HPE DSI 311
Introduction to Machine Learning

Spring 2023

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Overview

Assessing Model Capacity

- The Bias-Variance tradeoff

Supervised classification using deep learning models

- Neural Nets

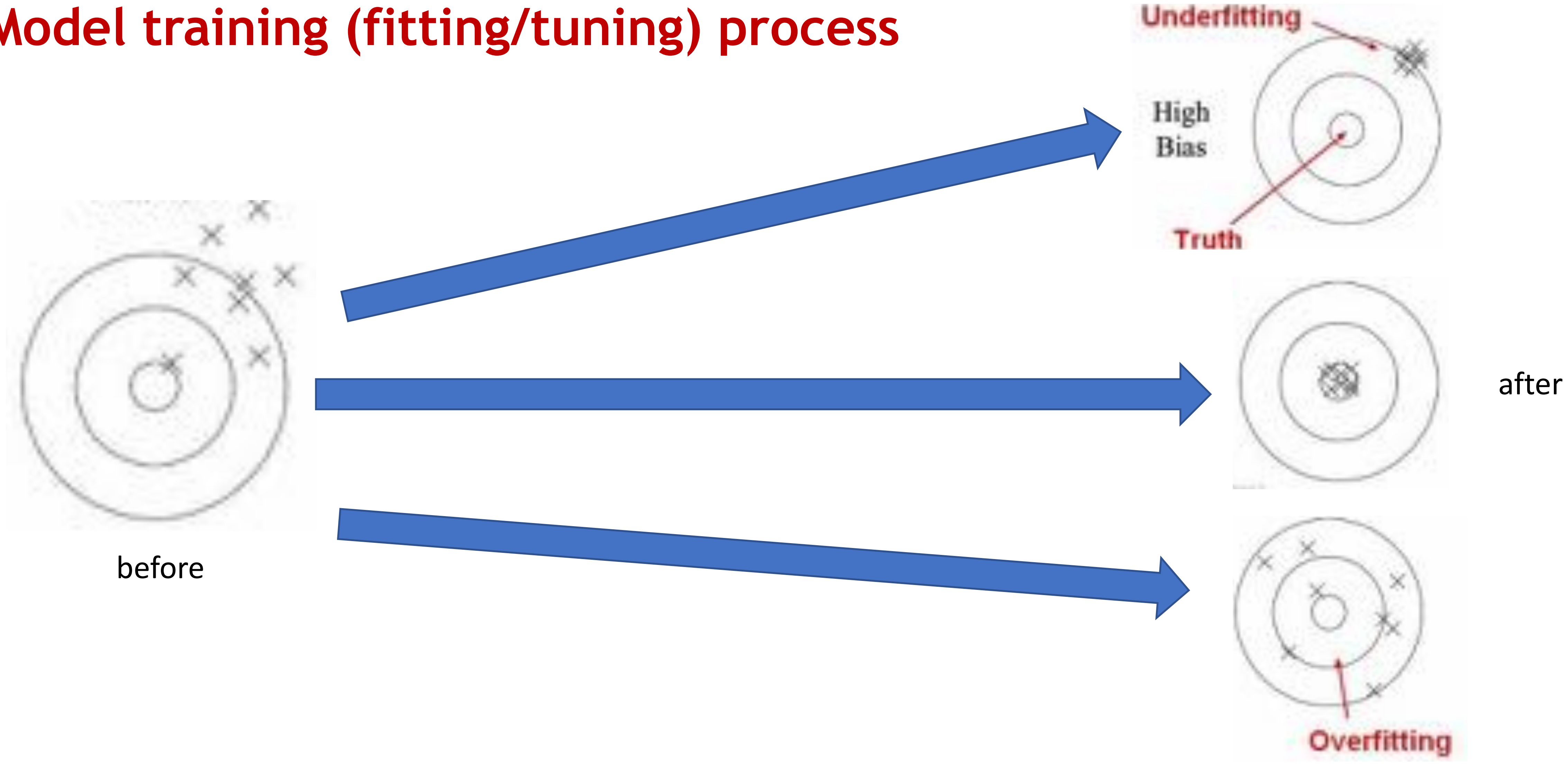
The bias-variance tradeoff

Model tuning: the over/under (fitting)

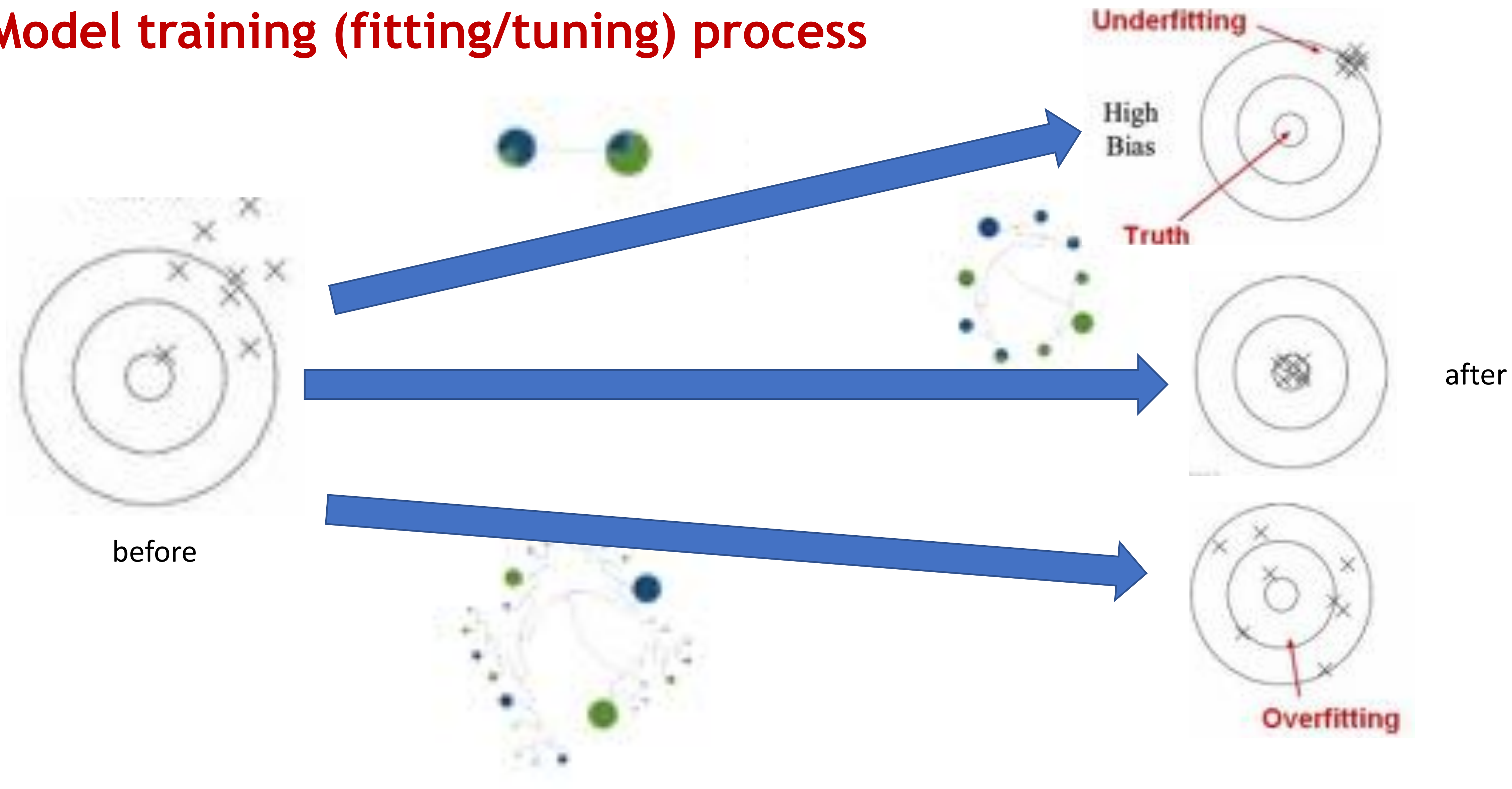
Interactive visualization of the main idea

