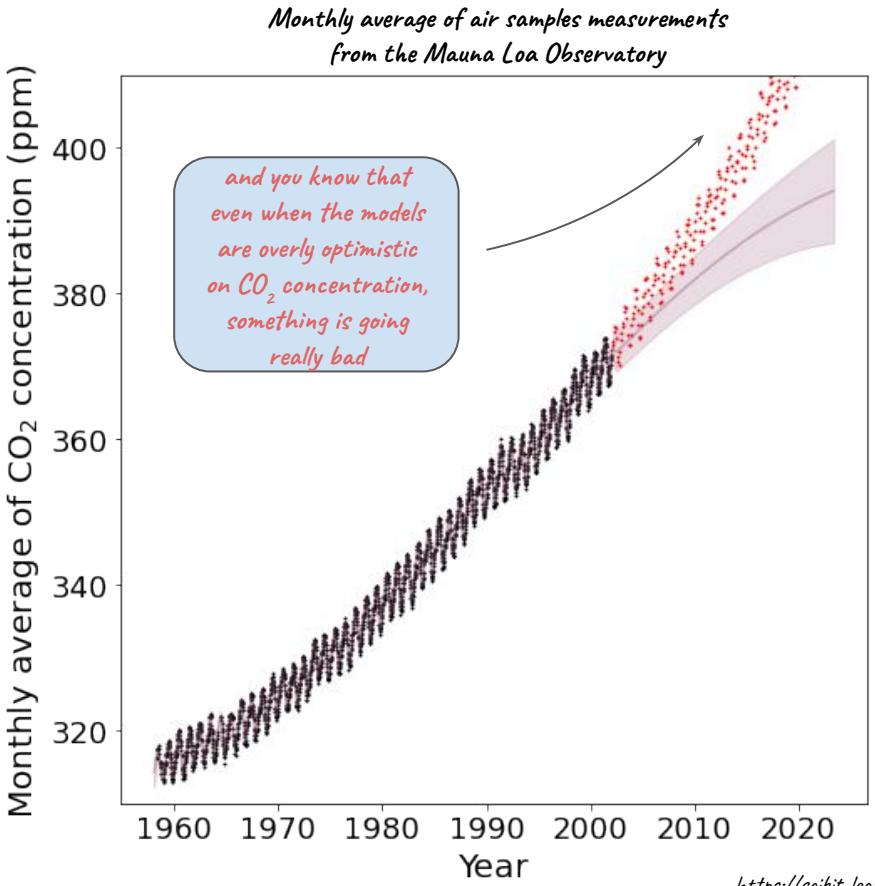

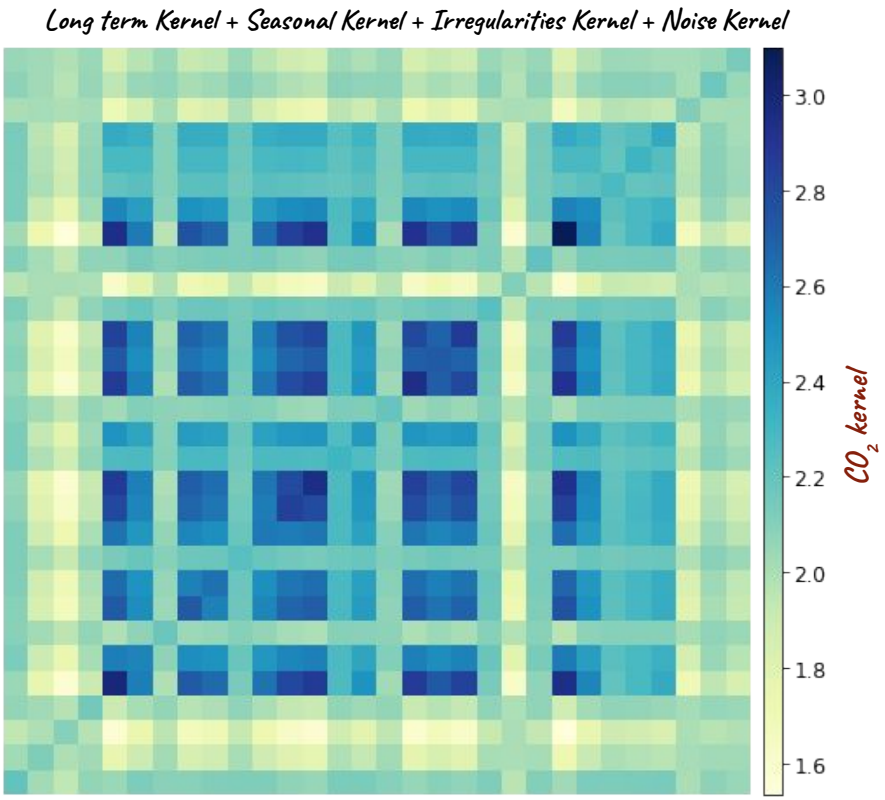

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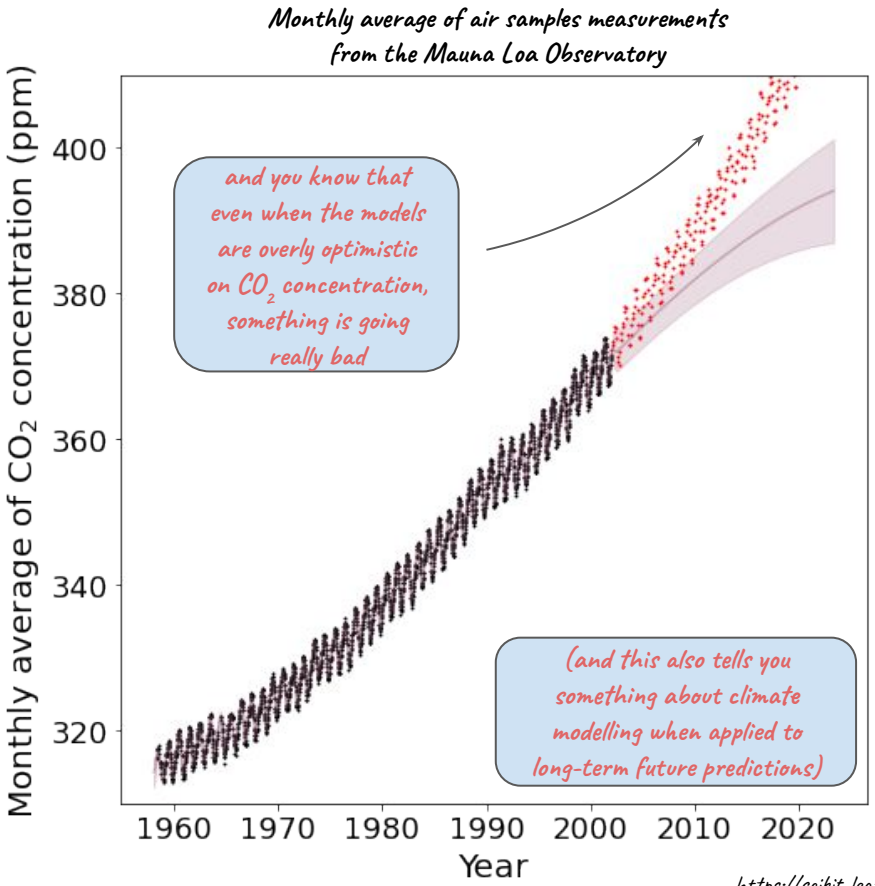

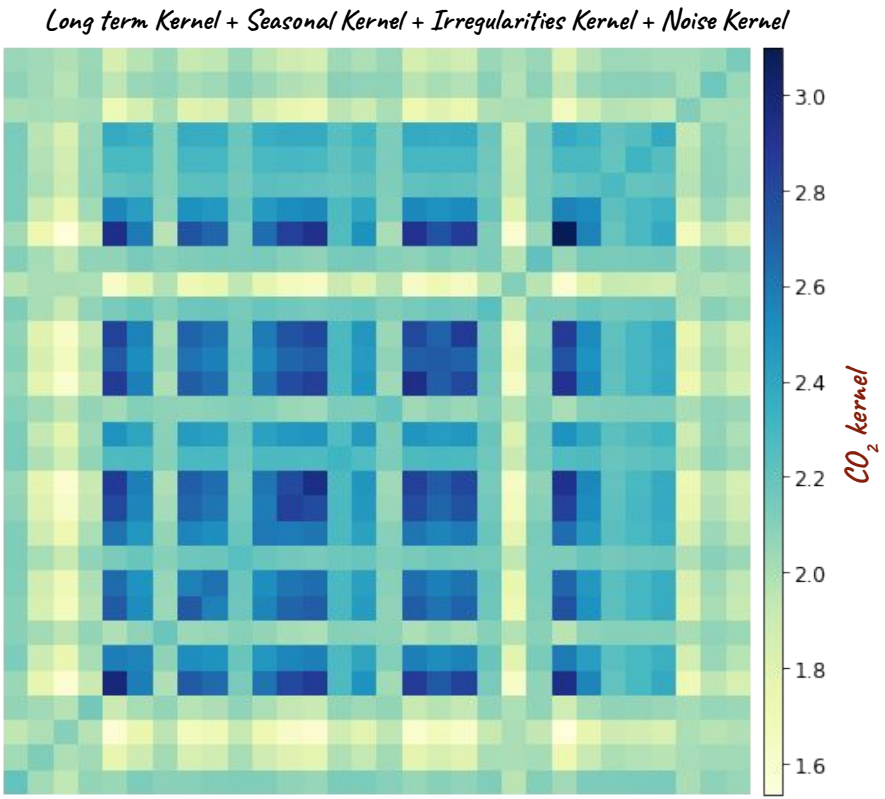

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means normal distribution centred on 0 and with variance σ_ε, which is another model hyperparameter

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That covariance matrix is made up of our kernel similarities between all inputs

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For the submatrix governing y, we add the noise variance to the diagonal

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Assuming that the covariance matrix is just the similarities of x's has the effect of smoothing the whole models (which is common in ML)

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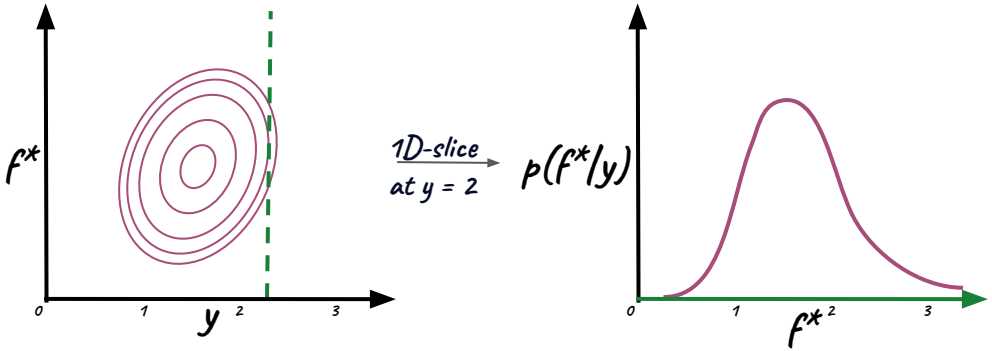
This is called *conditioning*. Let's see a simple example 1D example:



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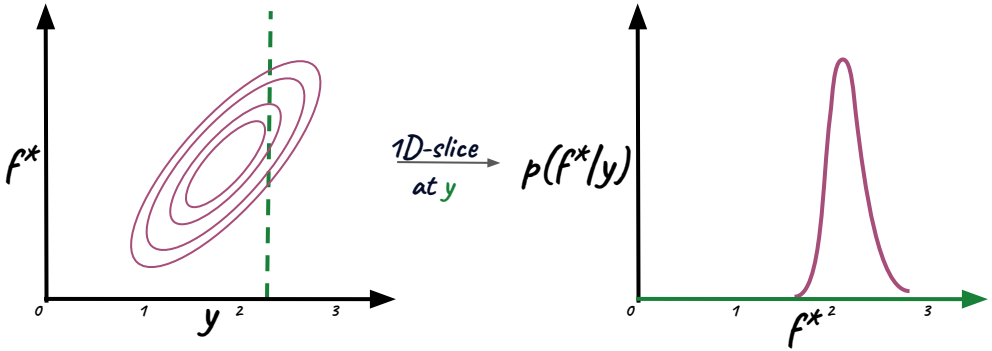

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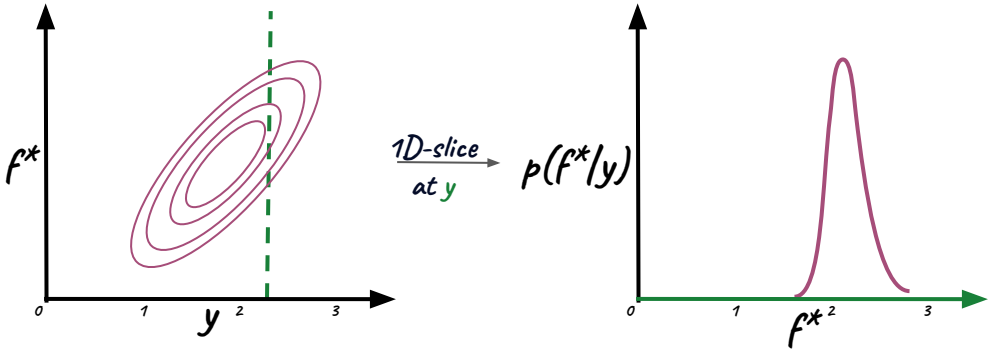

So, all this expression is doing is slicing a multivariate normal on multiple dimension, something that is computationally feasible on a Normal, but harder or impossible on a generic multivariate.

