HPE DSI 311
Introduction to Machine Learning

Summer 2021

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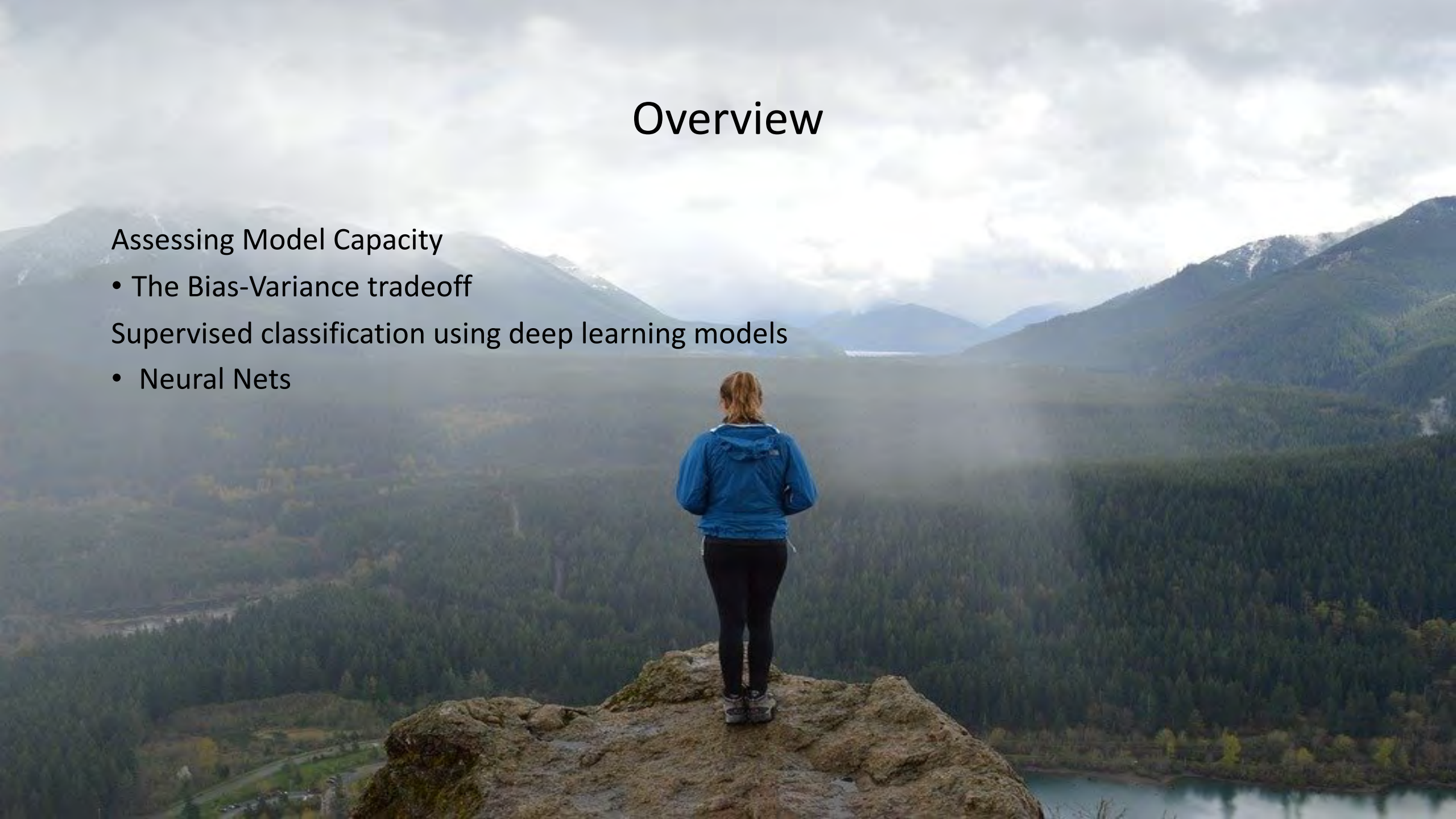
DIVISION OF RESEARCH
HEWLETT PACKARD ENTERPRISE DATA SCIENCE INSTITUTE