http://www.r2d3.us/visual-intro-to-machine-learning-part-2/

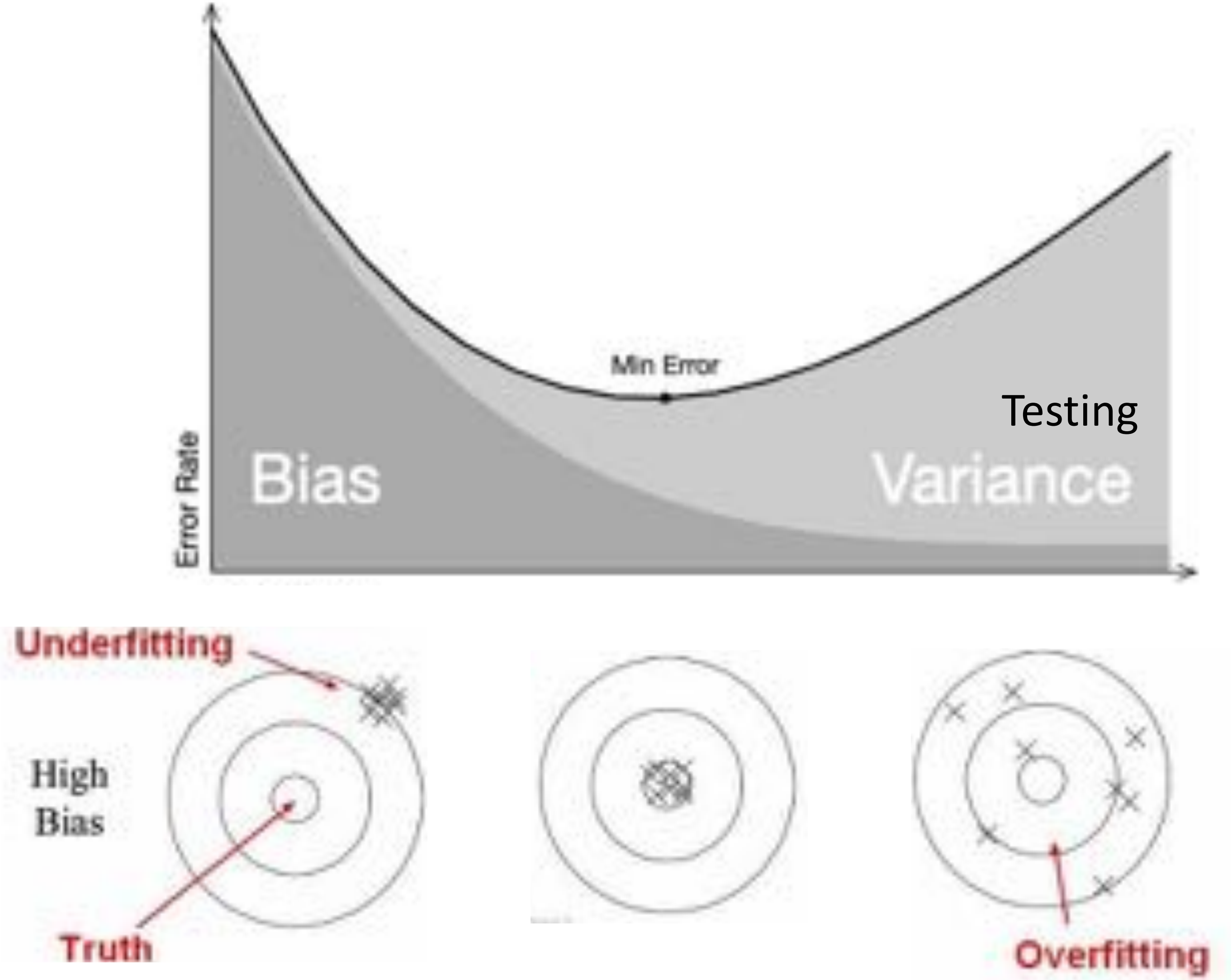
Model training (fitting/tuning) process



Model training (fitting/tuning) process



Some people think of it this way in ML



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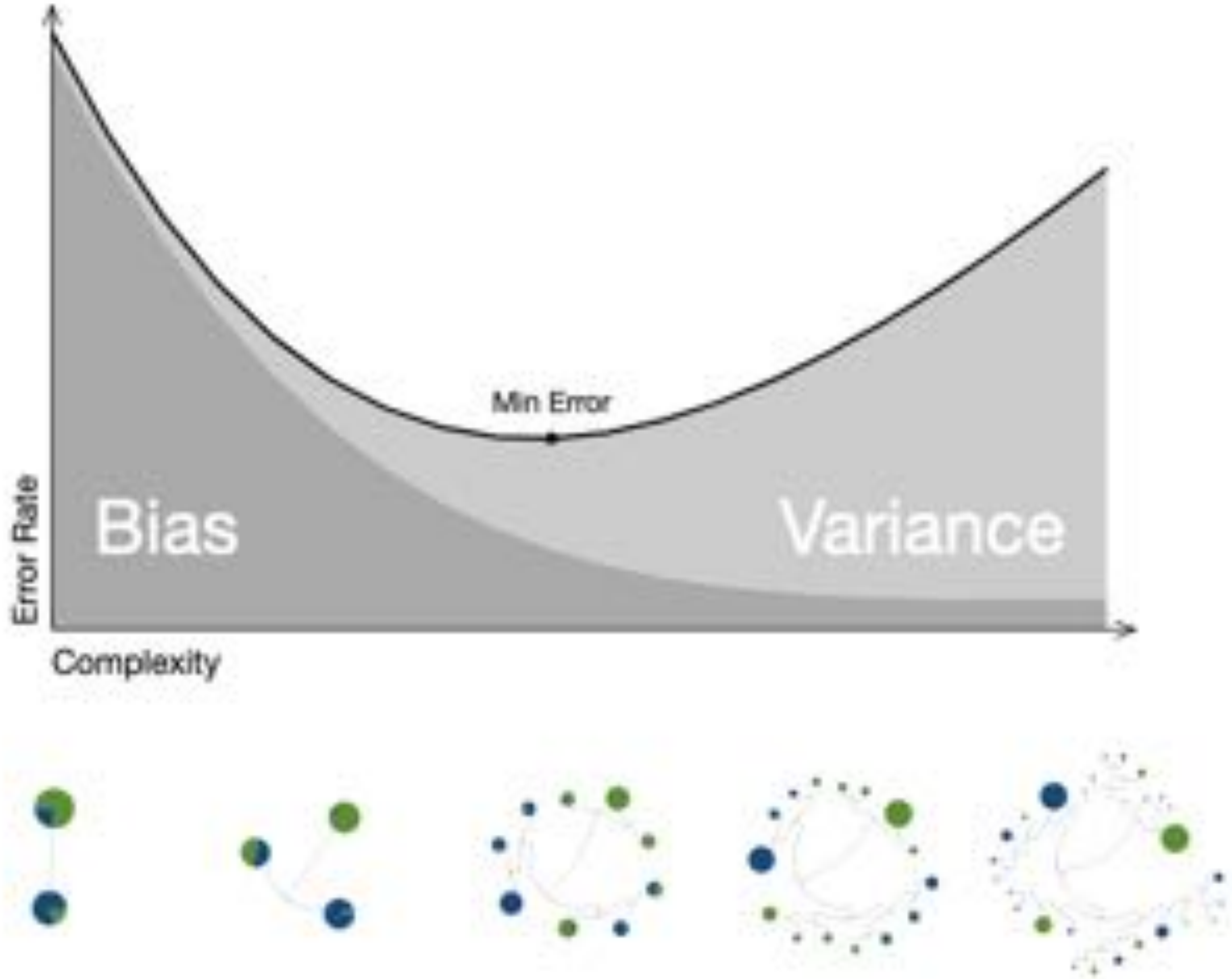
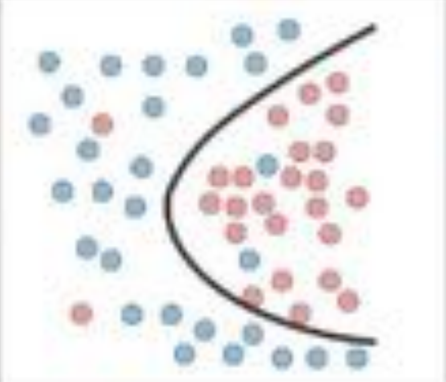
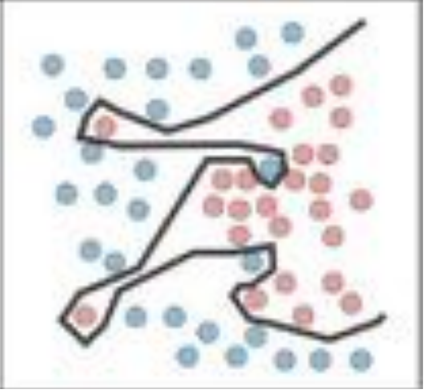


Some people think of it this way in ML

	Underfitting	Just right	Overfitting
Symptoms	- High training error - Training error close to test error - High bias	- Training error slightly lower than test error	- Low training error - Training error much lower than test error - High variance
Regression			
Classification			

Hands-on Example

Ready to move on

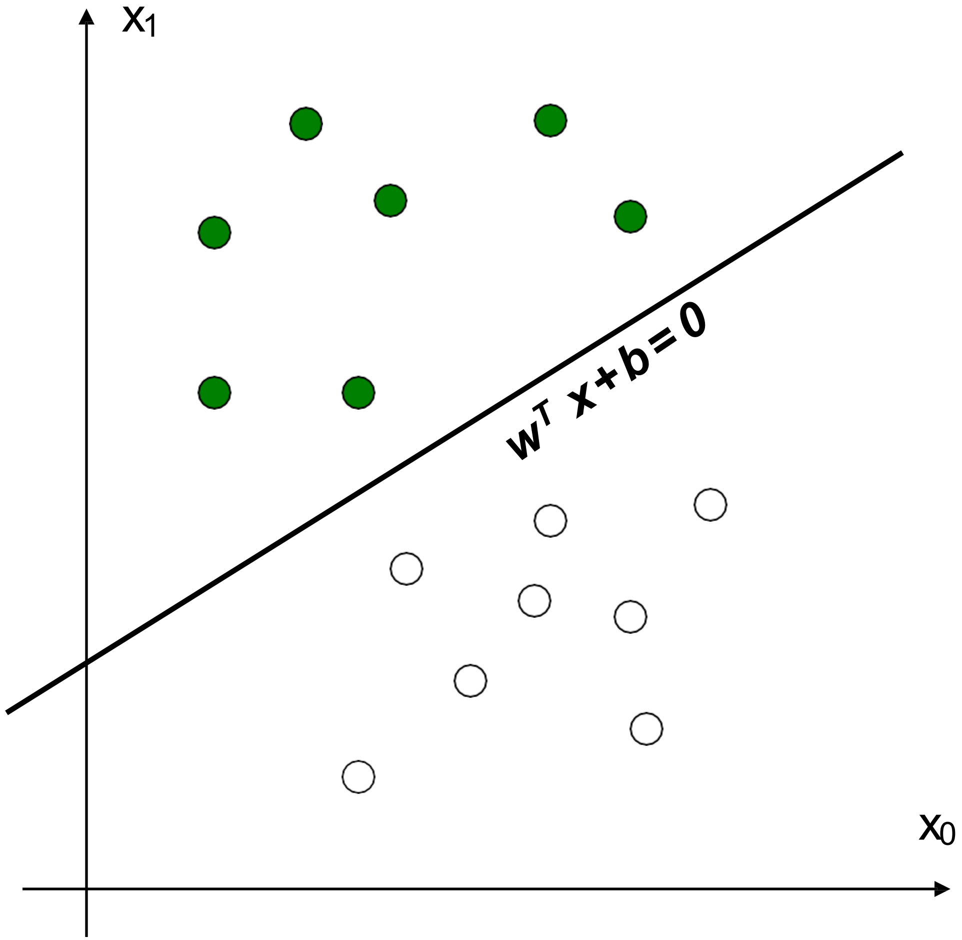
Remember Linear Discriminant Classifiers?

Linear Discriminant Classifier

$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b =$$

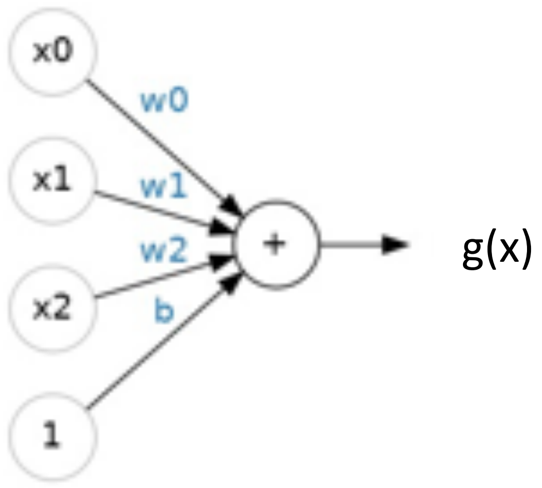
$$= \sum_{i \in SV} w_i \, x_i + b$$

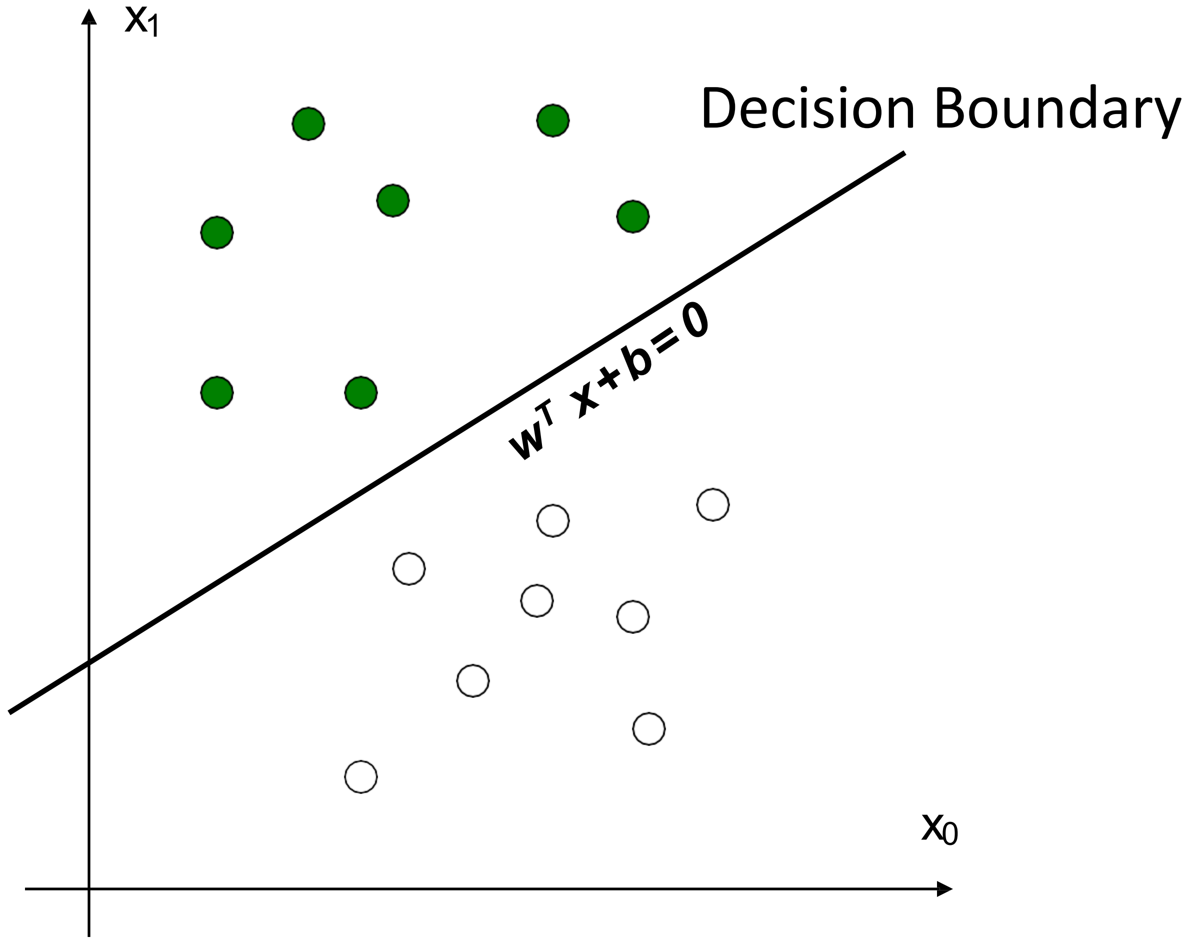
Decision function = sign(x)