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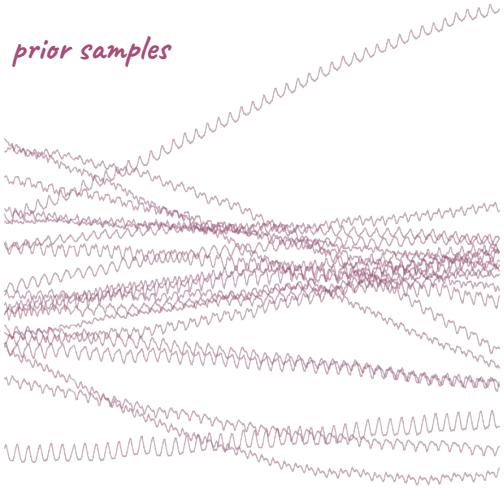

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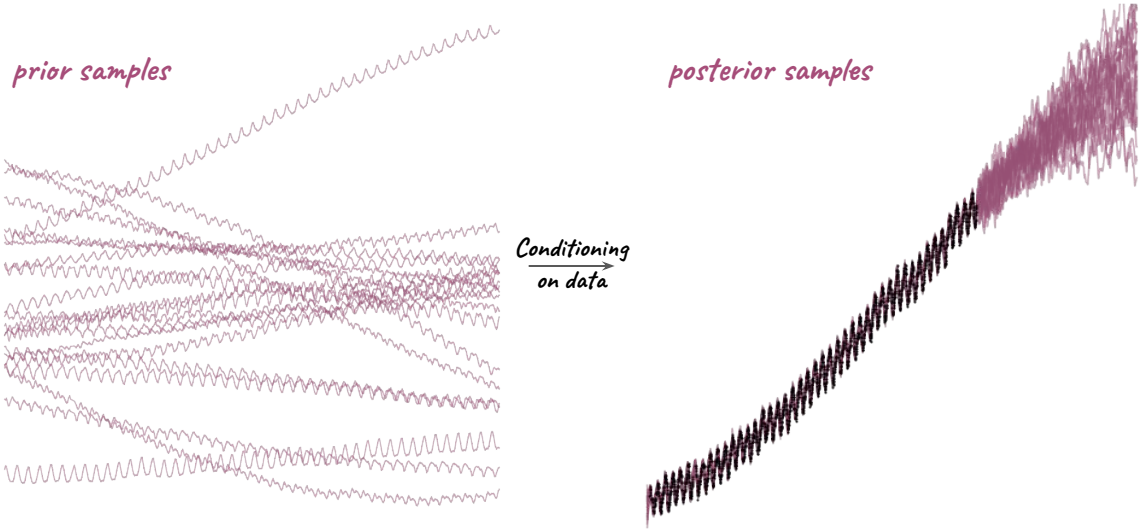

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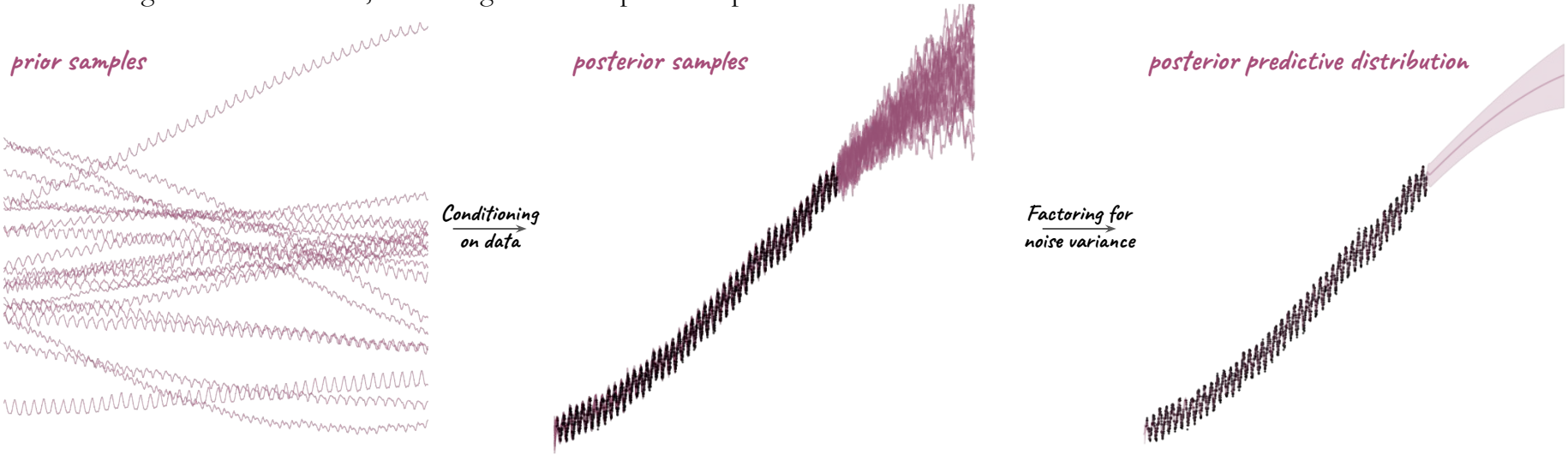
Once factoring for noise variance, this also gives us the posterior predictive distribution.



Gaussian Process Assumption

we assume that the observations *y* and the true function outputs at our test points *f
are jointly distributed as an (N+M)-dimensional multivariate Normal distribution:

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}^* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \hat{\mathbf{K}}_{\mathbf{X},\mathbf{X}} & \mathbf{K}_{\mathbf{X},\mathbf{X}^*} \\ \mathbf{K}_{\mathbf{X}^*,\mathbf{X}} & \mathbf{K}_{\mathbf{X}^*,\mathbf{X}^*} \end{bmatrix} \right) \qquad \hat{\mathbf{K}}_{\mathbf{X},\mathbf{X}} = \mathbf{K}_{\mathbf{X},\mathbf{X}} + \sigma_\epsilon^2 \mathbb{I}$$

Let's wrap it up.
The GP assumption gives us our *prior samples*. Each function comes from drawing a sample from the Normal (here with the CO_2 kernel).
To get the *posterior samples*, we just sample according to the Normal, after conditioning on the data.
Once factoring for noise variance, this also gives us the posterior predictive distribution.
How about the kernel hyperparameters ***τ*** and the noise variance σ_ϵ^2?
Those are picked by maximizing the log-likelihood of ***y*** after integrating out the possible functions:

$$\log p(\mathbf{y}|\mathbf{X}, \tau, \sigma_{\epsilon^2}) = \log \int p(\mathbf{y}|\hat{\mathbf{f}}, \sigma_{\epsilon^2}) p(\hat{\mathbf{f}}|\mathbf{X}, \tau) d\hat{f} = \log \mathcal{N}(\mathbf{y}|0, \hat{\mathbf{K}}_{\mathbf{X},\mathbf{X}})$$

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Drawbacks of GPs:

- inverting $K_{X,X}$ takes $O(N^2)$ time, which makes GPs slow for large values of N
- designing the kernel require **considerable** work, it's not out-of-the box
- for certain kernels (e.g. RBFs), prediction might break down in high dimensional feature spaces

Decision trees are the building block of random forest, ensemble methods and gradient boosted algorithms, three terms that "*squeeze squeeze*" ontologically refer to the same thing. As all the best things in life, they are extremely simple and yet powerful: gradient boosted algorithms are the lone ML technique that is able to compete with (deep) Neural Networks in terms of performances.
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Brutally taken from Andrew Ng's Machine Learning Course, please Andrew don't sue me, big fan btw.

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The Sloan Digital Cats Survey – III, with five cats and five dogs.
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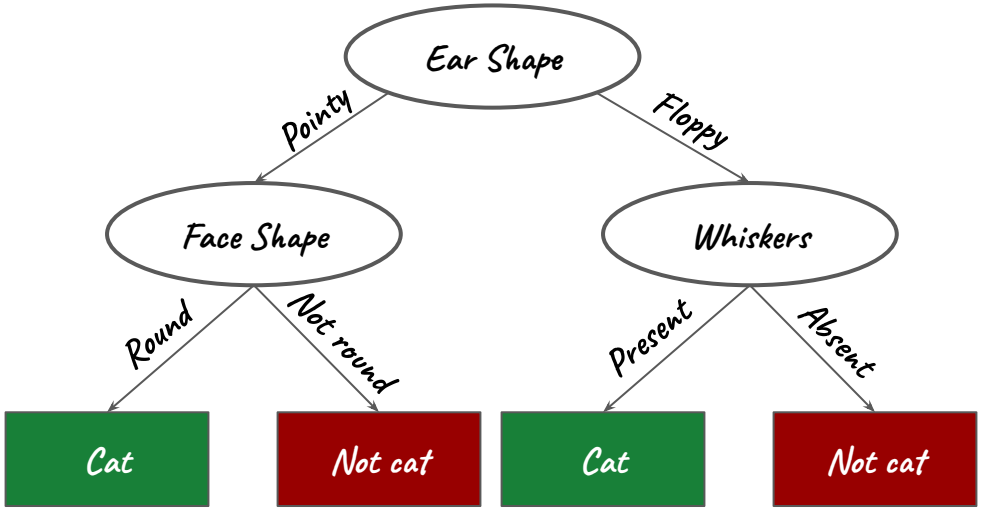

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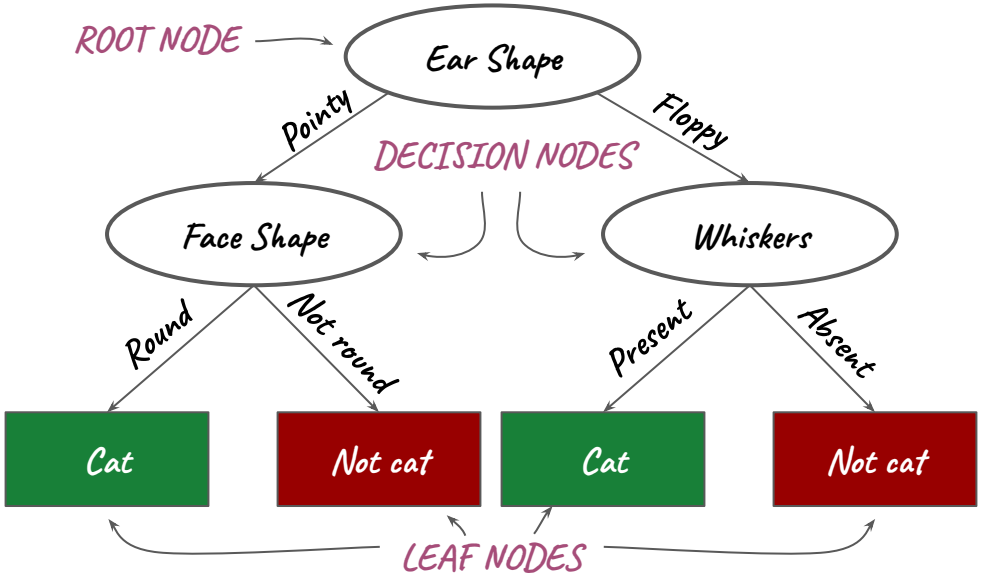

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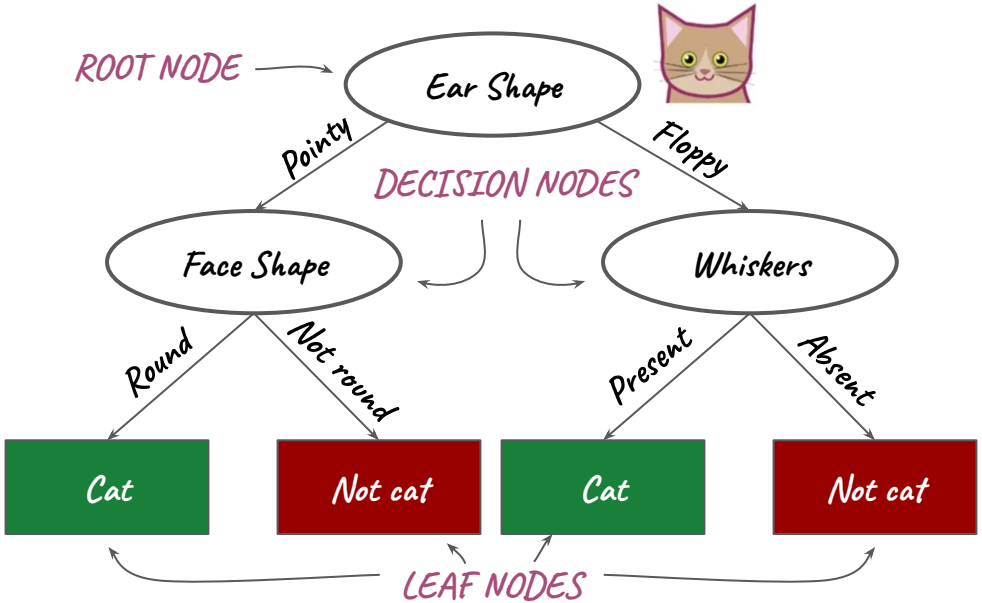

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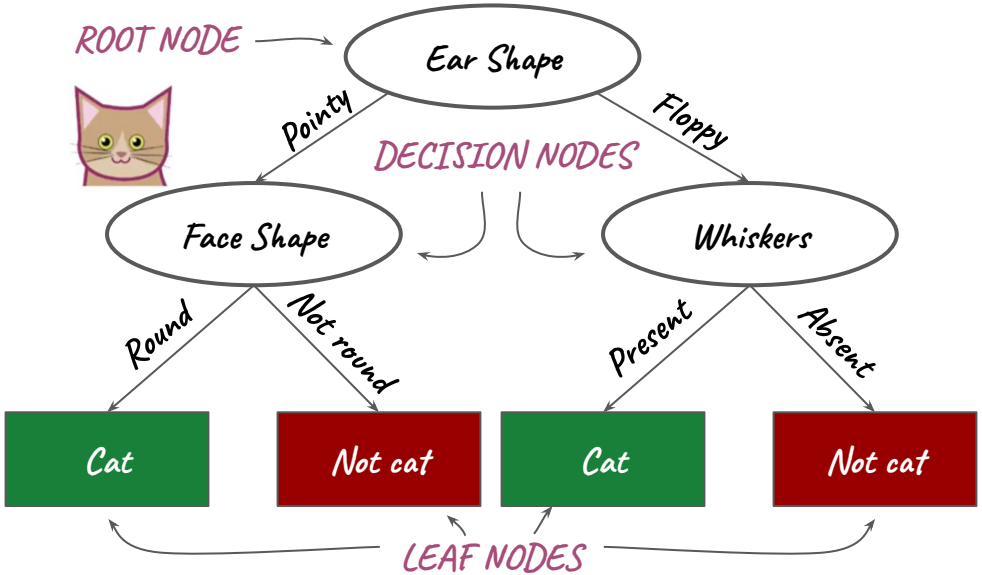