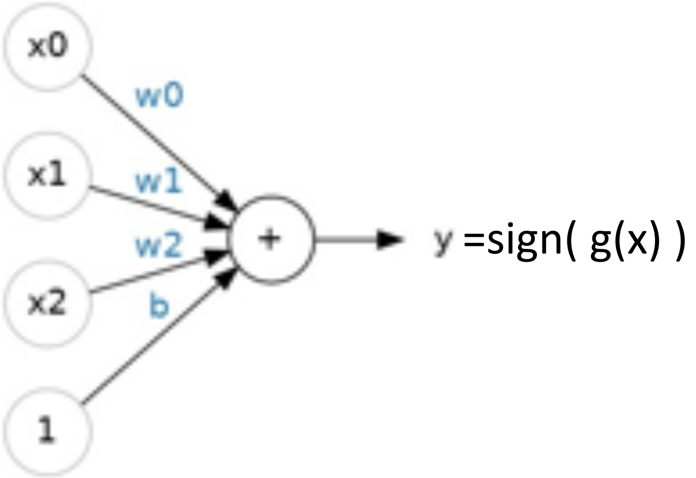
Linear units

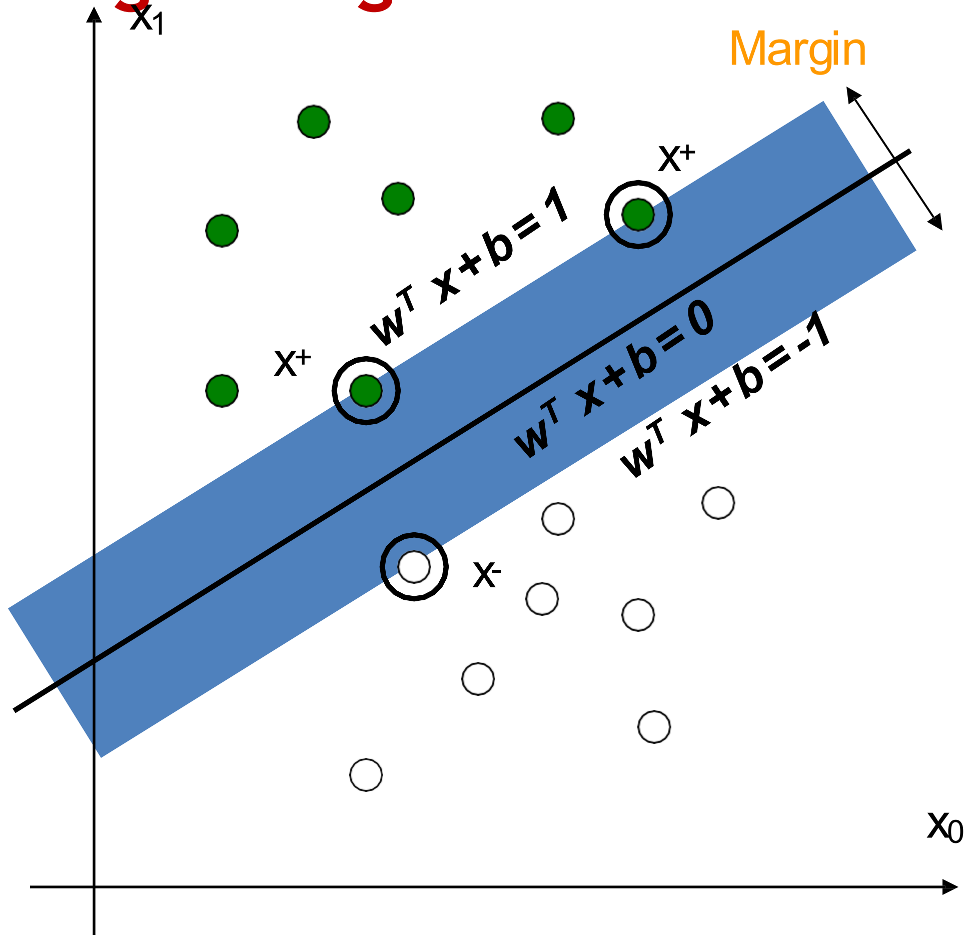
A linear unit:





SVM: linear unit with largest margin + sign





Speed vs. optimality

A 1080p digital image (most common screen size) comprises

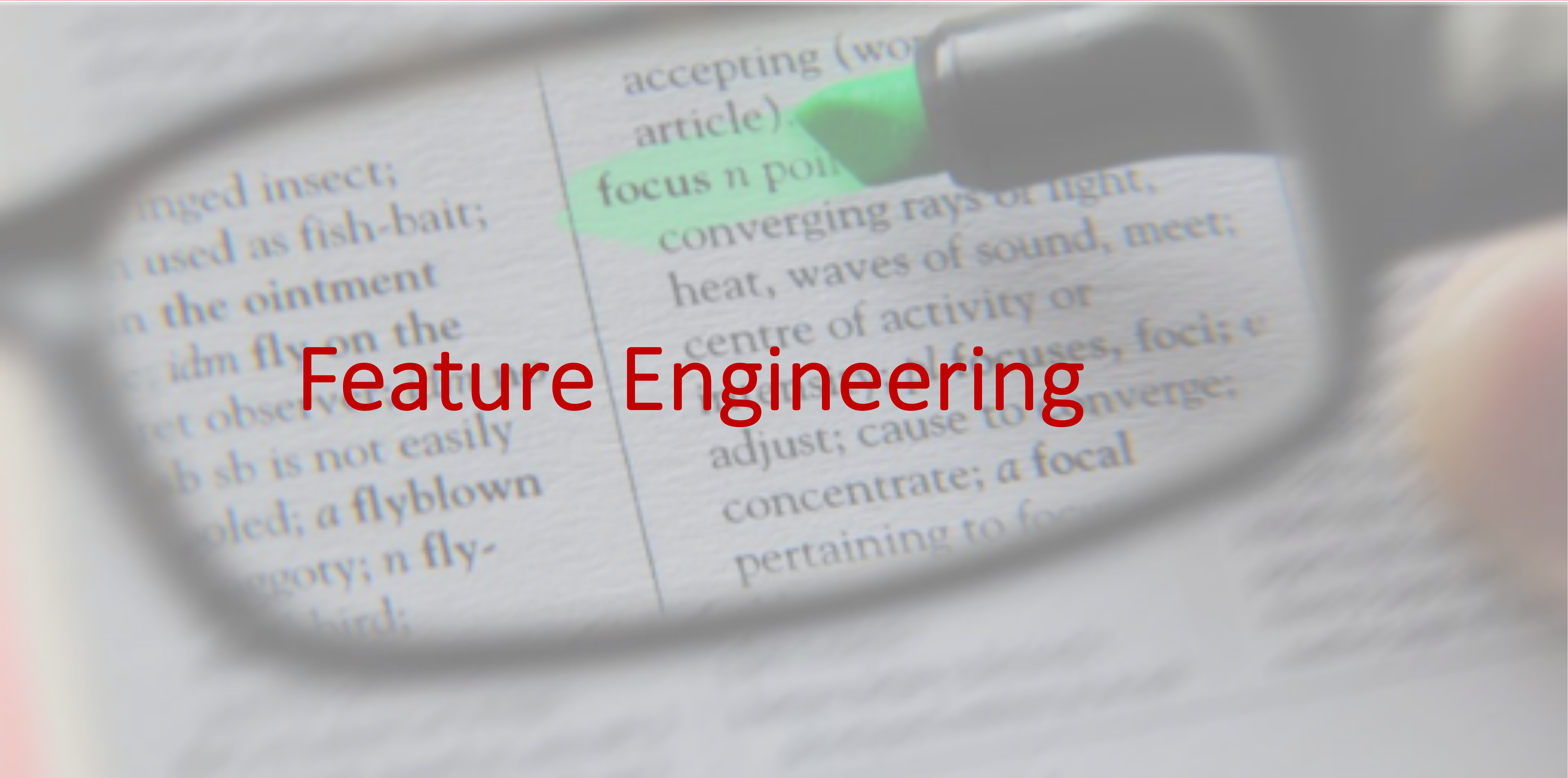
- 1920 x 1080 pixels (1080 lines of vertical resolution) and
- three color channels (RGB)

A total of more that 6 million variables!

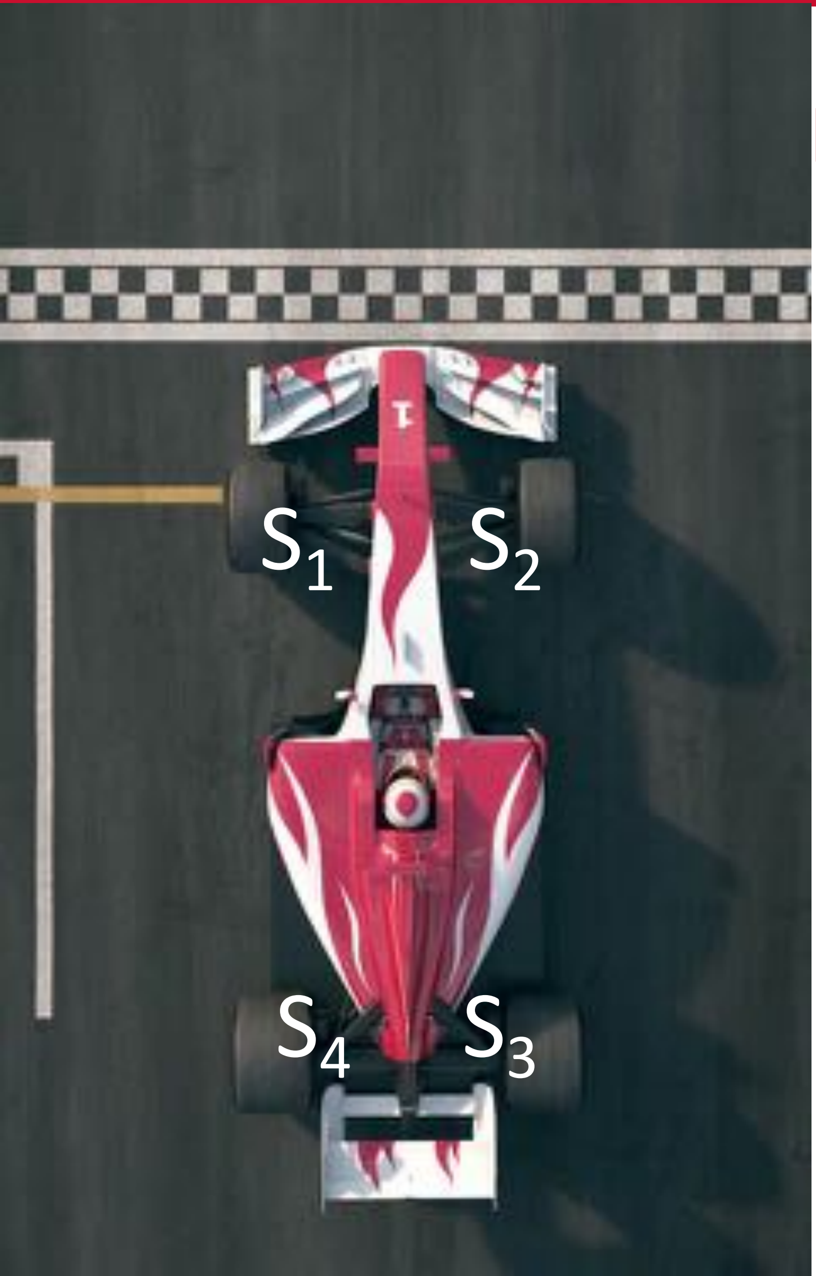
➢unlikely the points will line up nicely for linear class separation to work; also,