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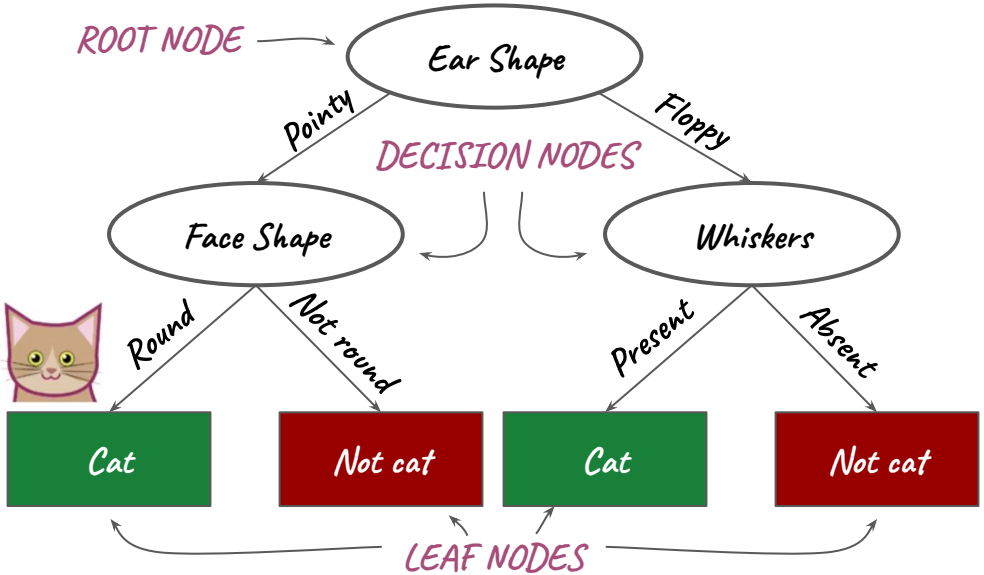
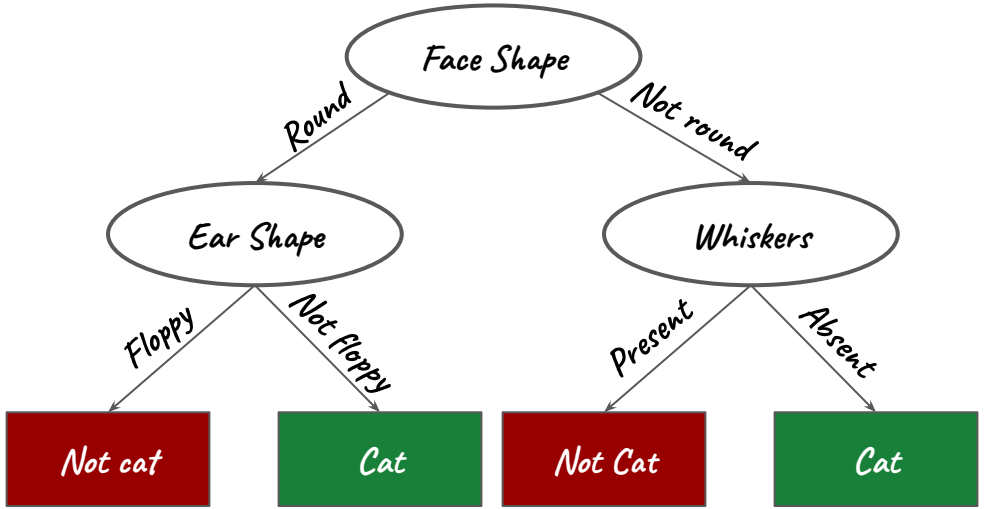


Of course, that's not the only possible decision tree that can be built from that **training** set.



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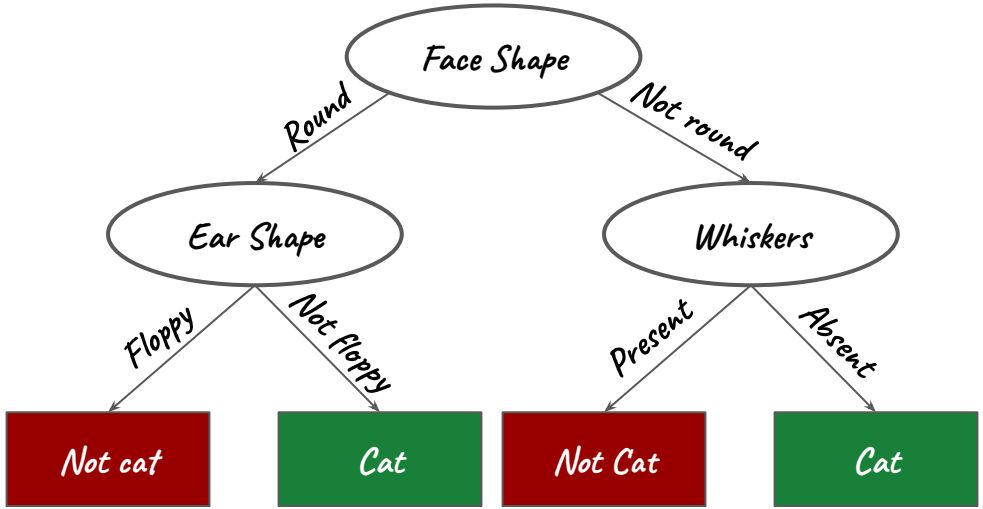

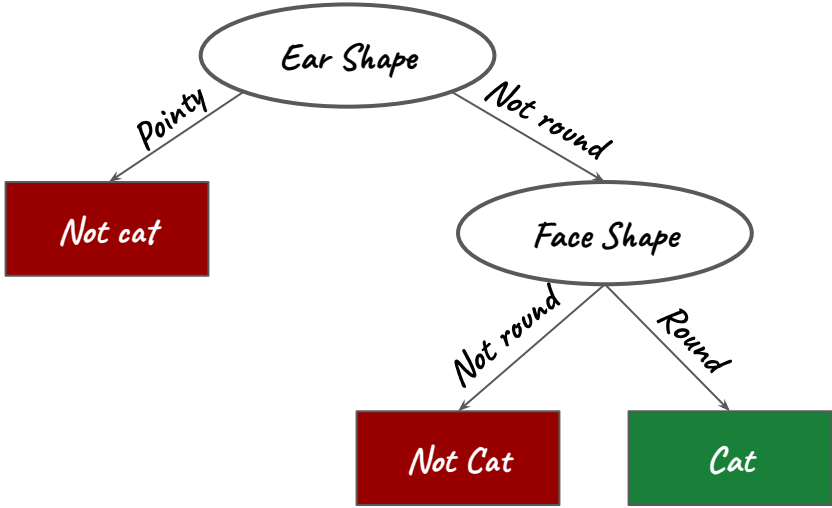

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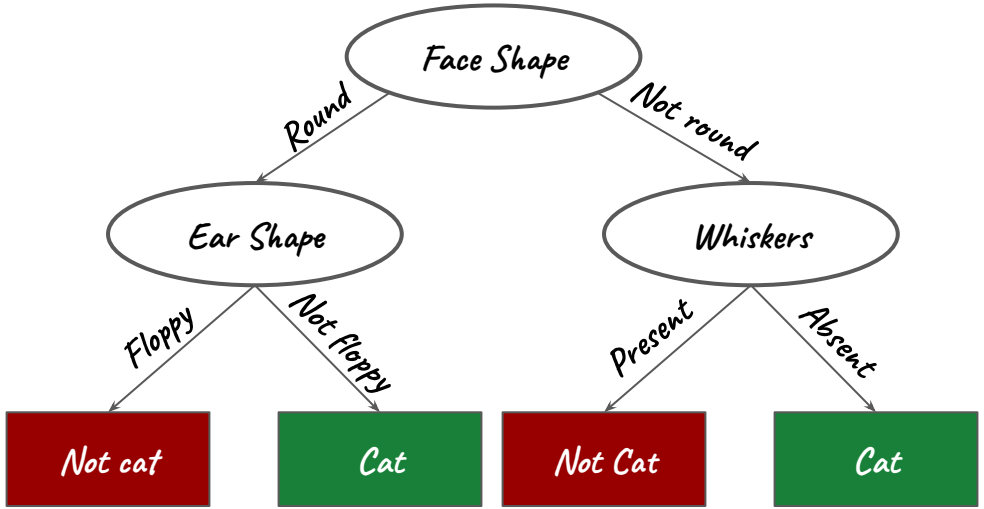
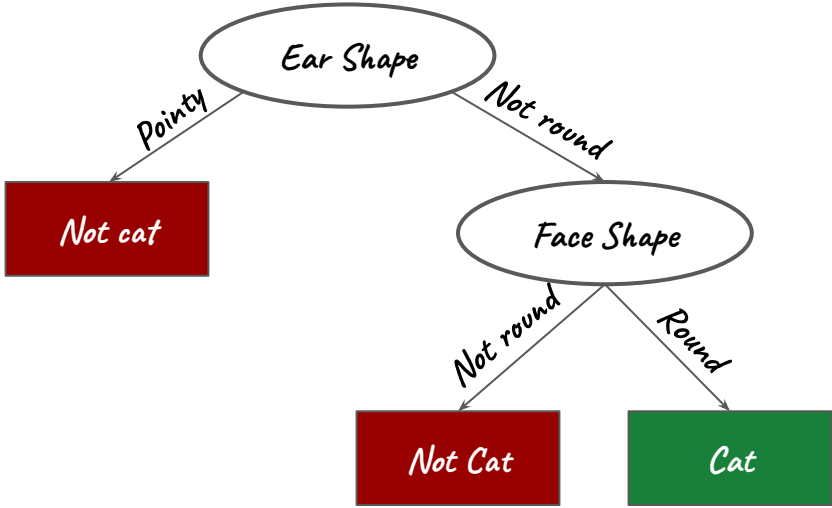
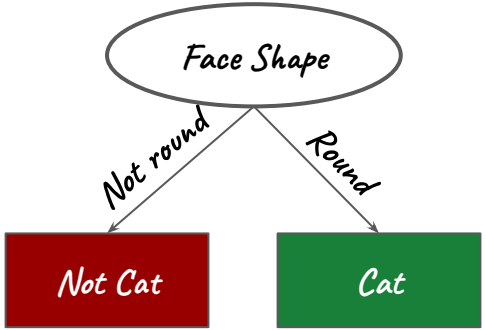




Some will do worse on the **training** / **dev** set, some will do better, etc …
The question is: out of all the possible decision trees, how to choose the one that generalizes to the data the most? How do you get an algorithm to automatically pick the best one?



Decision Trees - Information Gain

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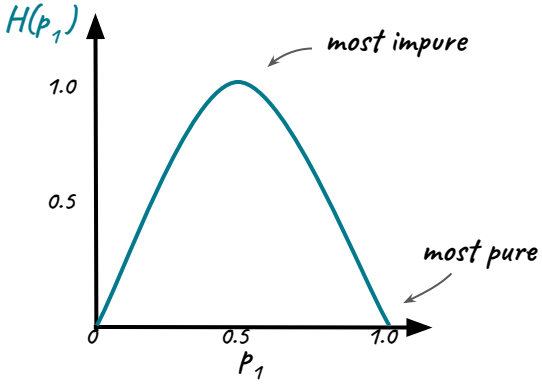

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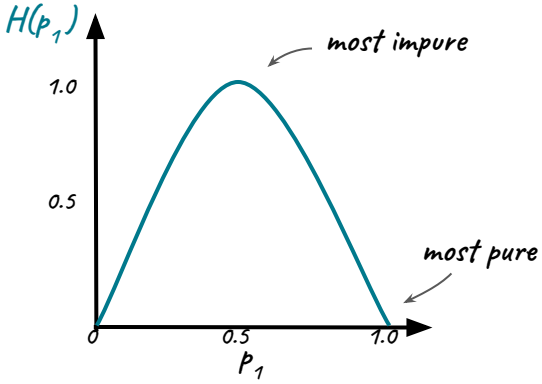

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if $p_1 = 0.50 \rightarrow H(p_1) = 1.00 \leftarrow$ ***most impure***

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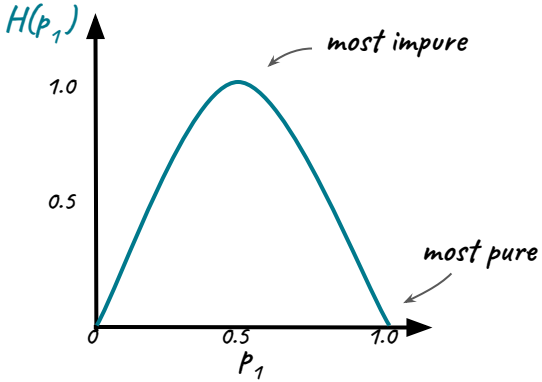

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In decision trees, the reduction of entropy is called the ***INFORMATION GAIN***, upon which the split choice is based.

e.g.
ear shape split $\rightarrow$ ***left*** $H = 0.72$; ***right*** $H = 0.72$
face shape split $\rightarrow$ ***left*** $H = 0.99$; ***right*** $H = 0.92$
whiskers split $\rightarrow$ ***left*** $H = 0.81$; ***right*** $H = 0.91$

Take the mean of the left/right split, weighted by the number of examples going in the sub-branch, subtracted to the entropy of the root node

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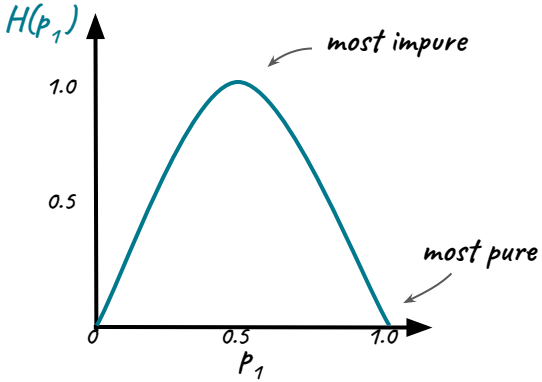

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$$\text{Information Gain} = H(p_1^{\text{root}}) - (w^{\text{left}} H(p_1^{\text{left}}) + w^{\text{right}} H(p_1^{\text{right}}))$$

the fraction of examples going to the left/right branch

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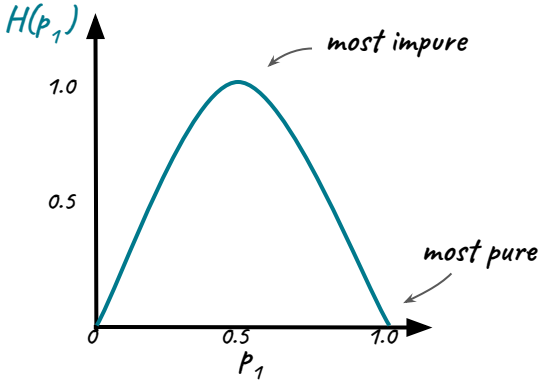

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IG (ear shape split) = 0.28
IG (face shape split) = 0.03
IG (whiskers split) = 0.12

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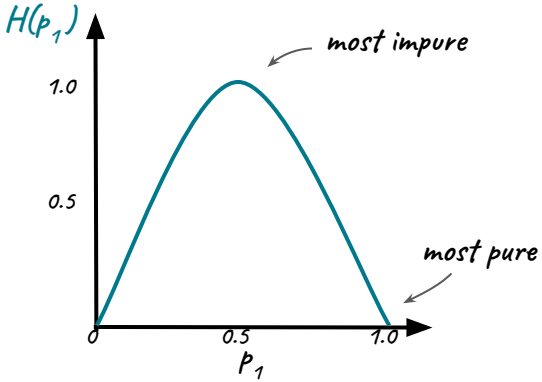

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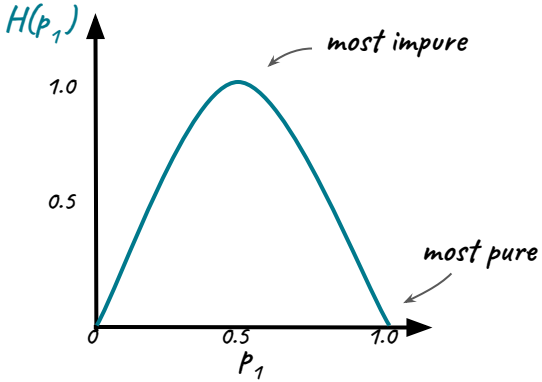
and that's why the first split was on the ear shape feature

The feature upon which split the data at each node is chosen as the one that maximizes the *purity* *(or minimizes impurity)*
The sample *purity/impurity* is measured from the *entropy H*, function of the fraction *p* of examples in the sample that belong to a category.



$$H(p_j) = -\sum_j p_j \log_j(p_j)$$

$$H(p_1) = -p_1 \log_2(p_1) - p_0 \log_2(p_0) = -p_1 \log_2(p_1) - (1-p_1)\log_2(1-p_1)$$

e.g. $p_1 \rightarrow$ fraction of examples that are cats; $H(p_1)$ is the *entropy* of p_1; $p_0 = 1 - p_1$
if $p_1 = 0.50 \rightarrow H(p_1) = 1.00 \leftarrow$ *most impure*
if $p_1 = 0.83 \rightarrow H(p_1) = 0.65$
if $p_1 = 1.00 \rightarrow H(p_1) = 0.00 \leftarrow$ *most pure*

Another commonly used metric for purity/impurity is the Gini coefficient

In decision trees, the reduction of entropy is called the *INFORMATION GAIN*, upon which the split choice is based.

e.g.
ear shape split → *left H = 0.72; right H = 0.72*
face shape split → *left H = 0.99; right H = 0.92*
whiskers split → *left H = 0.81; right H = 0.91*

Take the mean of the left/right split, weighted by the number of examples going in the sub-branch, subtracted to the entropy of the root node

$$\text{Information Gain} = H(p_1^{\text{root}}) - (w^{\text{left}} H(p_1^{\text{left}}) + w^{\text{right}} H(p_1^{\text{right}}))$$

the fraction of examples going to the left/right branch

The chosen feature split is the one with the **highest** *INFORMATION GAIN*.

IG (ear shape split) = 0.28
IG (face shape split) = 0.03
IG (whiskers split) = 0.12

and that's why the first split was on the ear shape feature

So, at each step a decision tree measures the *IG* for all possible features, and picks the one with the highest *IG*.

Decision Trees Recursive Algorithm

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	Floppy	Round	Absent	15	No
	Pointy	Not round	Present	42.1	No
	Pointy	Round	Present	4.6	Yes
	Pointy	Round	Absent	5.7	Yes
	Floppy	Not round	Absent	15.2	No
	Pointy	Round	Absent	10.3	Yes
	Floppy	Round	Absent	13.4	No
	Floppy	Round	Absent	19.4	No

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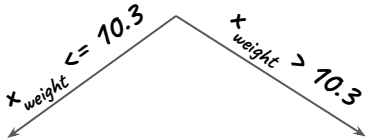
The concept is still the same: the feature is chosen by maximizing the *IG*, so the algorithm will measure the one obtained by splitting on the ***weights*** feature.
In this case, there are various possible x_{weight} values upon which to split: the decision tree will try all the different thresholds, measure the *IG* for each one, and pick the one carrying the highest, to compare with the *IG* arriving from splitting at the other features.

In this case, is 10.3 kg, so the eventual split would be on:



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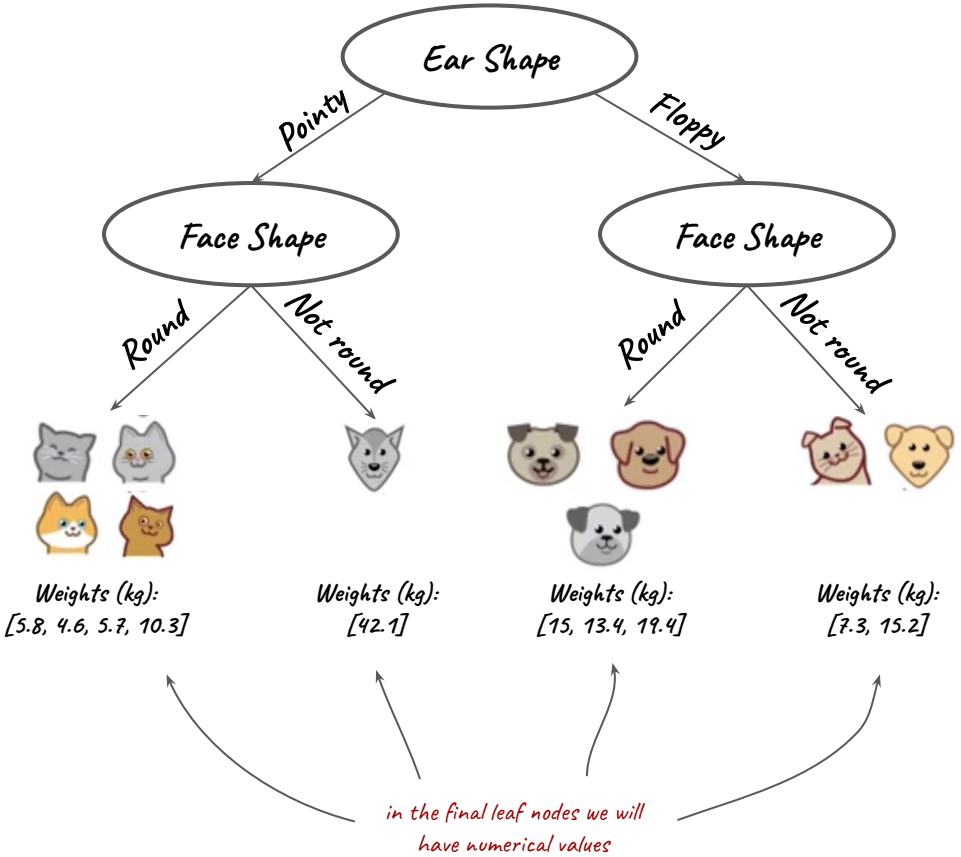

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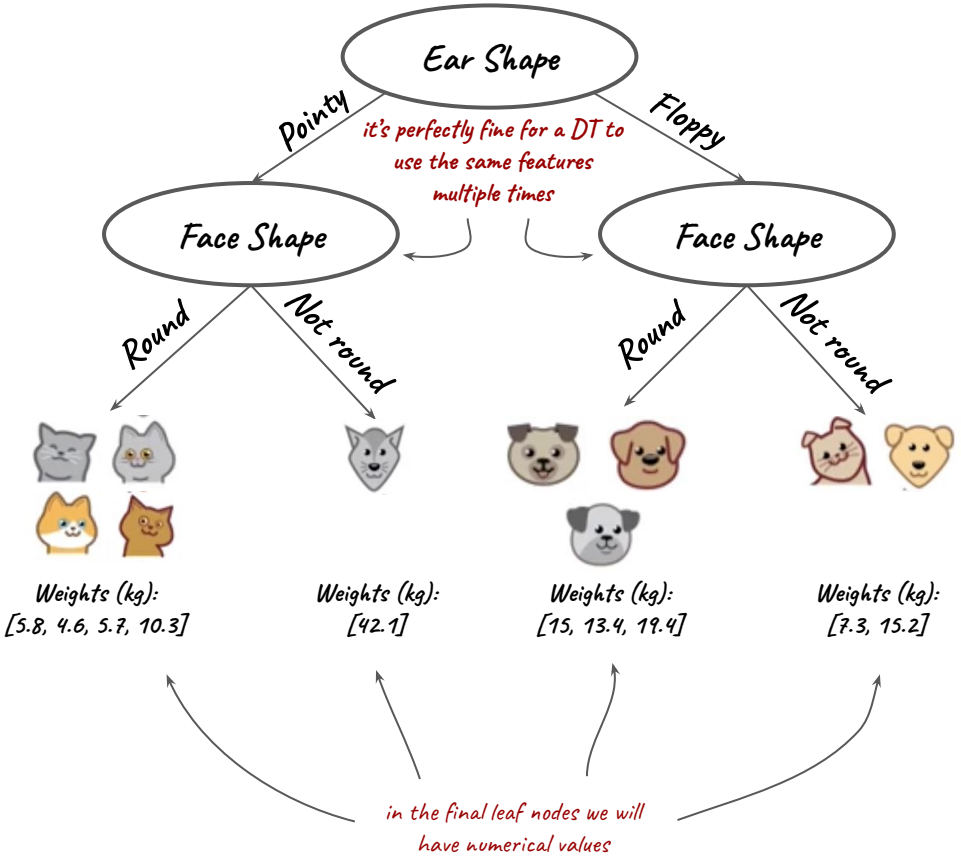

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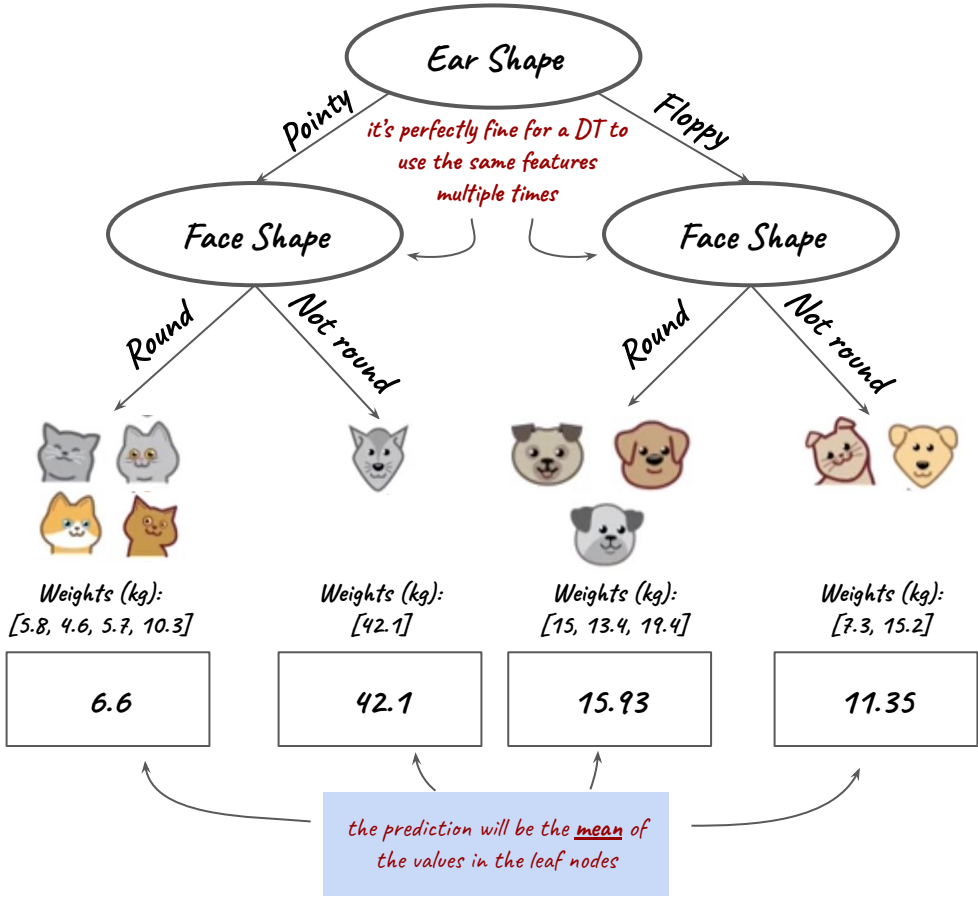

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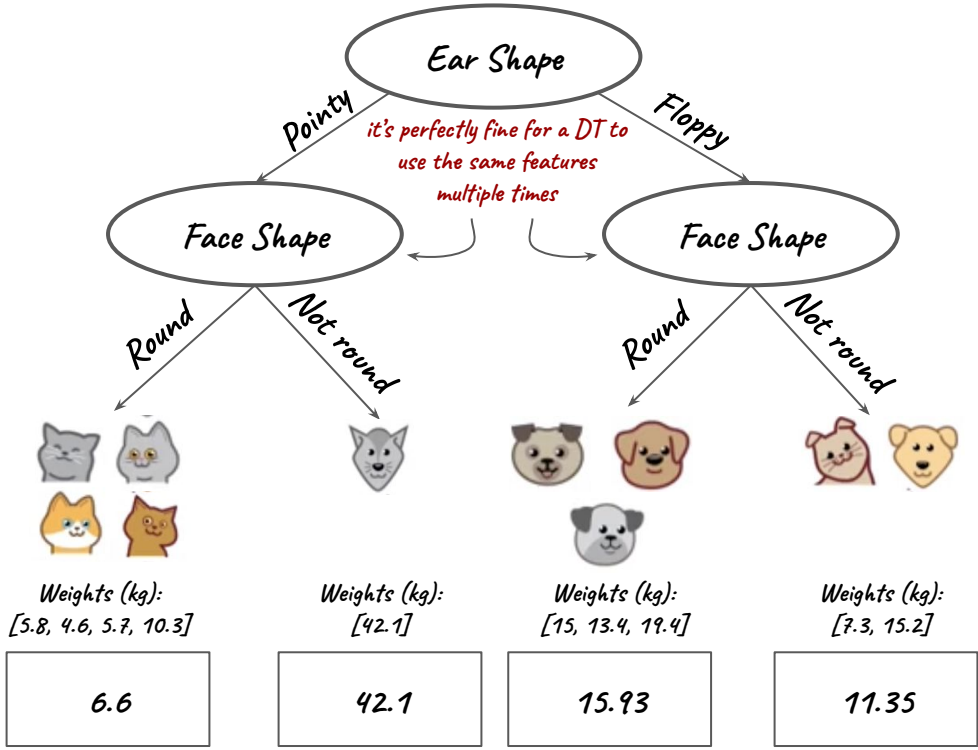

$$\Delta\text{Var} = \text{Var}(\text{root}) - (w^{\text{left}}\,\text{Var}(\text{left}) + w^{\text{right}}\,\text{Var}(\text{right}))$$

The feature to split on is chosen as the one that reduces the most the VARIANCE between the root node and the weighted left/right branches.