➢computing the optimal margin takes a lot of effort (quadratic programming)

Need feature extraction / dimension reduction



Feature Engineering



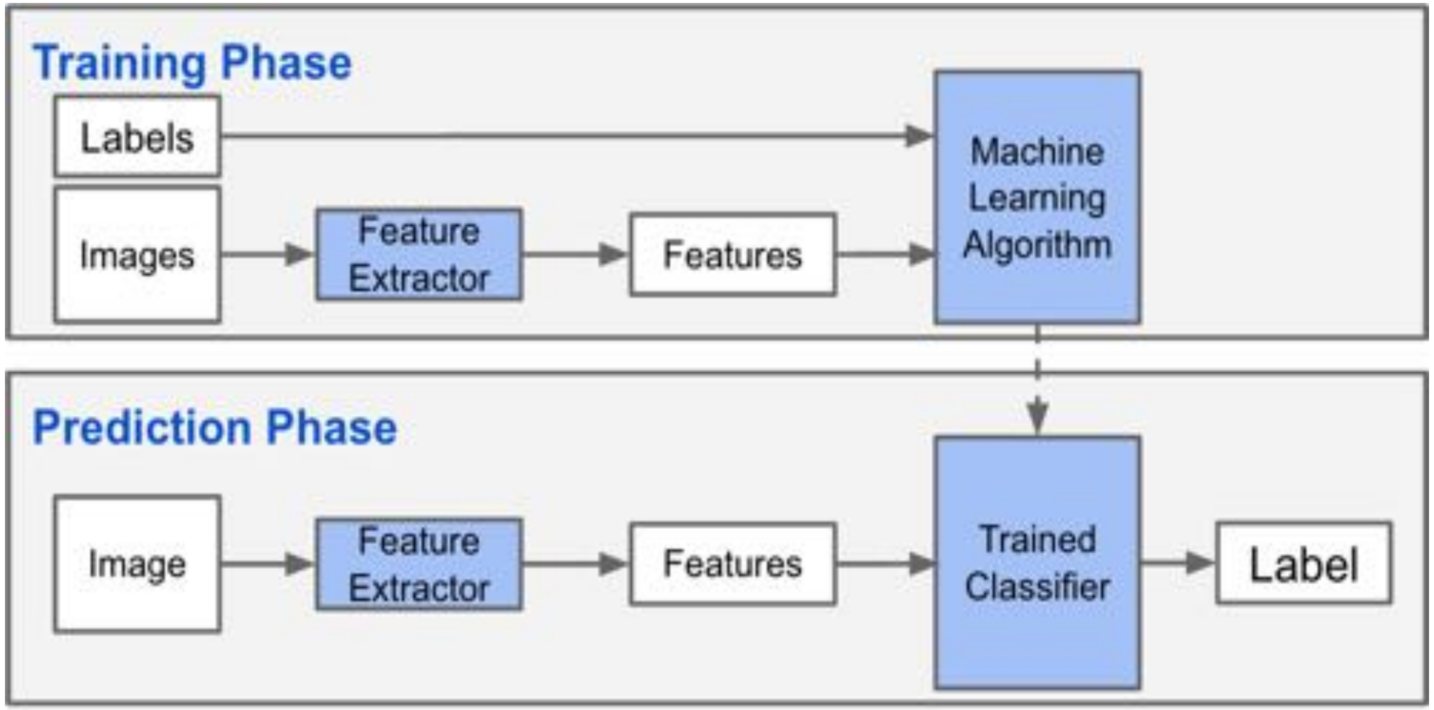
Features: domain knowledge

RAW DATA
Four sensors measuring rotation speed (spin) at each wheel: S_1, S_2, S_3, S_4

NEW FEATURES
$$T_1 = \{ (\frac{S_2 + S_3 + S_4}{3}) - S_1\} / 2 = -\frac{1}{2} S_1 + \frac{1}{6} S_2 + \frac{1}{6} S_3 + \frac{1}{6} S_4$$

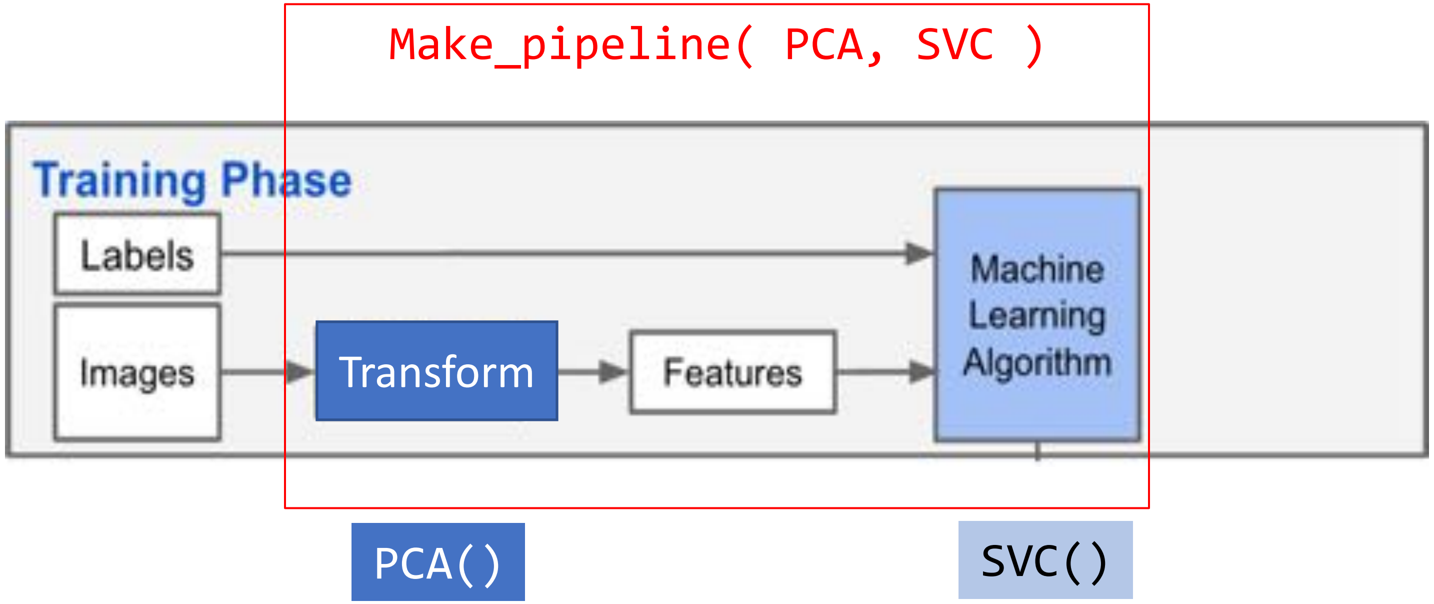
EXPERT KNOWLEDGE
If a feature starts to veer away from zero, then a tire is spinning faster than the others (possible flat)

Feature extractors help unscramble the features from the raw data, and prioritize features for selection



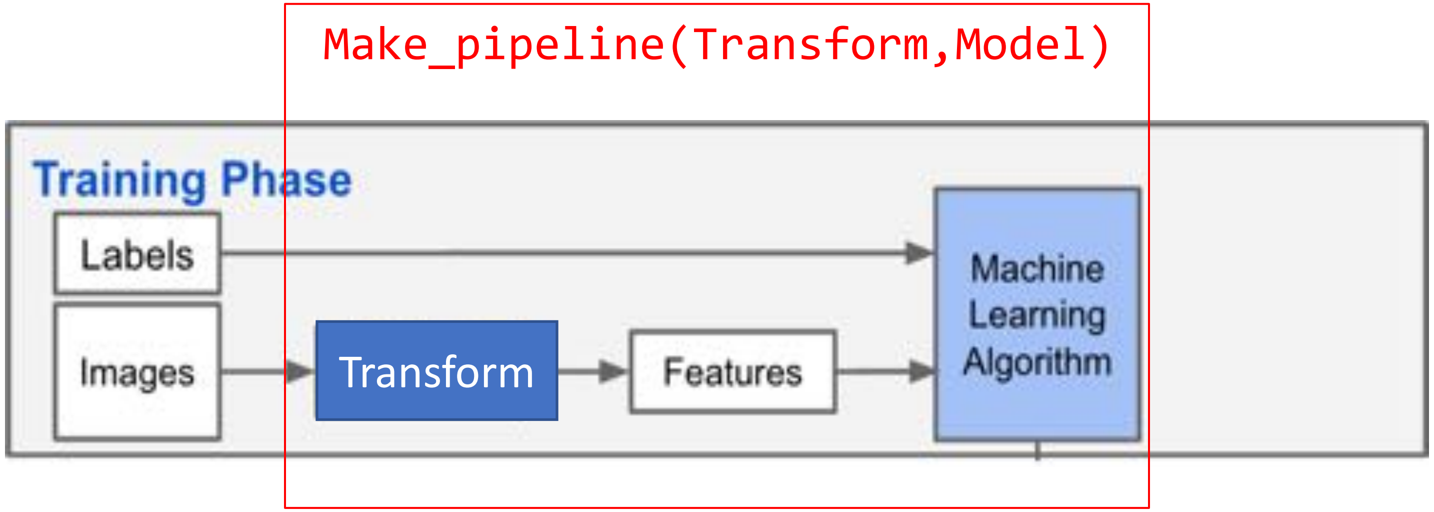
Machine Learning Phases

Feature engineering example: PCA



PCA is most commonly available data transform, because it is the most generic

Feature engineering: a lot of possibilities

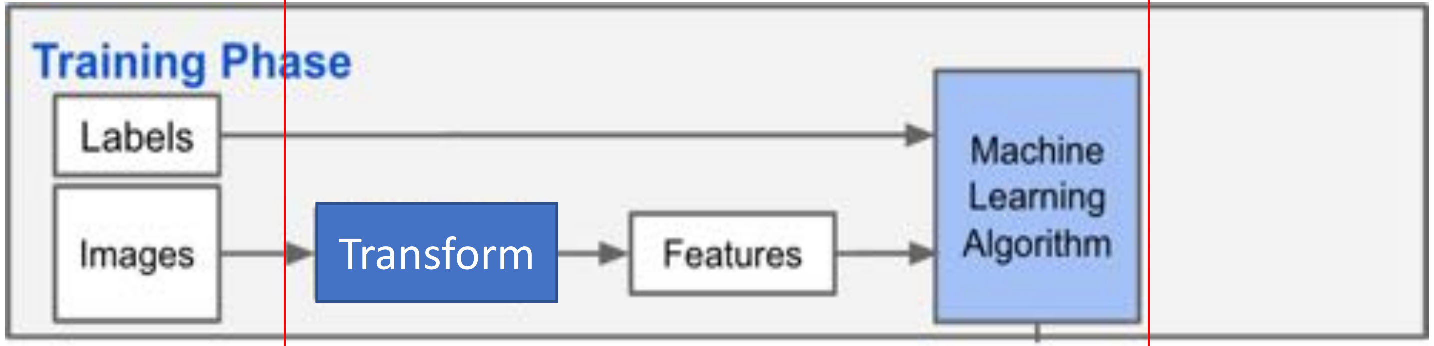


PCA is most commonly available data transform because it is the most generic

There are many other choices

Feature engineering: a lot of possibilities

```
Make_pipeline(Transform,Model)
```