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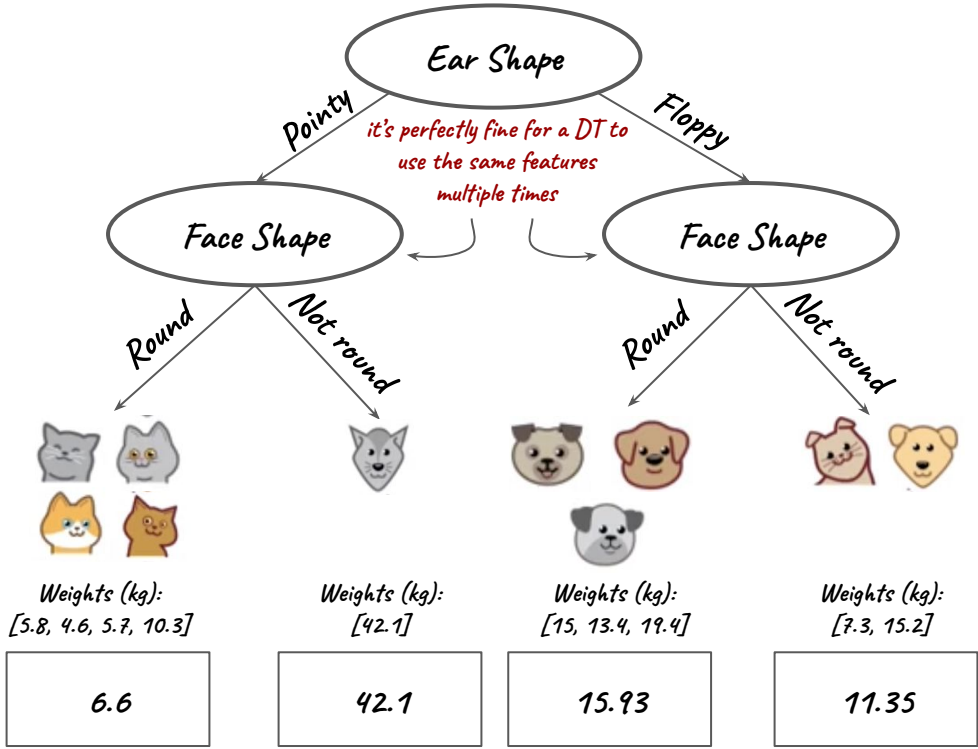

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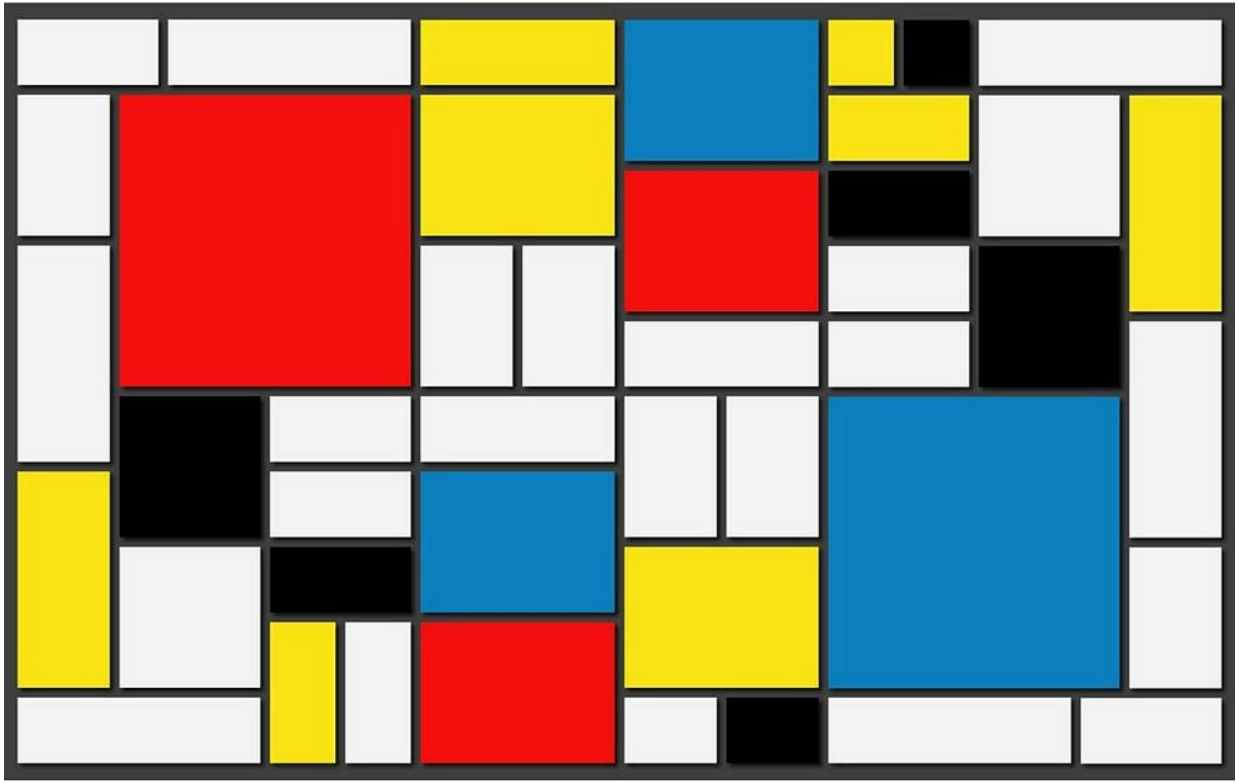
The whole thing works also for **multilabel (multi-output)** predictions (e.g. weight and height). The algorithms will chose the feature that reduces the **average** variance.

The feature to split on is chosen as the one that reduces the most the VARIANCE between the root node and the weighted left/right branches.

What is a decision tree actually doing on the feature space?

A decision tree is partitioning the feature space, grouping together close training examples in the a bag (***leaf***) with the least possible variance. When a new target examples rolls down the tree, it arrives in the final leaf, and the prediction comes from averaging the training values. That's similar to what NN is doing, but with a smarter/ad hoc feature space partitioning.



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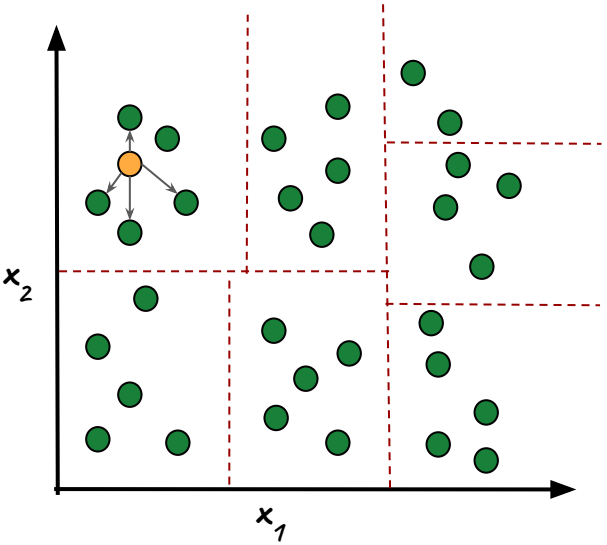

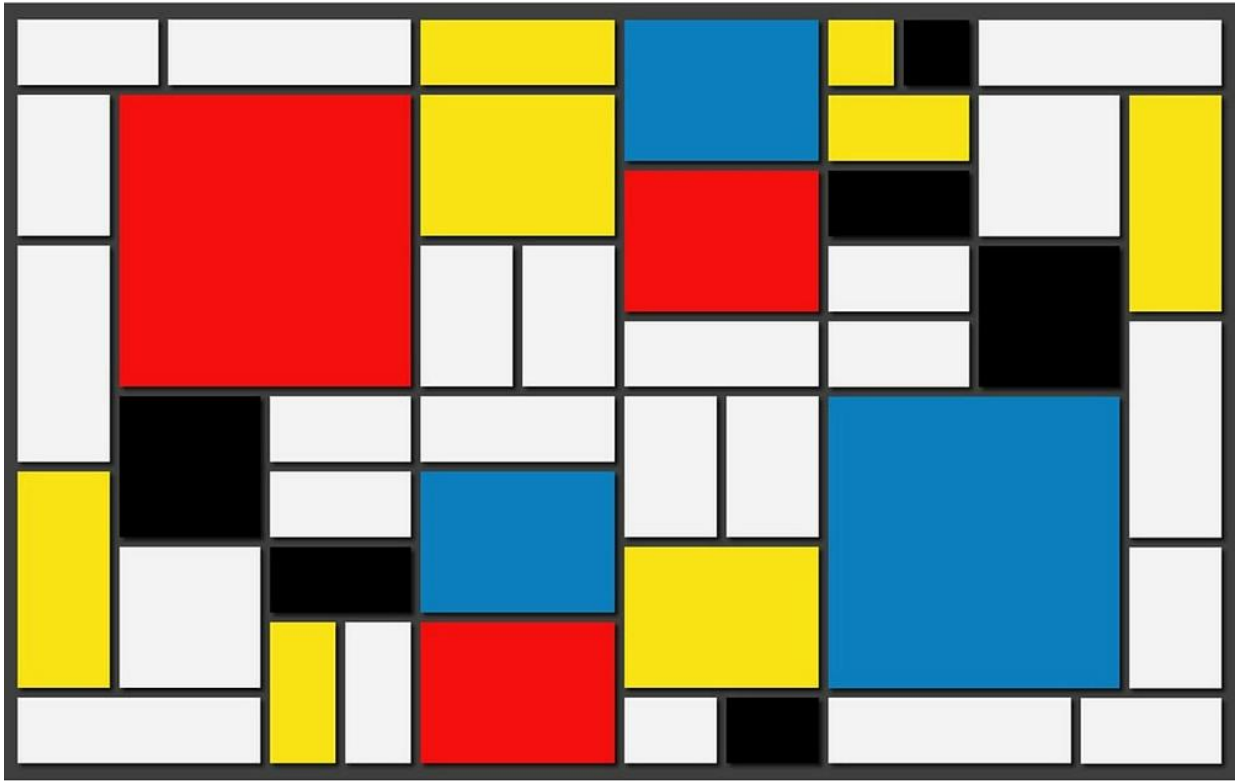

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The solution is to use multiple decision trees, a **tree ensemble**.
Every tree in the ensemble is built from a *sampling-with-replacement* version of the **training set**.

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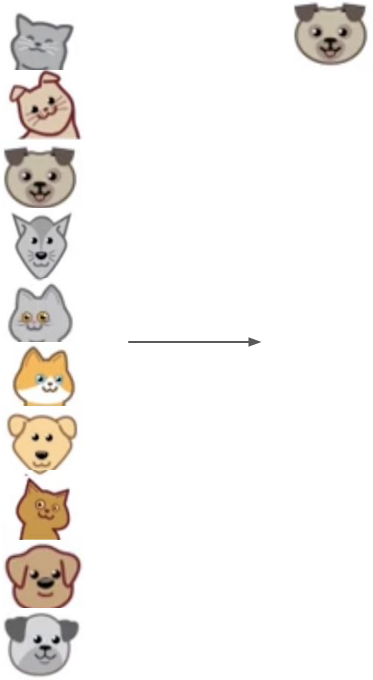

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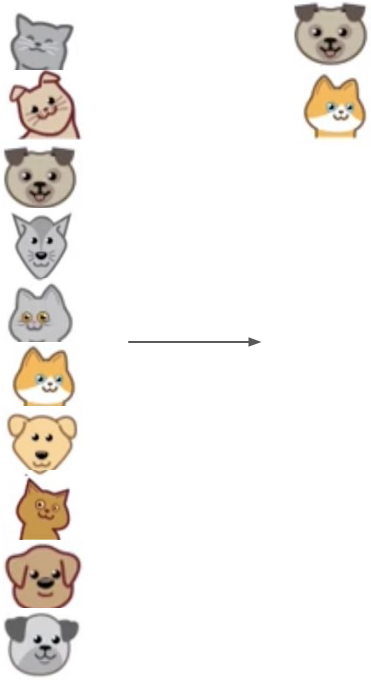

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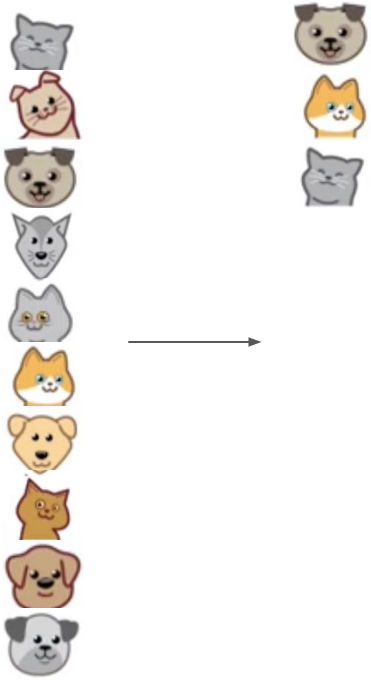

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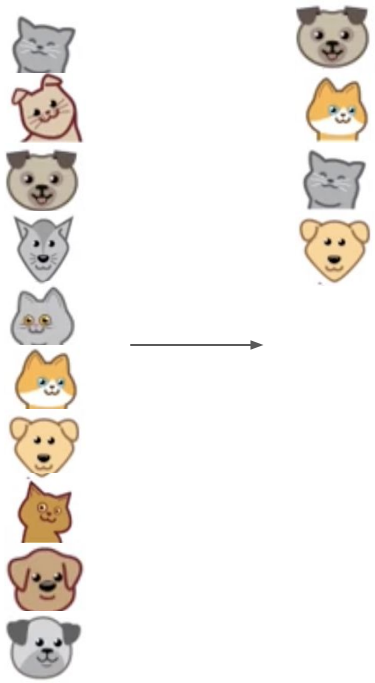

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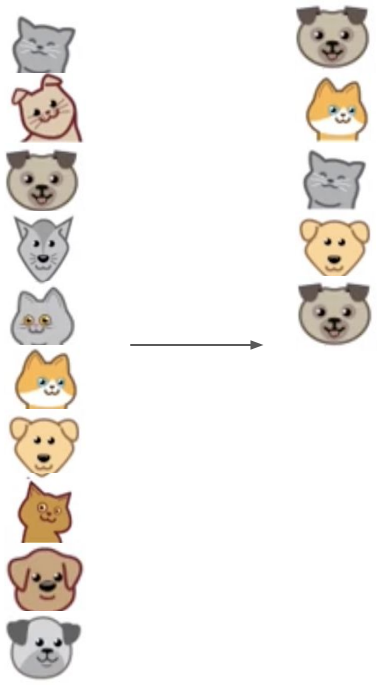

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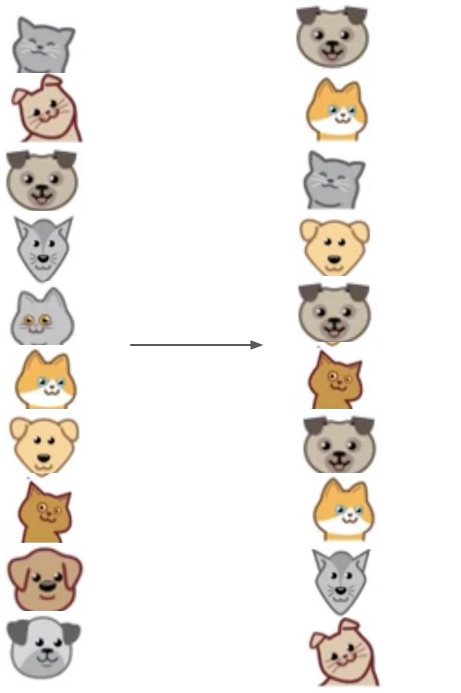

training set *Set #1 → DT#1*

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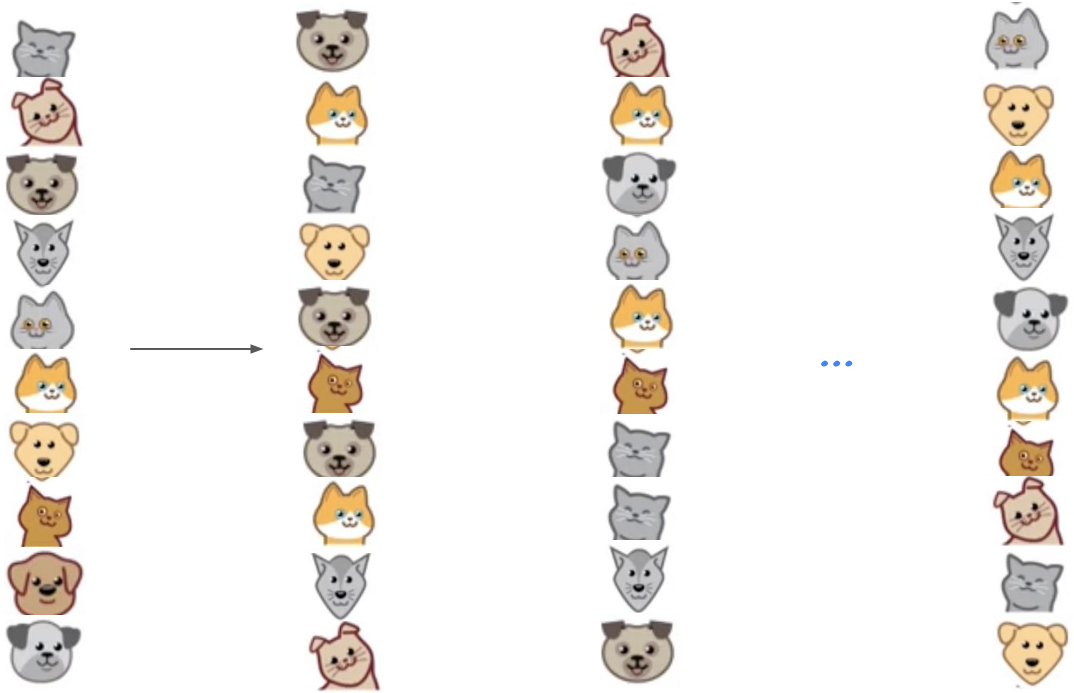

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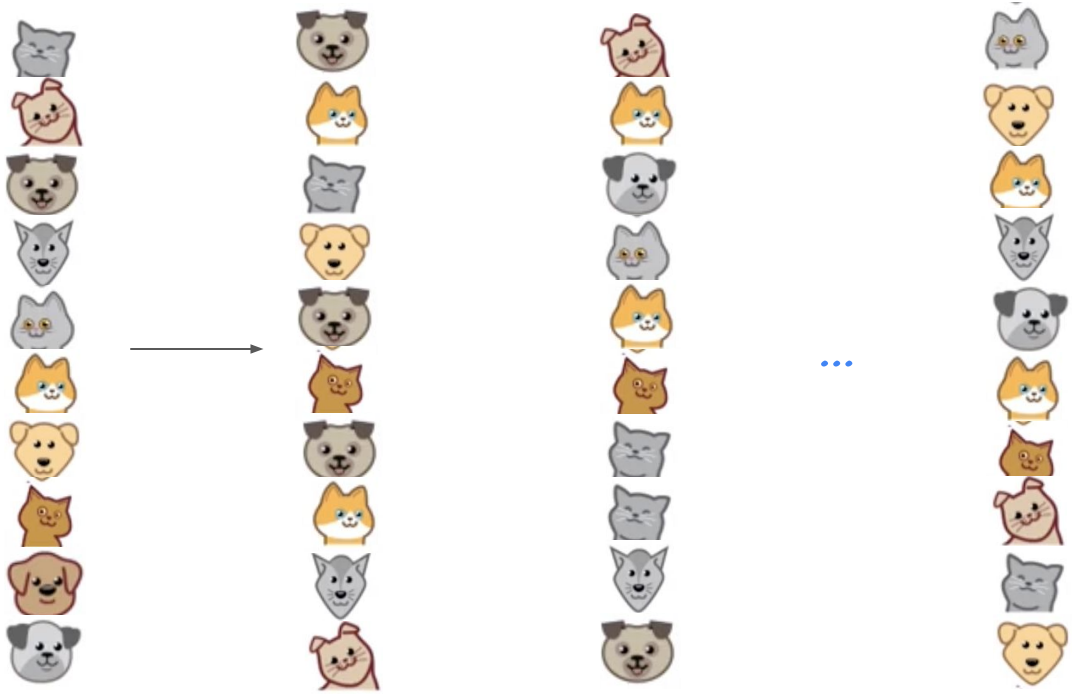

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This technique is called *BAGGING*, short version for bootstrap aggregating.

For $i = 1 \ldots B$ use sampling with replacement to create a new training set of size m and train a **decision tree** on the new dataset.

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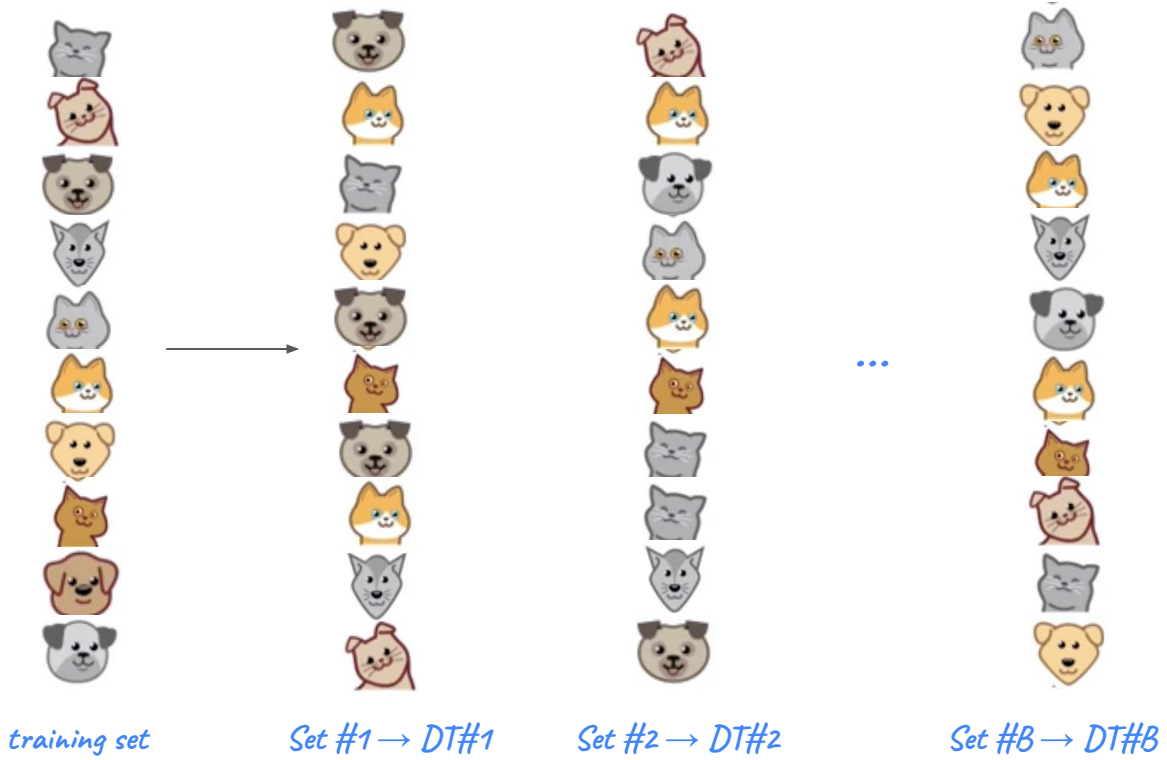

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This is the *random forest* algorithm.

Tree Ensemble and Random Forest

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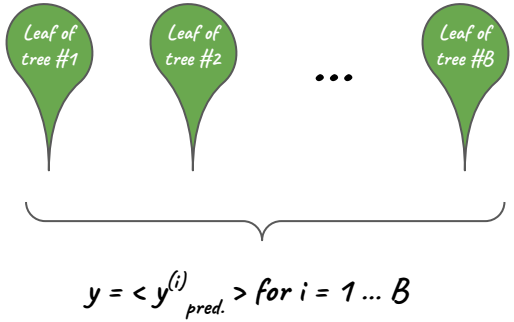
Classification

For classification tasks, the predicted label y is taken by choosing the class of the single leaf of the whole forest with the highest probability, or by either a majority vote coming from the final leaves of each classifier (the DTs), or (as scikit-learn does) by averaging the classifiers probabilistic predictions.

Regression

For regression tasks, the predicted label y is computed as the mean of the predictions made by the trees in the forest.



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In this way, a random forest regressor is able to give a punctual prediction given a certain set of features.

Random Forests and the posterior distribution function

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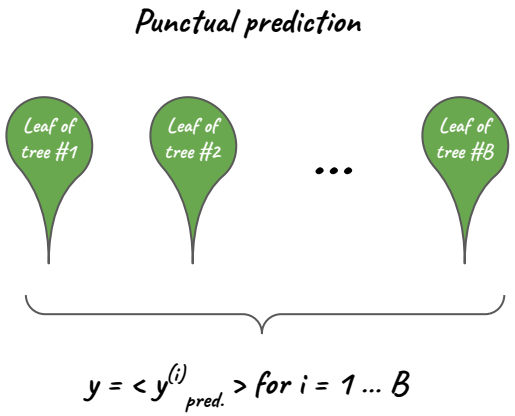
As in NN algorithms, there is a trick to extract a sort of posterior distribution function for that predicted label ***y***, under the same assumption that similar observations will lead to similar PDFs:

- the punctual prediction ***y*** is the mean of all the predictions made by the trees in the forest, e.g. between the values in the final leaves

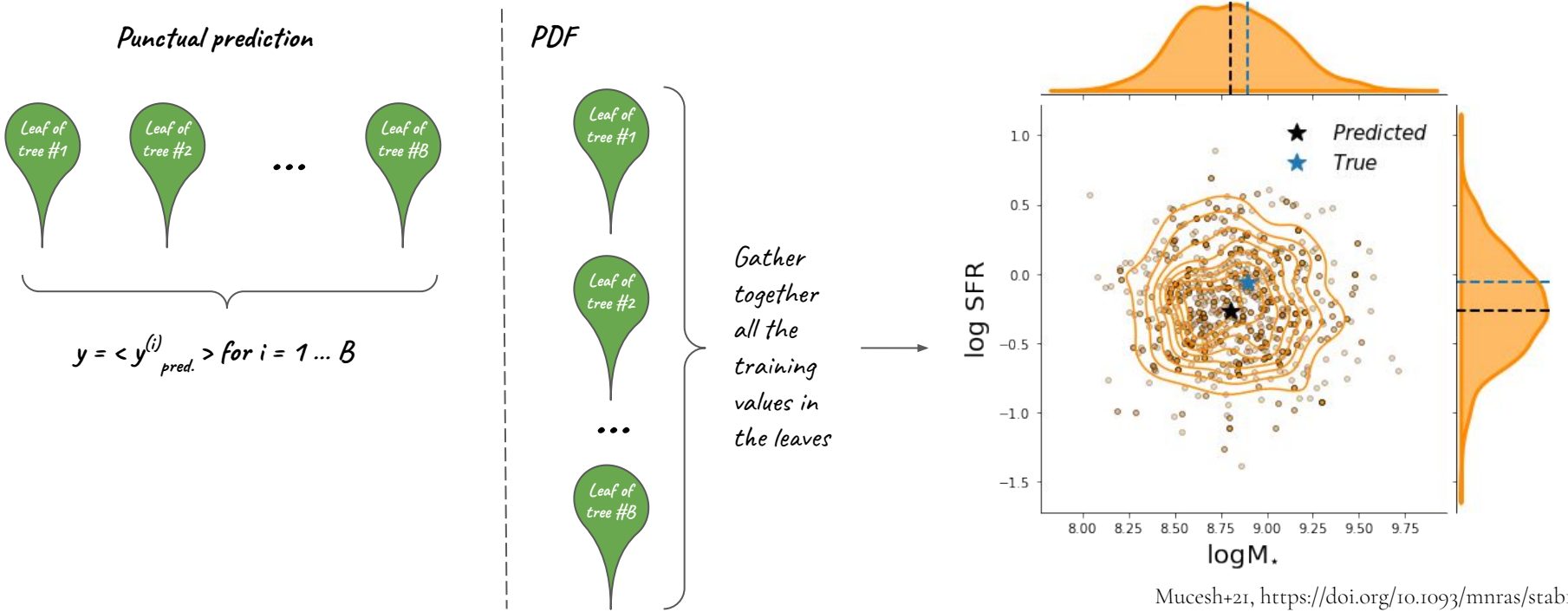


Mucesh+21, https://doi.org/10.1093/mnras/stab164

Random Forests and the posterior distribution function

In this way, a random forest regressor is able to give a punctual prediction given a certain set of features.
As in NN algorithms, there is a trick to extract a sort of posterior distribution function for that predicted label ***y***, under the same assumption that similar observations will lead to similar PDFs:

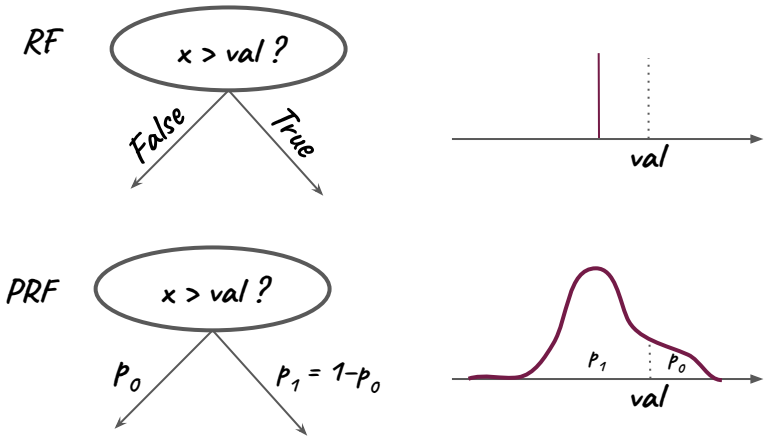
- the punctual prediction ***y*** is the mean of all the predictions made by the trees in the forest, e.g. between the values in the final leaves
- the posterior distribution function ***PDF*** is obtained by putting together the training values in the final leaves, and estimate their density (e.g. with KDE)



Mucesh+21, https://doi.org/10.1093/mnras/stab164

Turns out there is also a way for factoring in the noise in the features/labels.
Probabilistic Random Forest (PRF) algorithm treats the features and labels as probability distribution functions, rather than deterministic quantities.