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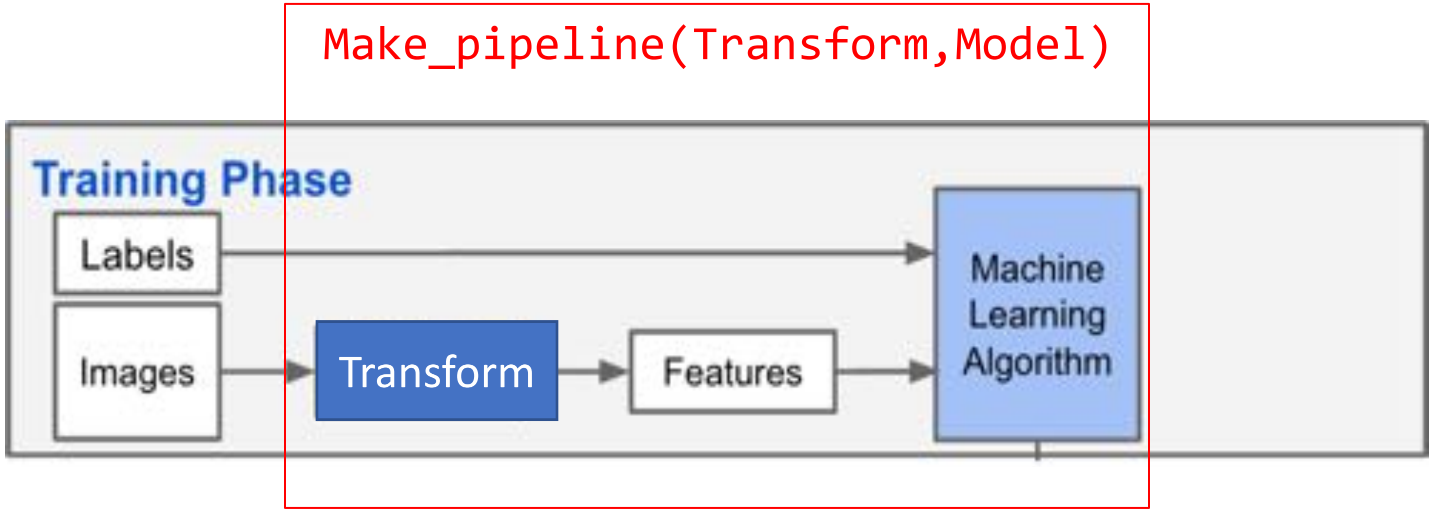
There are many other choices:

- Fourier Transform: extract frequencies from wave signals

Feature engineering: a lot of possibilities



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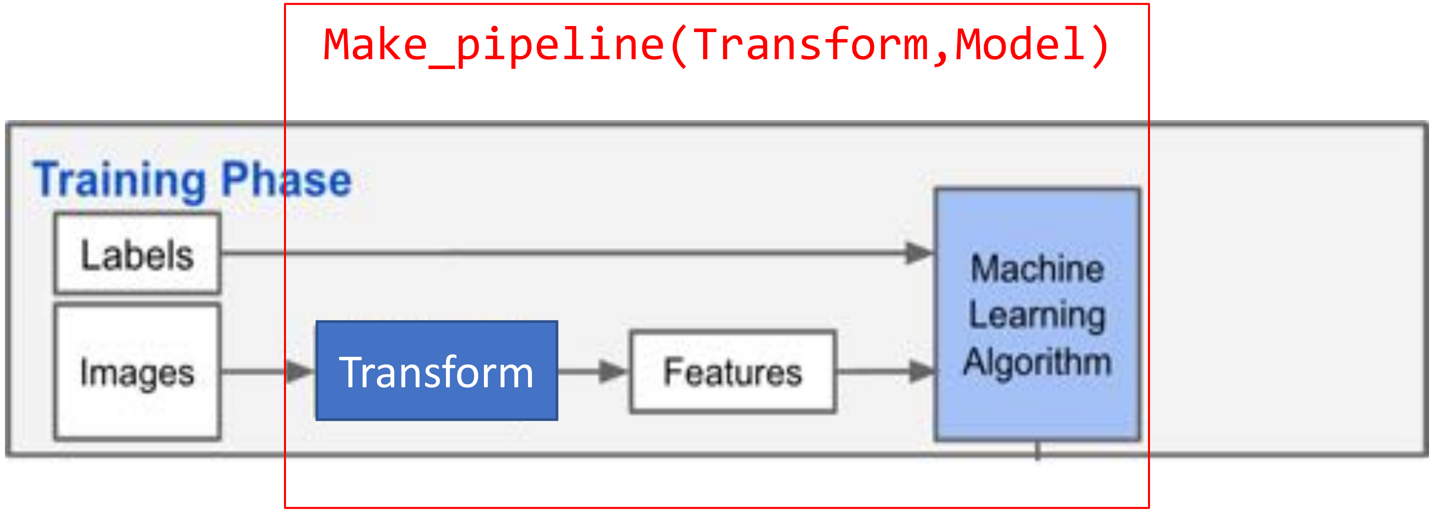
There are many other choices:

- Fourier Transform: extract frequencies from wave signals
- Wavelet Transform: extract levels of detail from images

Feature engineering: a lot of possibilities

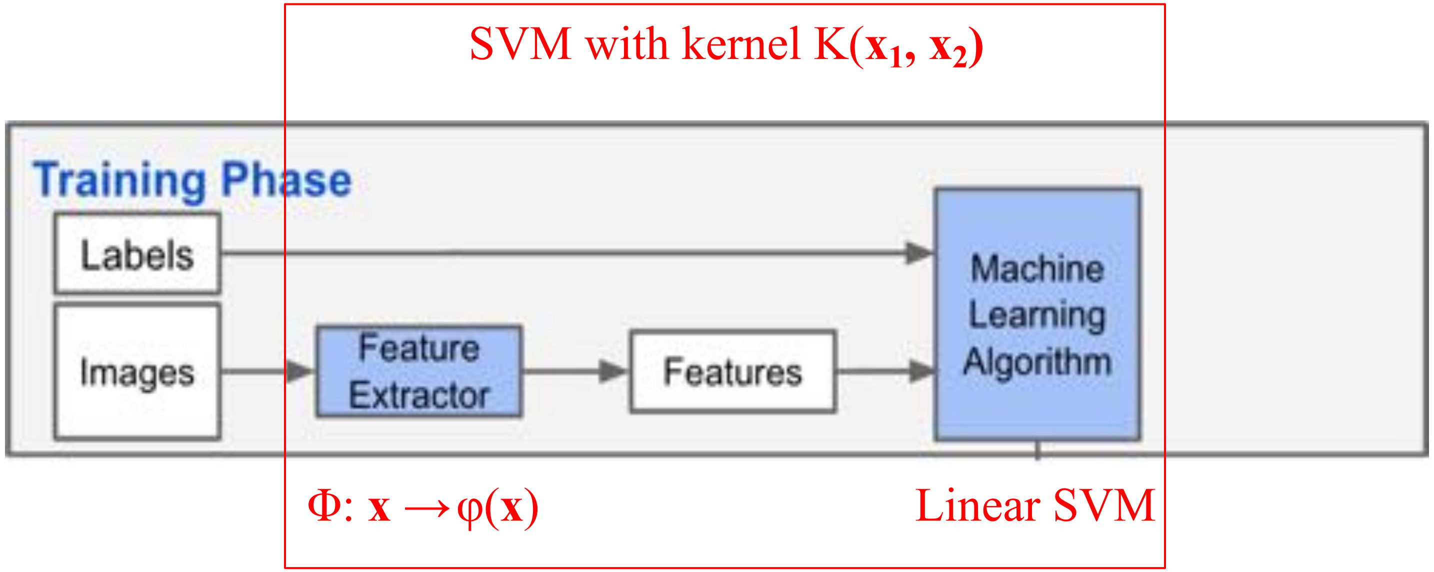


PCA is most commonly available data transform because it is the most generic

There are many other choices:

- Fourier Transform: extract frequencies from wave signals
- Wavelet Transform: extract levels of detail from images
- Kernel Trick!

The kernel trick masks a data transform



Think of

```
    SVC( kernel=‘rbf’ )
```

as being the same as

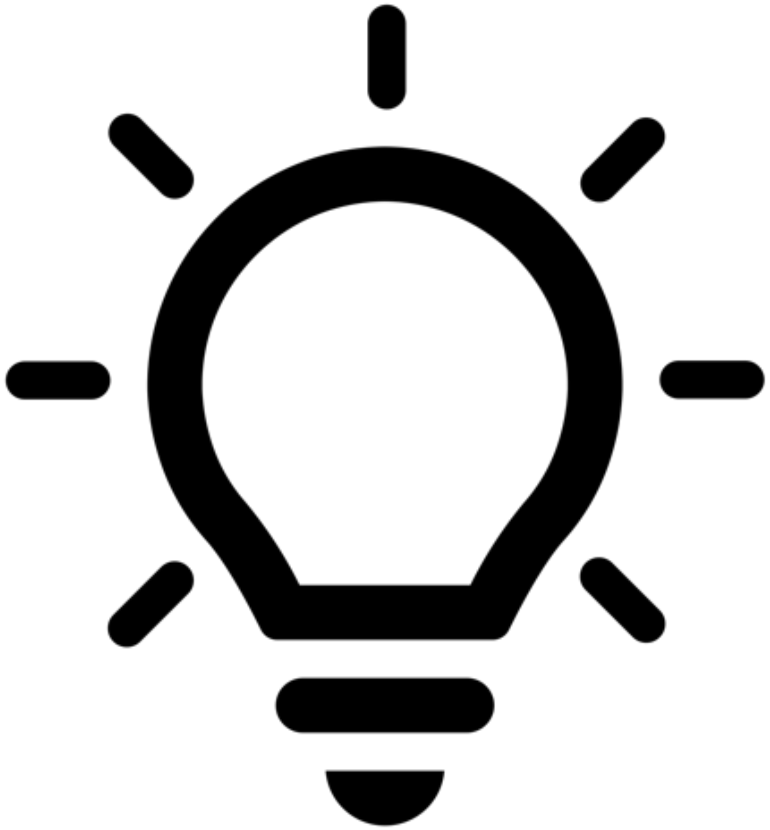
```
    make_pipeline( rbfTransform, SVC )
```

Feature engineering: drawbacks

- Feature engineering is difficult, time-consuming, and requires domain expertise.
- It is in the spirit of symbolic AI, instead of the modern connectionist paradigm

Can we try something different?