Labels and features as PDFs



"In the presence of feature uncertainty the split is not deterministic. At every node each object may propagate into both branches with some probability. Therefore, while in an RF tree an object goes through a single trajectory, in a PRF tree the object may propagate through all the tree nodes, with some probability."

The final probability of each object at the leaf nodes is the combined probability for it to take all the turn that led to it from the root node.

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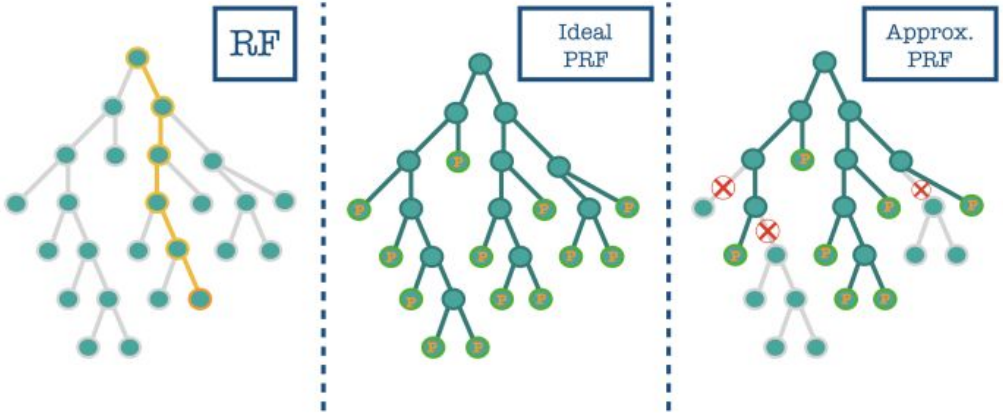

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Training of a PRF

Training is done by choosing the most homogeneous possibile splits, as in RF, but using a modified version of the *Gini impurity* as the cost function. Stopping criterion and other details are the same as in a normal RF.

Prediction by a PRF

The prediction is determined via majority vote (as in the scikit-learn version of RF), where the vote of each tree comes from the leaf that achieved the *highest* probability.

Selective propagation scheme

This works as smooth as silk from a theoretical point of view, but it is computationally ***EXTREMELY*** expensive. Therefore not all the possible propagation schemes down the trees are maintained, but only the ones over a certain threshold (e.g. 5%).

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Random forests are fine, but there is a way to increase their ability to generalize and make accurate predictions, up to the levels where only NN now are used to play: **gradient boosting**.
The idea is quite simple: focus more on the subsets that are underperforming, and learn how to make them perform better. Combine multiple badly performing trees (weak learners) to make one performing strong learner.
This is achieved with a tweak to the bagging technique:

For $i = 1 \dots B$ use sampling with replacement to create a new training set of size m and train a decision tree on the new dataset.

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AdaBoost:

a split made on a single feature

> In the first iteration of AdaBoost, each example is assigned an equal weight. After building and evaluating the first *stump*, increase the weights of those examples that are difficult to classify, lower the weights for those that are easily classified, and build a second stump. Repeat for a certain number of iterations. Predictions of the final ensemble model is therefore the weighted sum of the predictions made by all the previous stumps.

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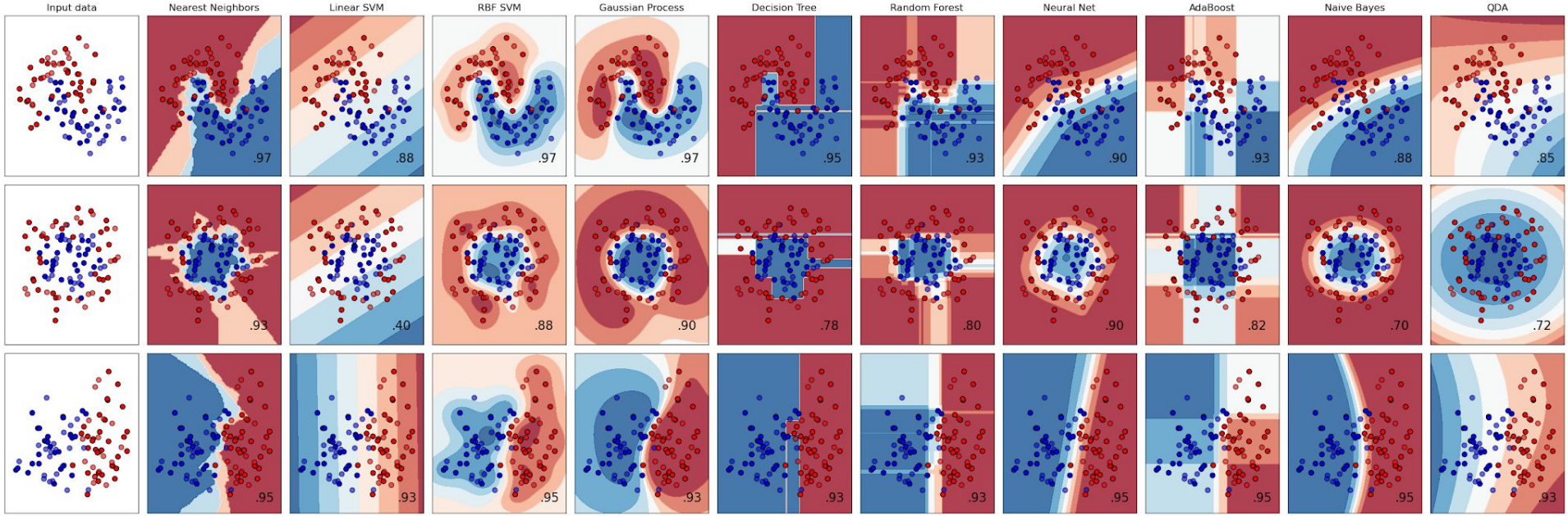
Gradient Boosted Decision Trees (e.g. scikit-learn):

Similar as above, but building full trees, and instead of trying to directly predict the labels y, the model will try to predict the ***residuals*** between the labels y and the predictions y' (MSE loss), trying to minimize them at each iteration. The trees predictions are scaled with a learning rate and the whole process is regularized in order to increase generalization and avoid overfitting.

XGBoost (eXtreme Gradient Boosting)

Similar as above, with small differences and details on tree growth policy, it is the most widely used ensemble methods, the one that is able to compete with Deep Learning algorithms in terms of performances.

Classifiers, classified



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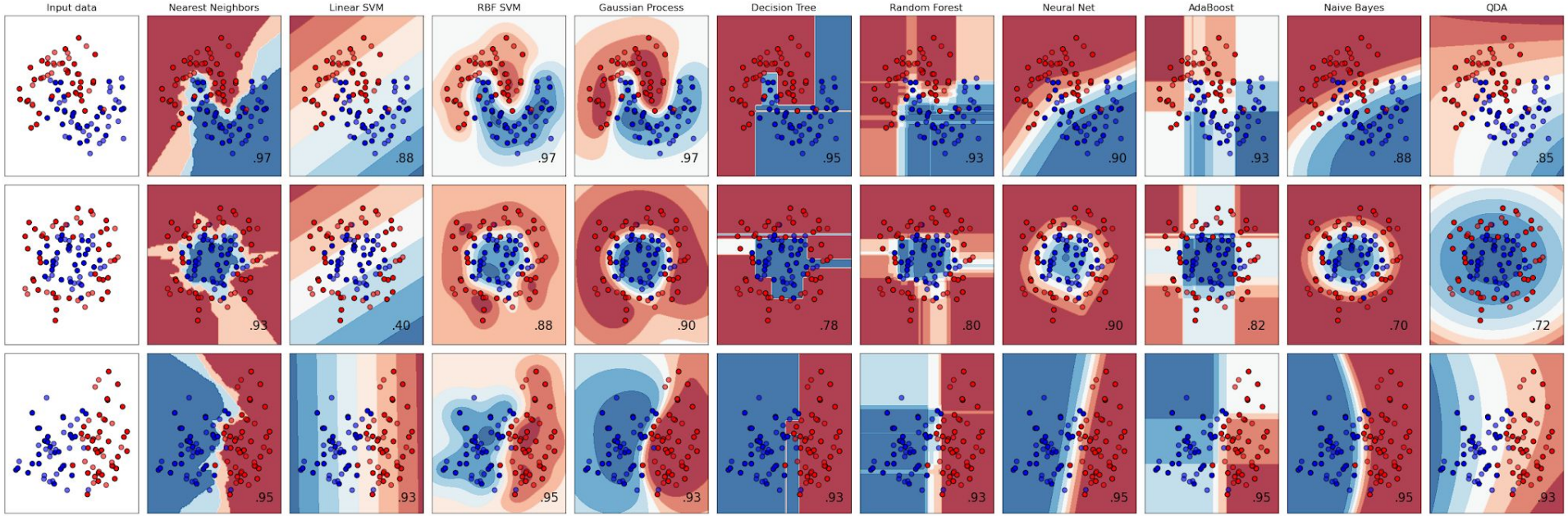

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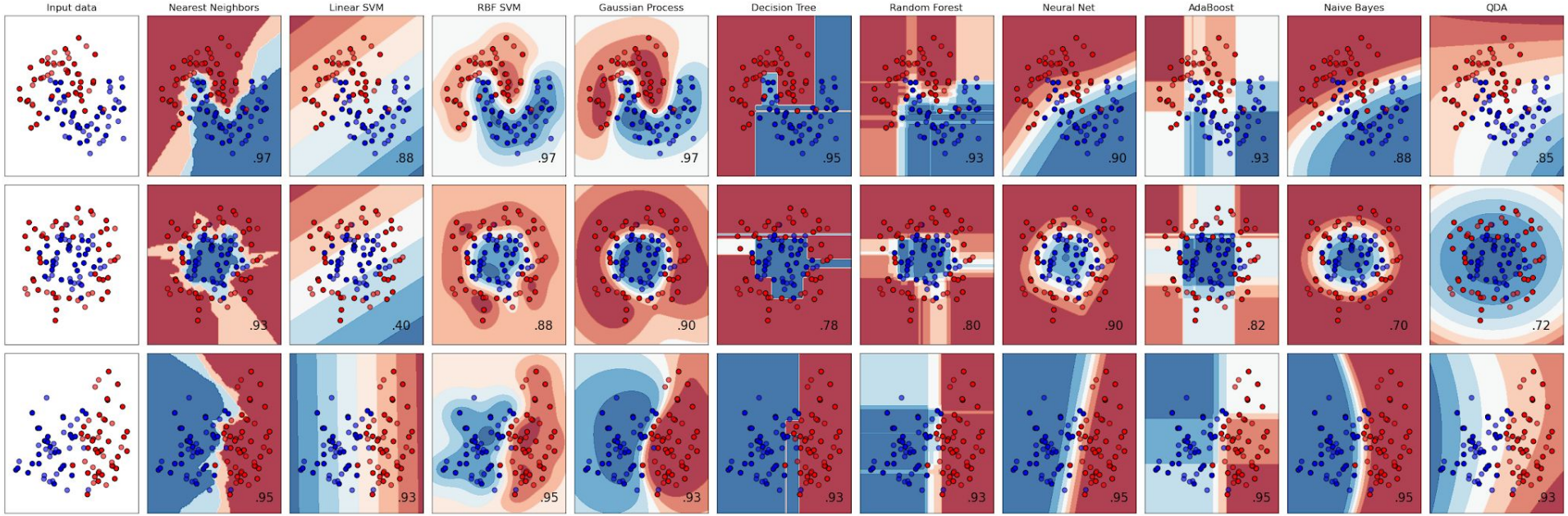

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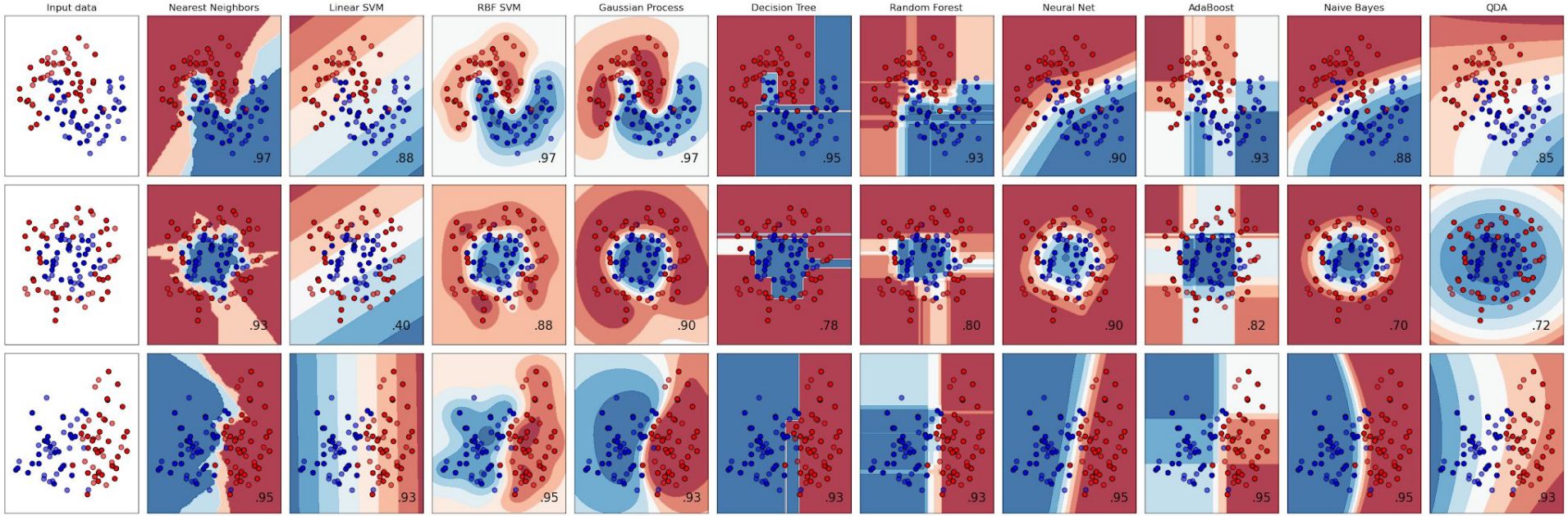

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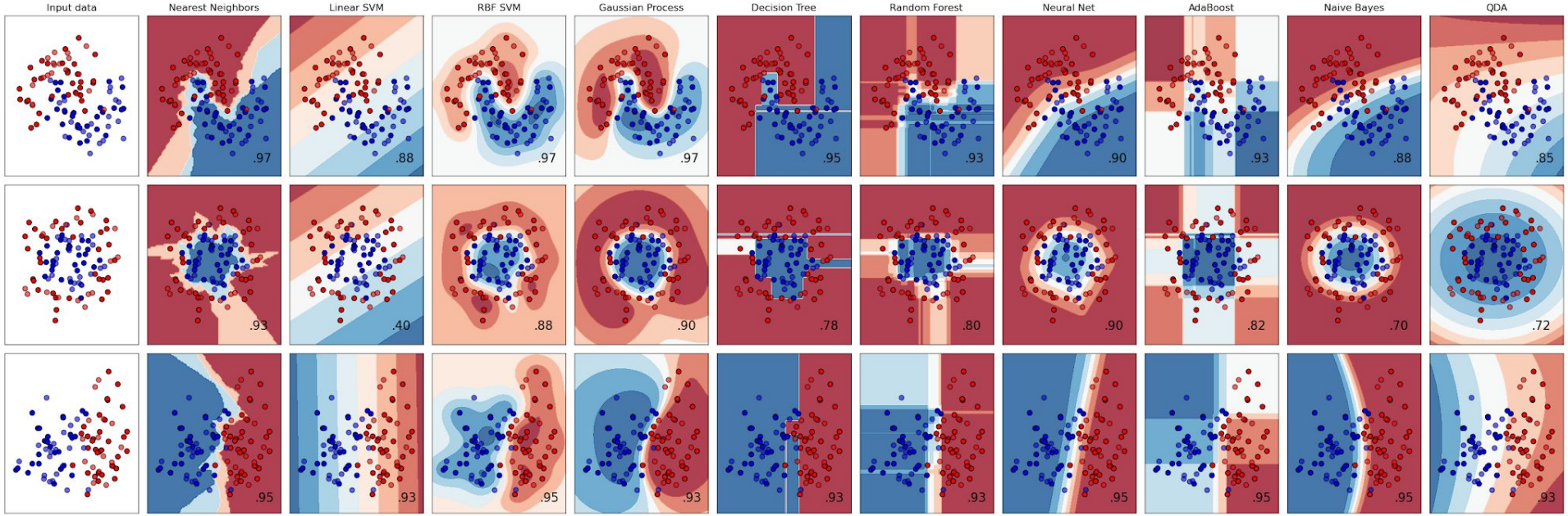

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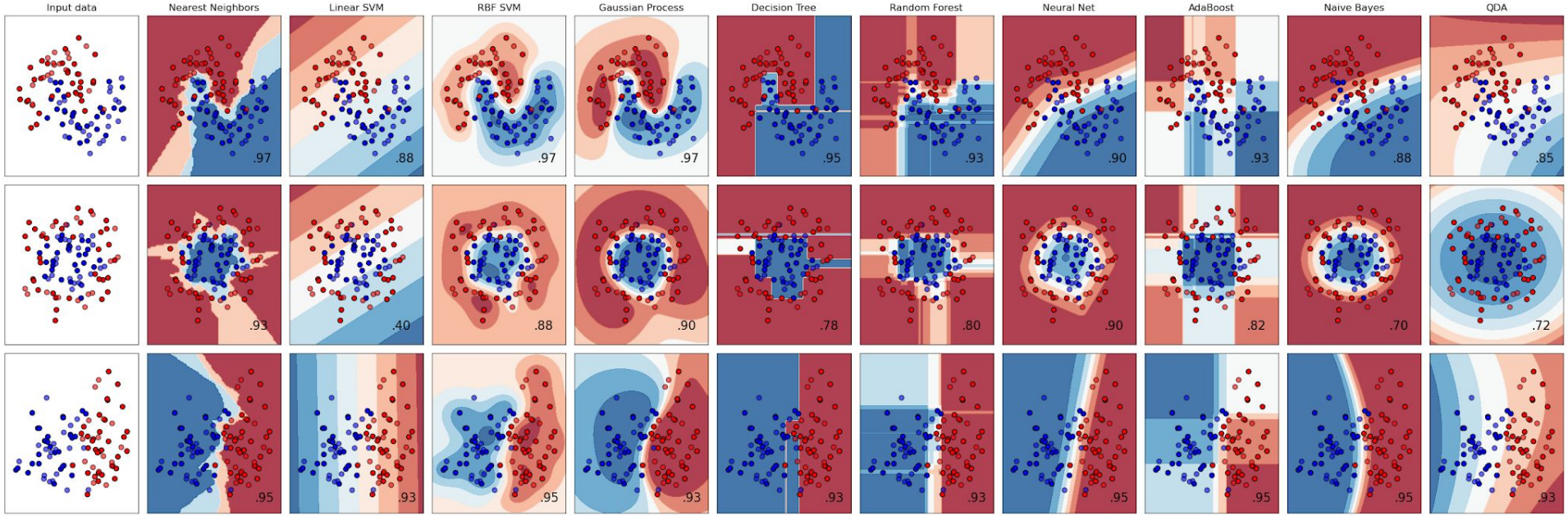

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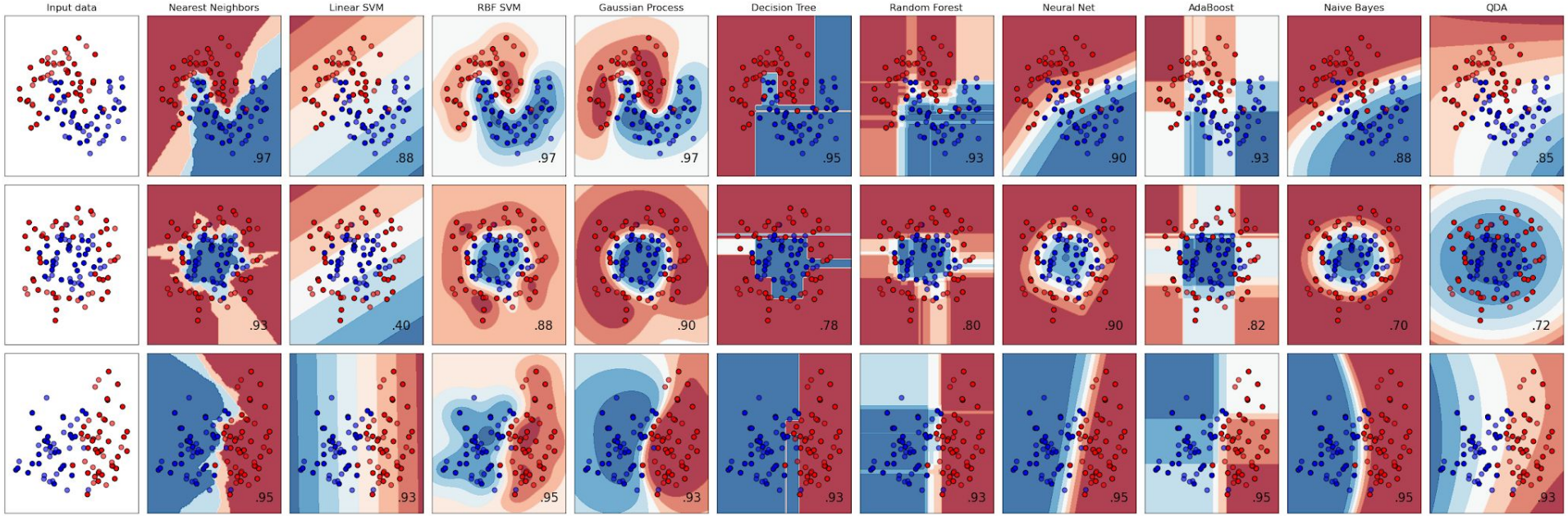

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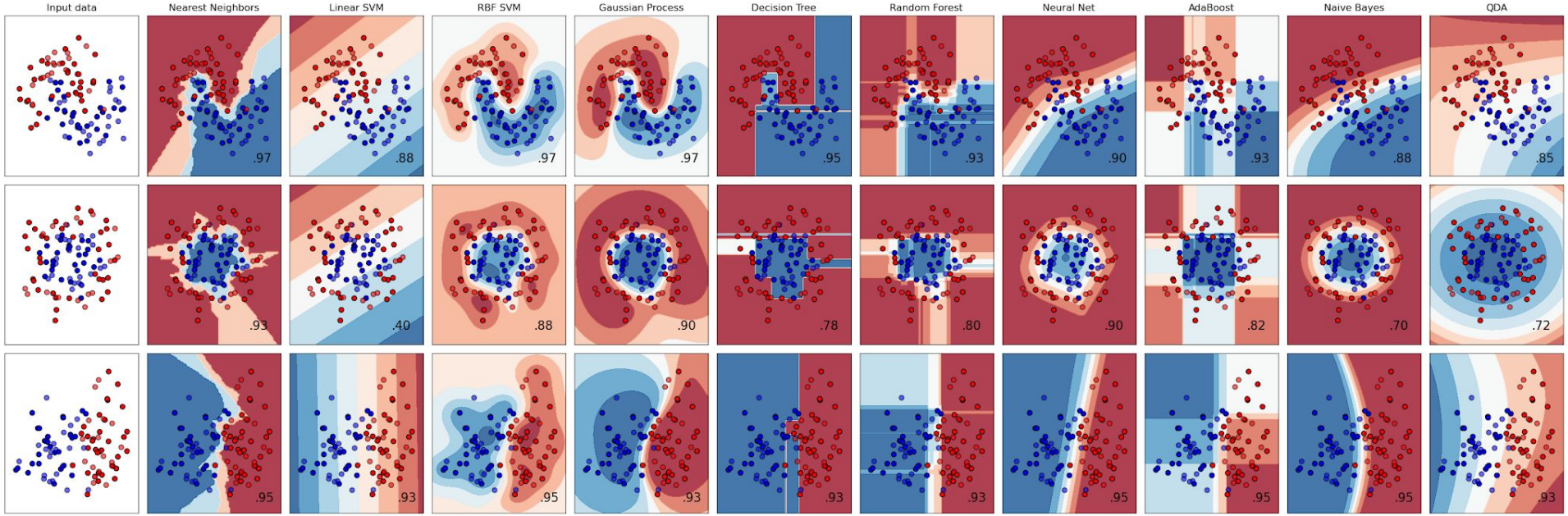

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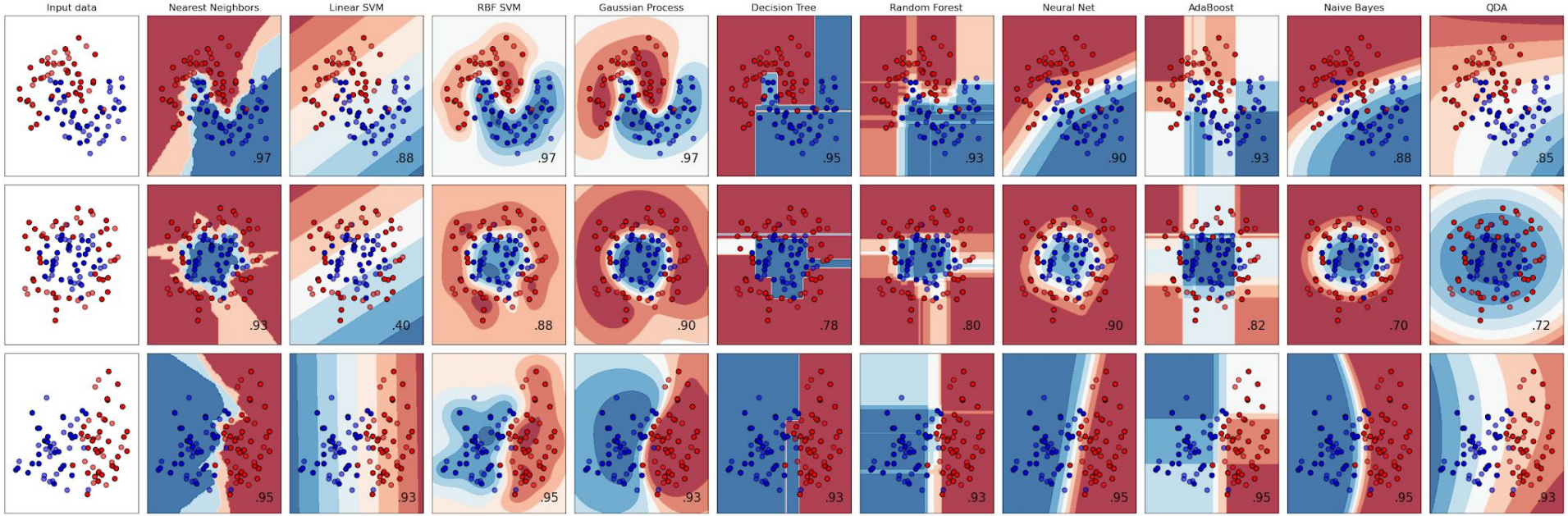

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