First Idea: Ensemble SVC

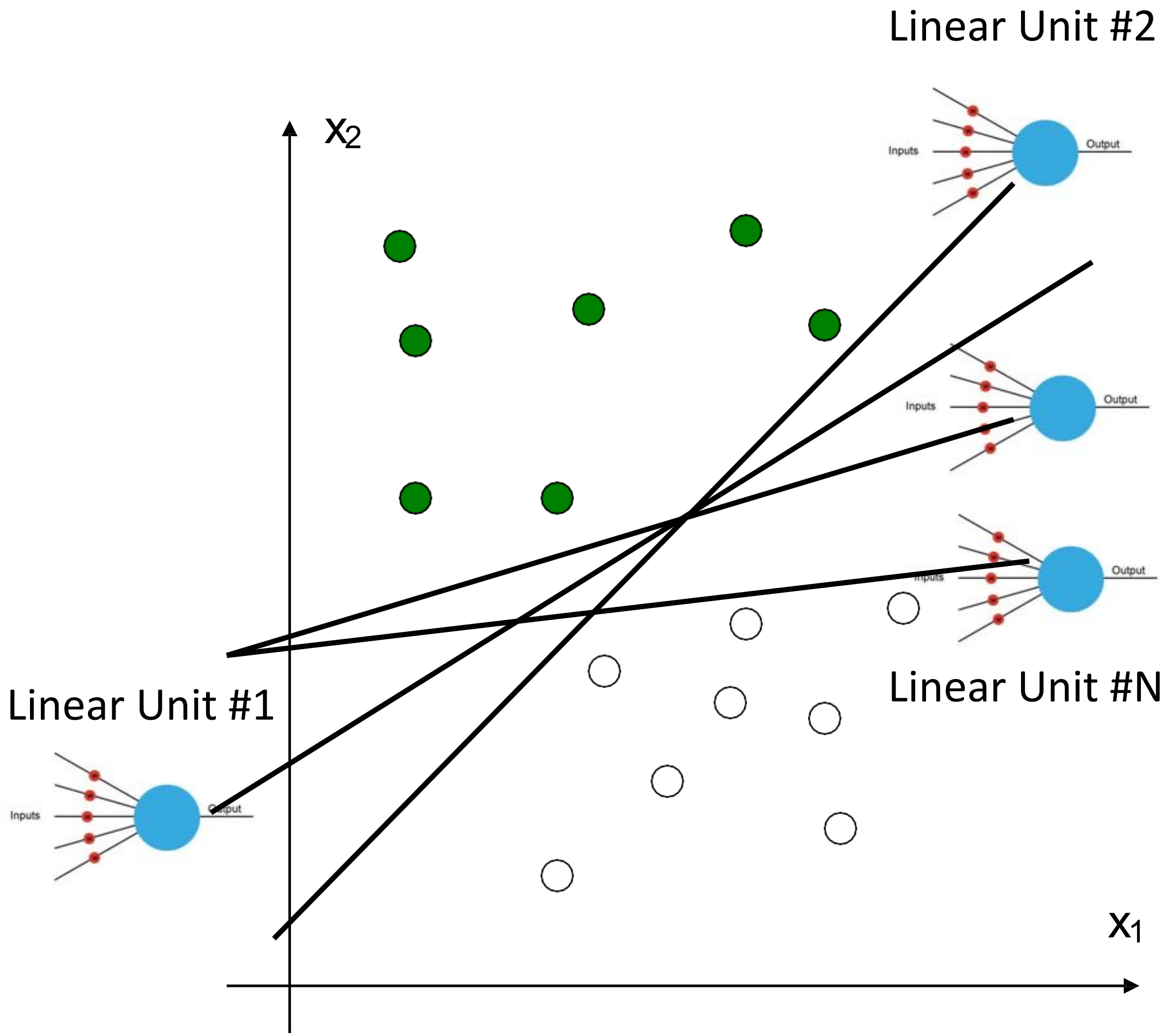


Aggregating activated linear units

Linear units

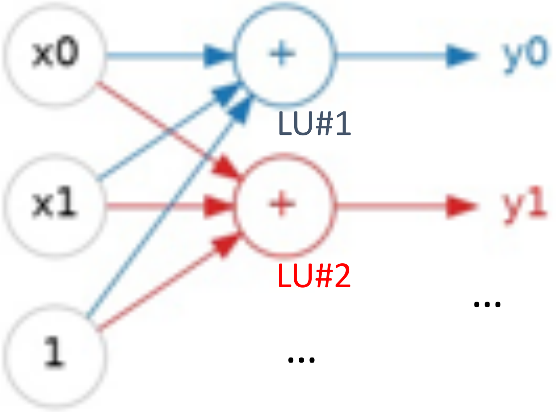
- Different hyperplanes correspond to different linear units

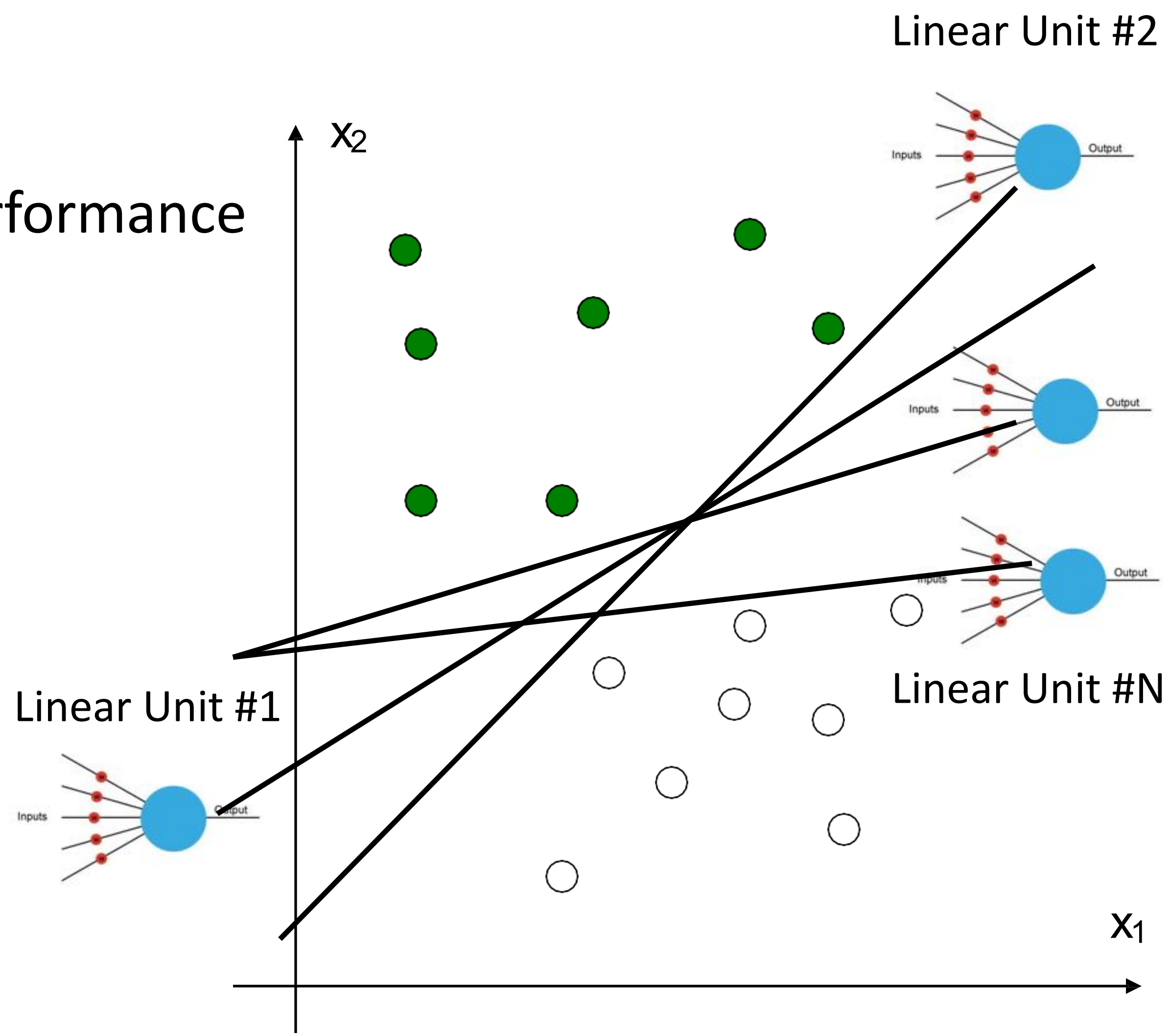
- They all classify the training set correctly, but are slightly suboptimal



Linear units

Aggregated as a group, their performance can be close to the SVM



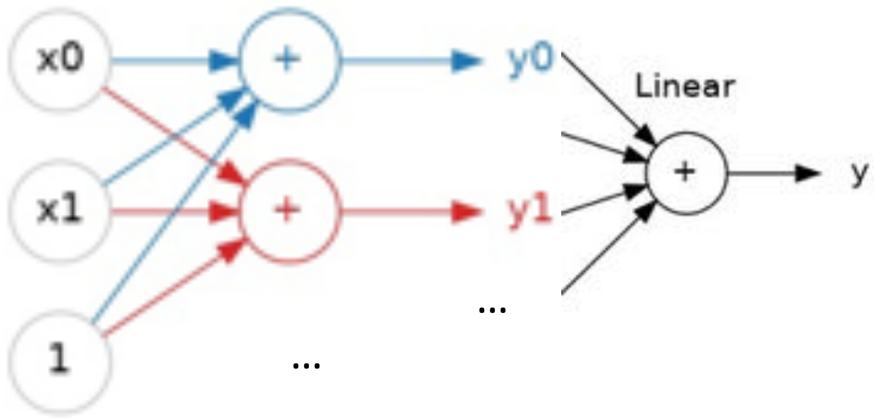


A simple ensemble

Decision function: Add the outcome of each unit to aggregate

Input Layer

Output Layer



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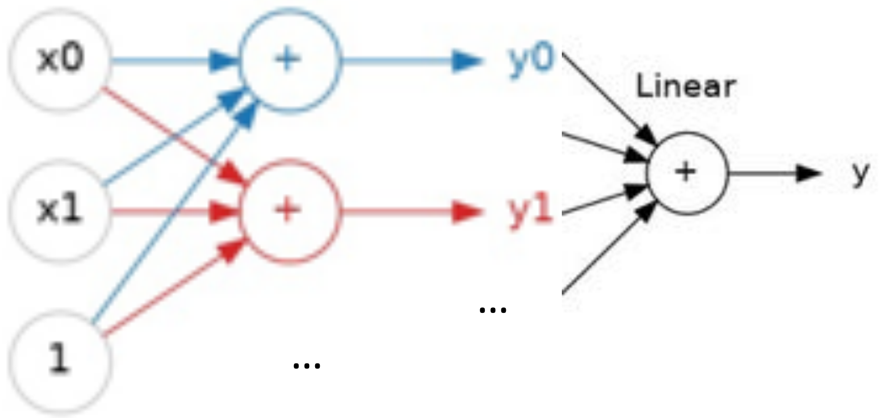
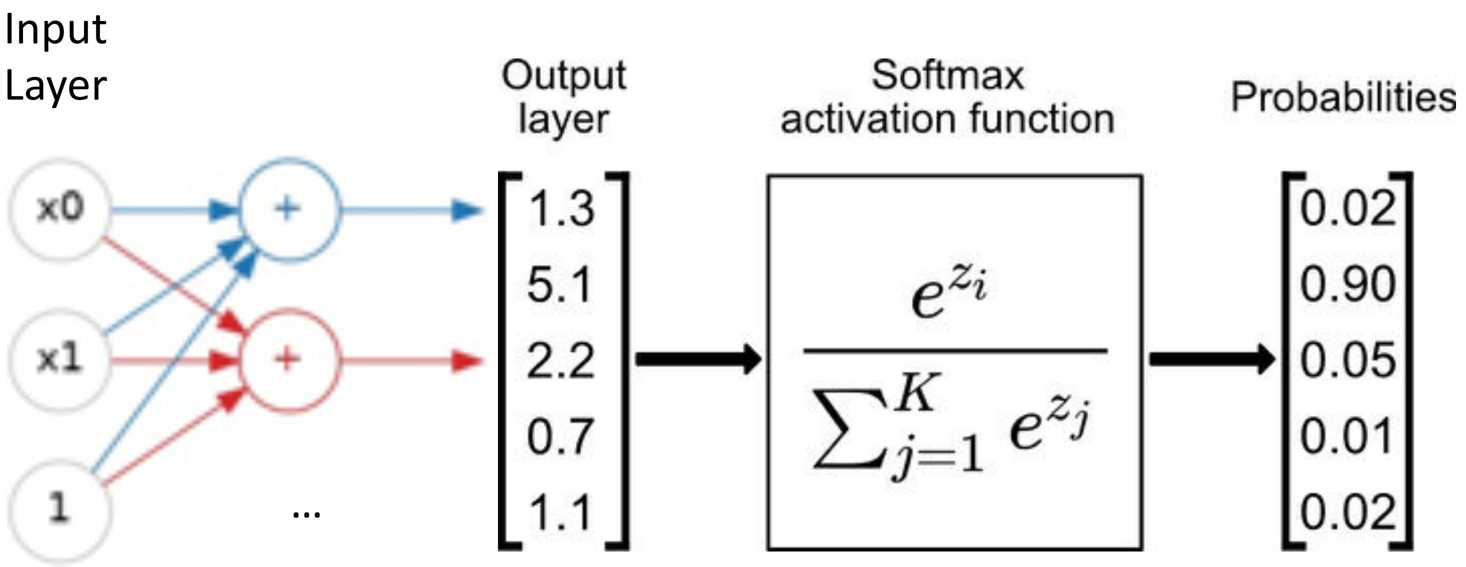


The final (output) layer is also a linear unit. That makes this network appropriate to a regression task, where we are trying to predict some arbitrary numeric value.

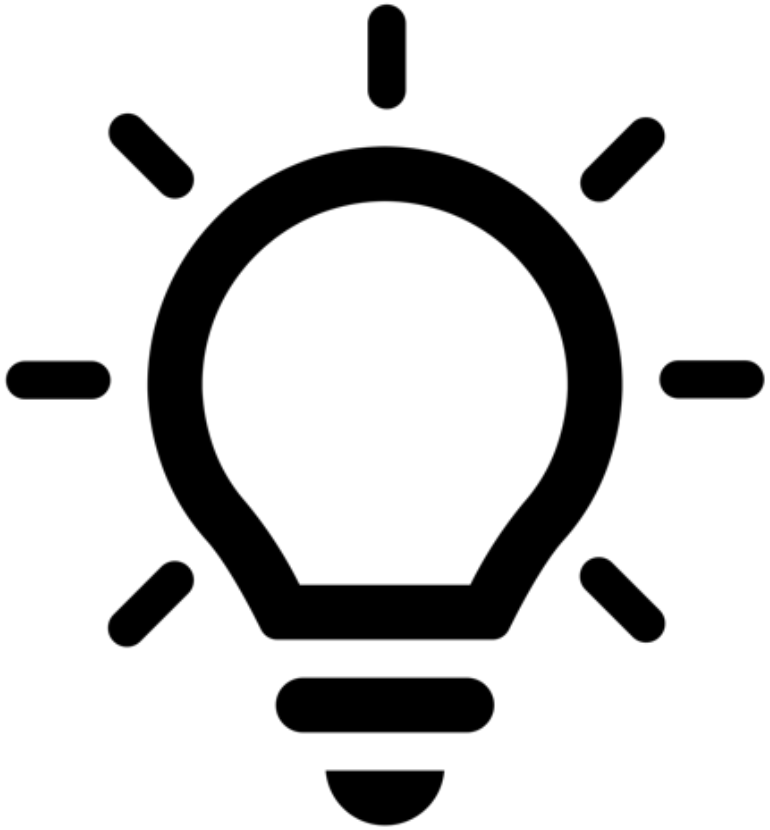
A simple ensemble

Decision function: Other tasks might require a different decision function on the output

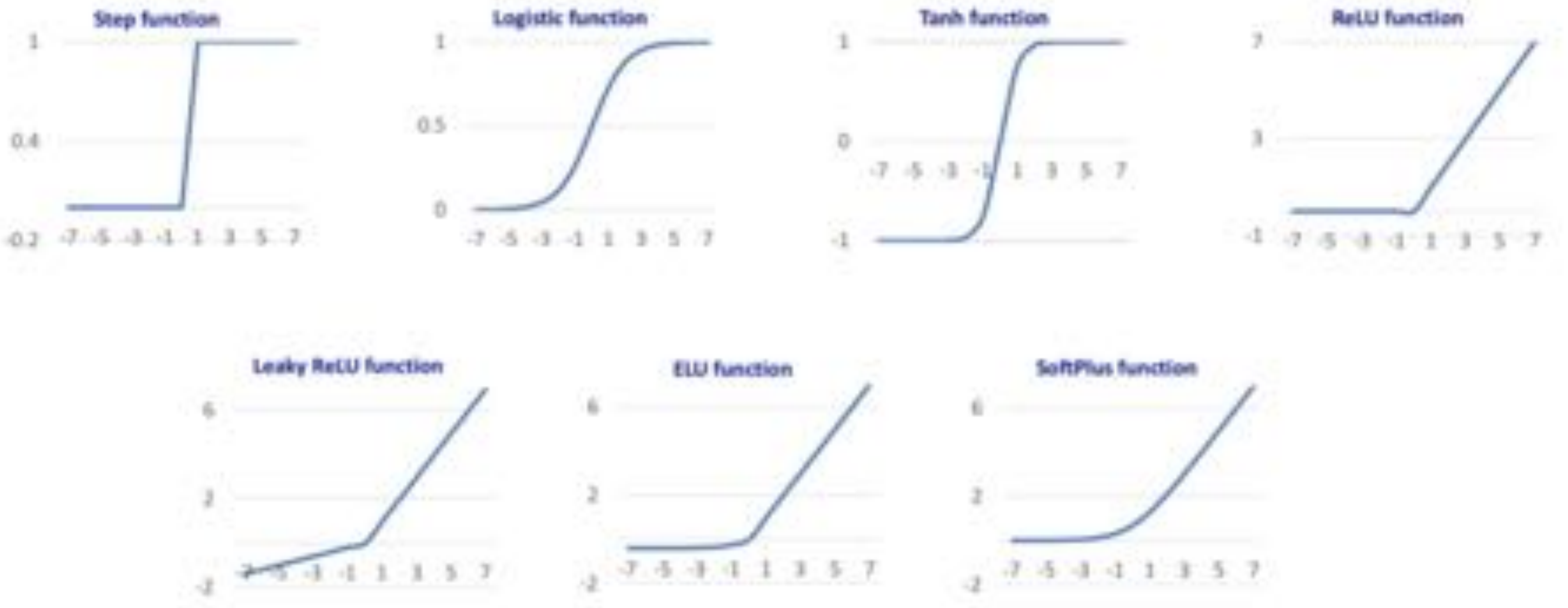


SoftMax is the most common for classification

Second Idea: sign, logit, … ?



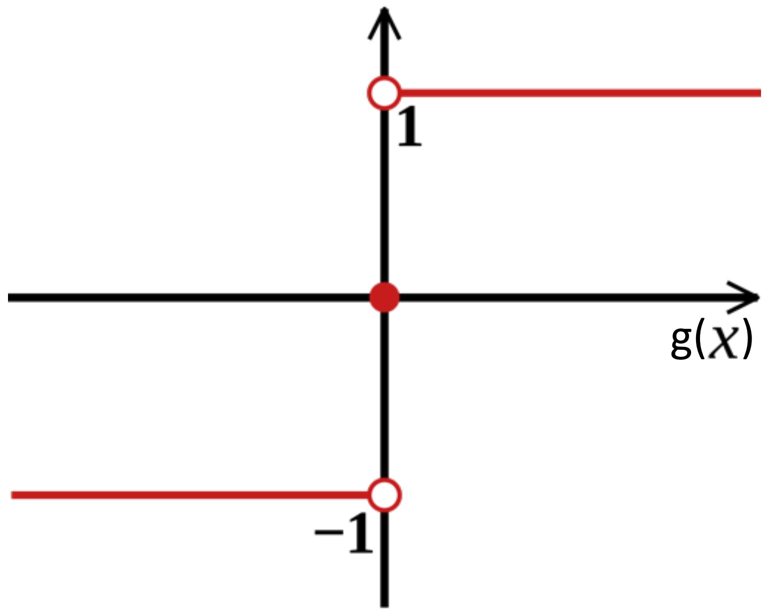
Many choices for the activation function



Logistic Regression: activate using the logistic function

$$\text{Probability(y)} = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$

SVC: activate using the sign function

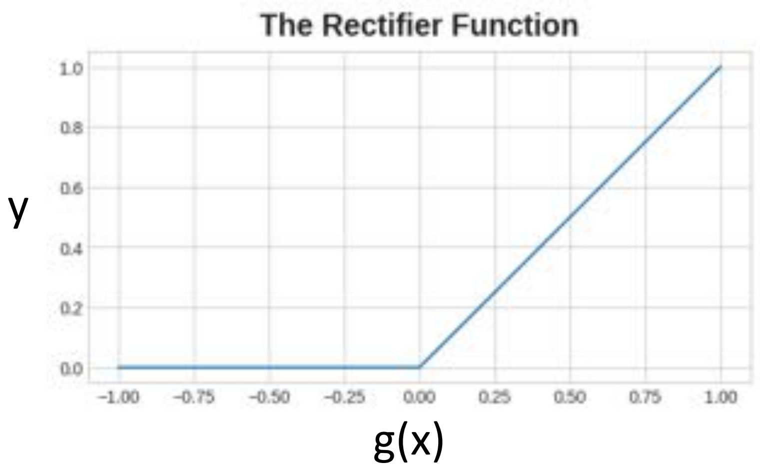


The output is sign(g(x))

decision = +1 if g(x) > 0

decision = -1 if g(x) < 0

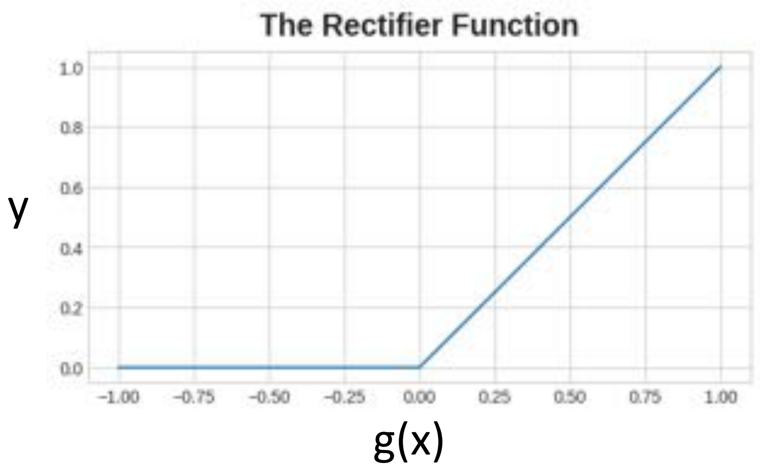
New: activate using the rectifier function

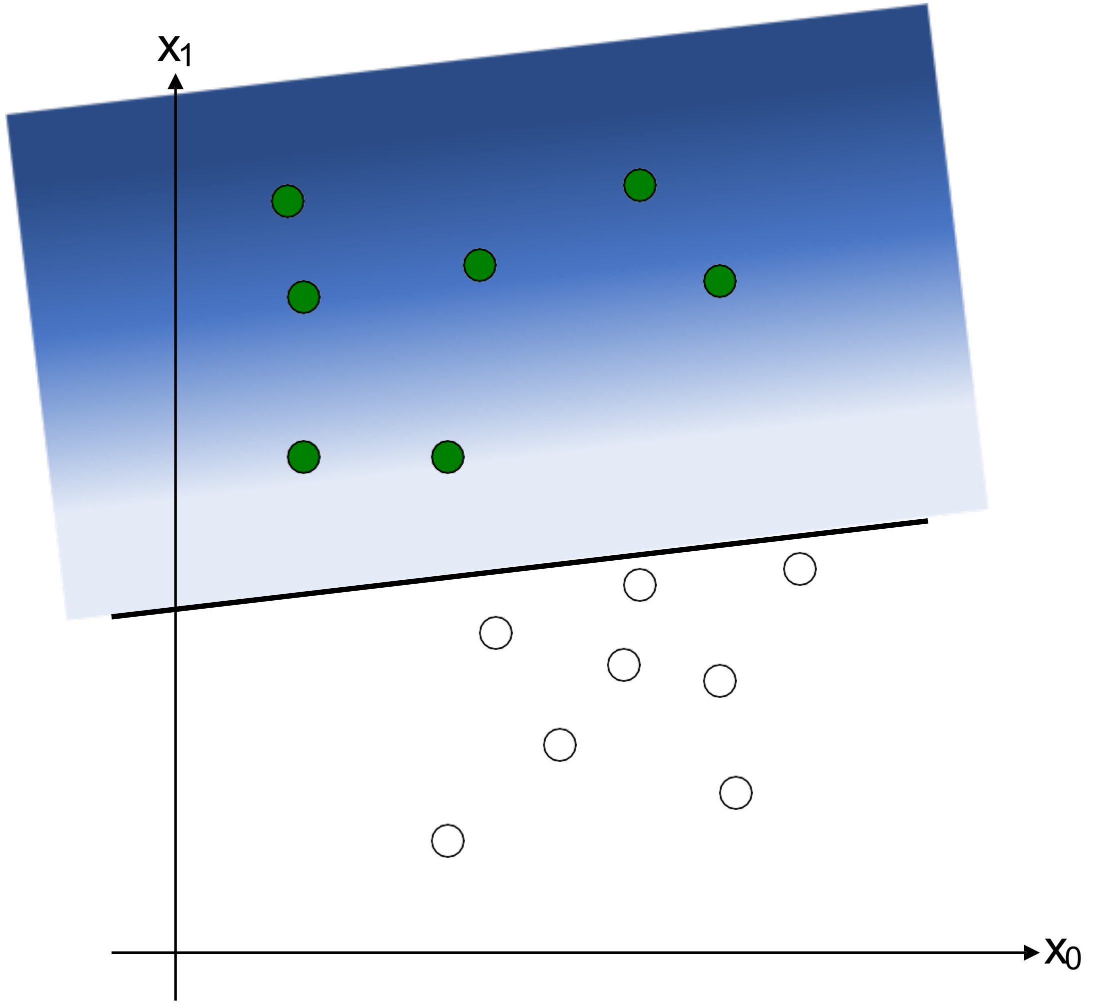


Instead of strict binary sign(g(x)), the output is max(0, g(x))

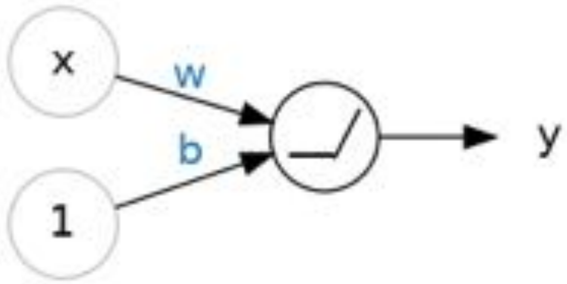
y = g(x) if g(x) > 0
y = 0 if g(x) < 0

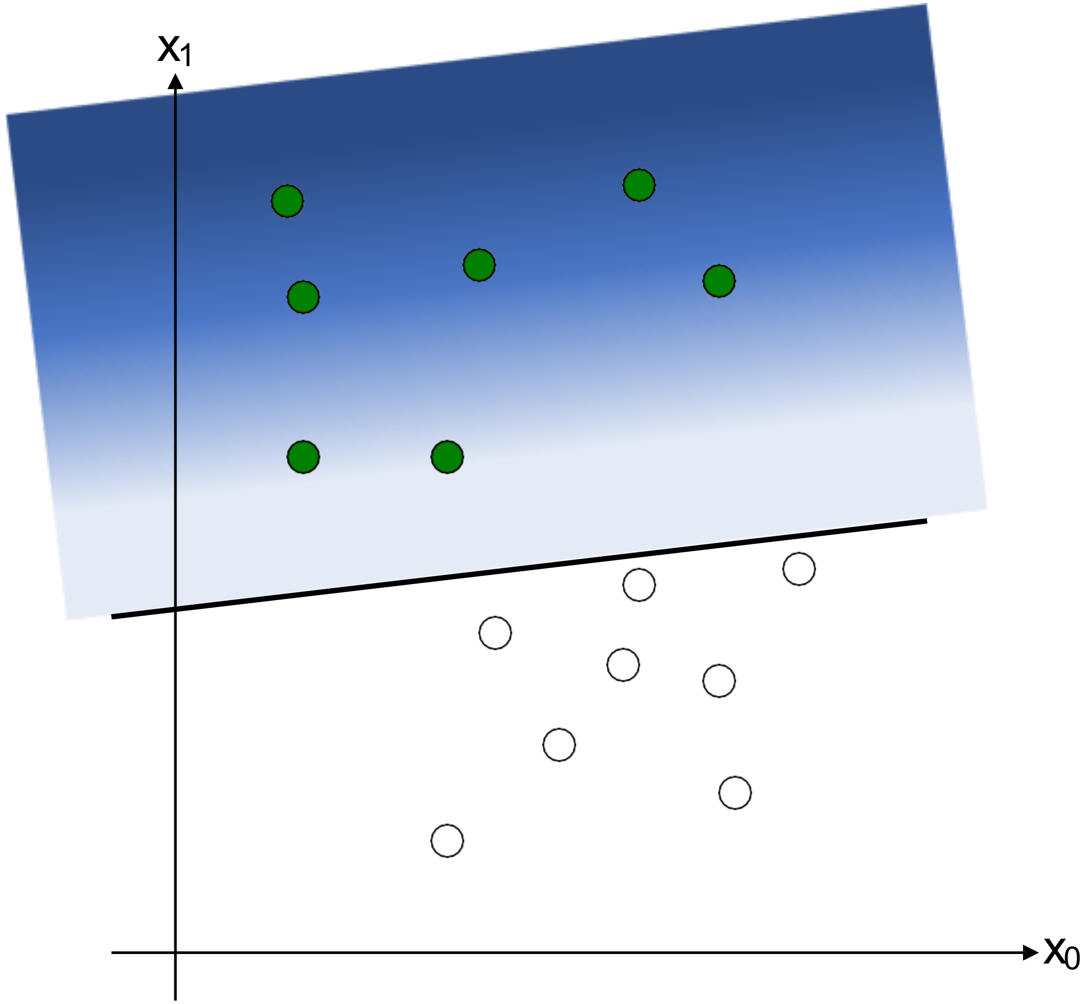
New: activate using the rectifier function





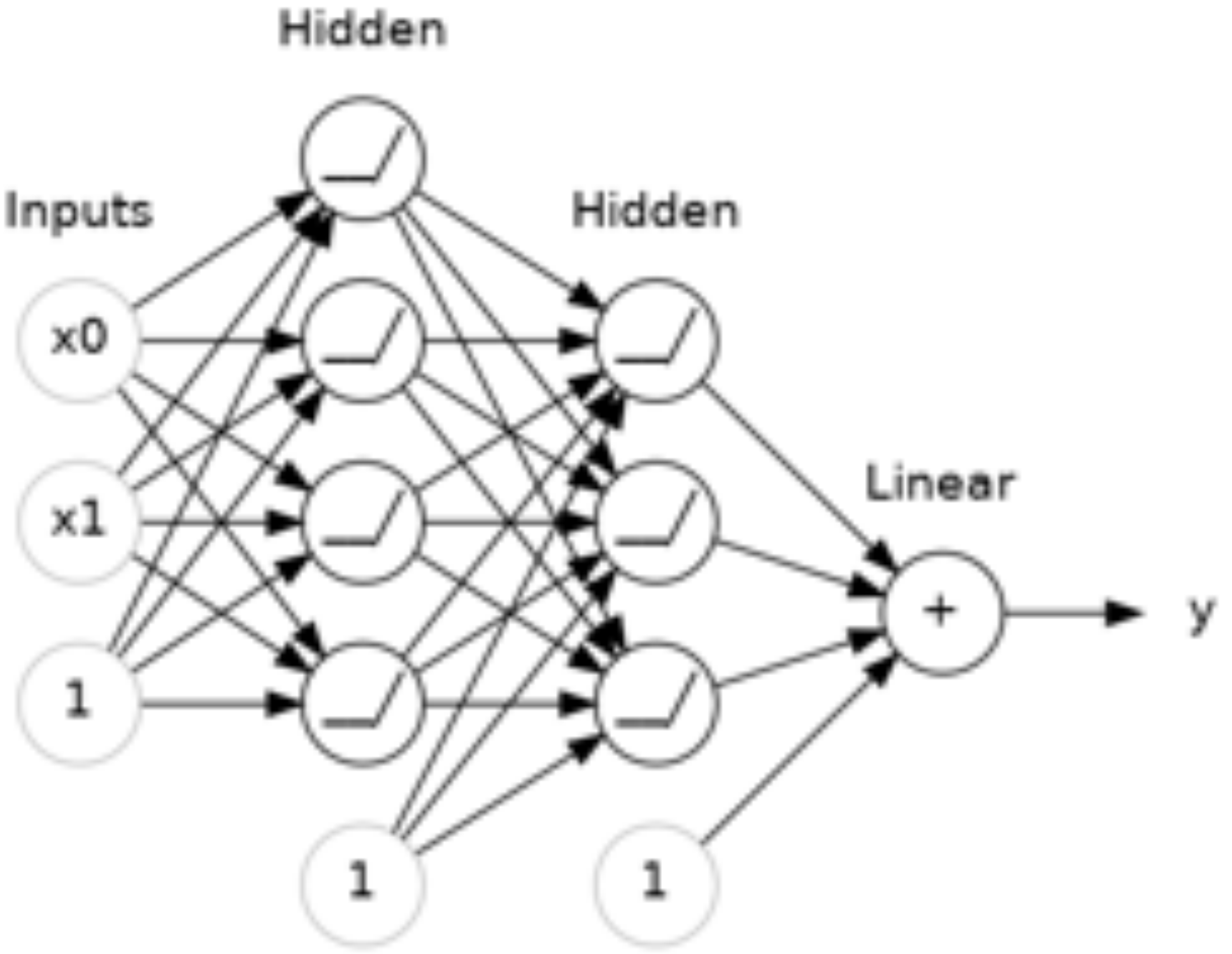
ReLU: a Linear Unit activated using the rectifier function





Putting it all together: Multi-Layer Perceptron

A fully-connected, feed-forward ReLU neural network with two hidden layers



Next time: Neural Nets

Supervised classification using deep learning models

https://playground.tensorflow.org/