Overview



Assessing Model Capacity

- The Bias-Variance tradeoff

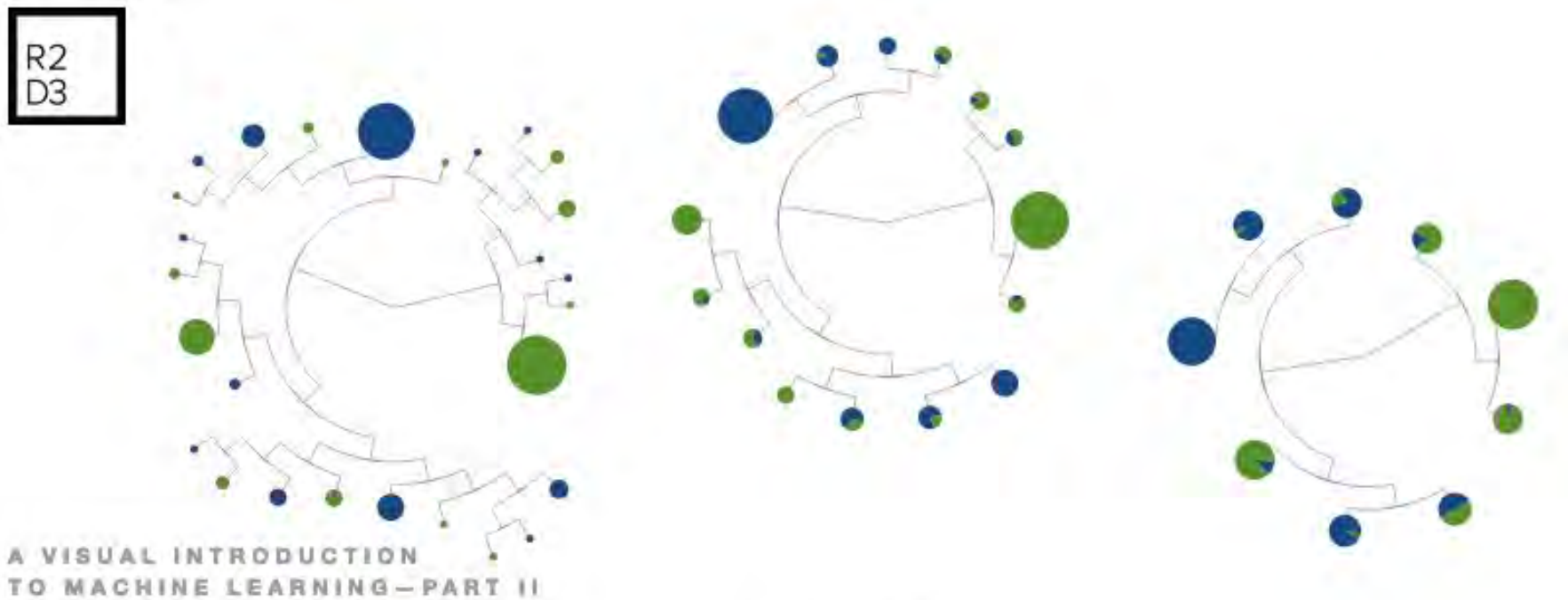
Supervised classification using deep learning models

- Neural Nets

The bias-variance tradeoff

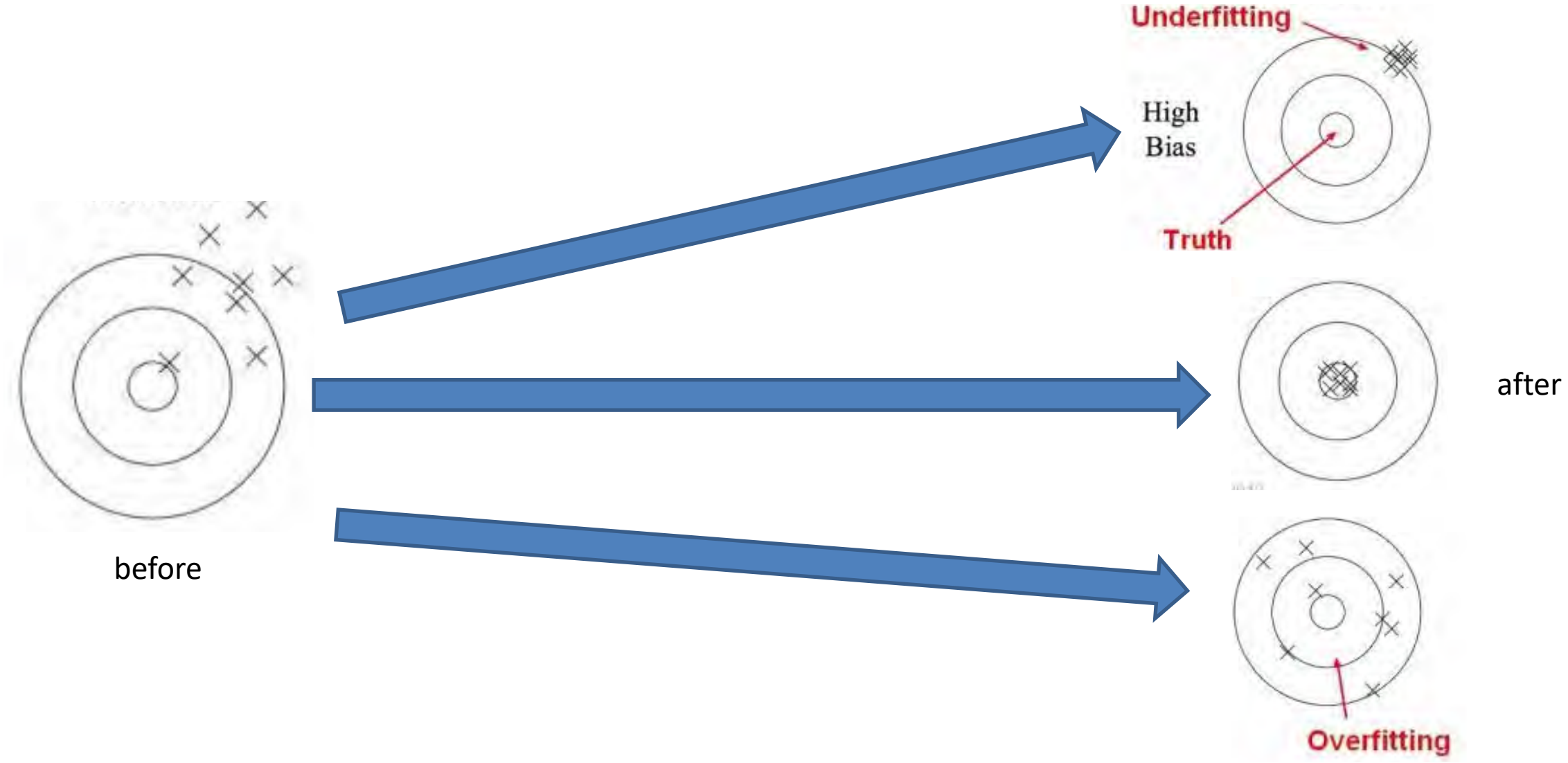
Model tuning: the over/under (fitting)

Interactive visualization of the main idea



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

Model training (fitting/tuning) process



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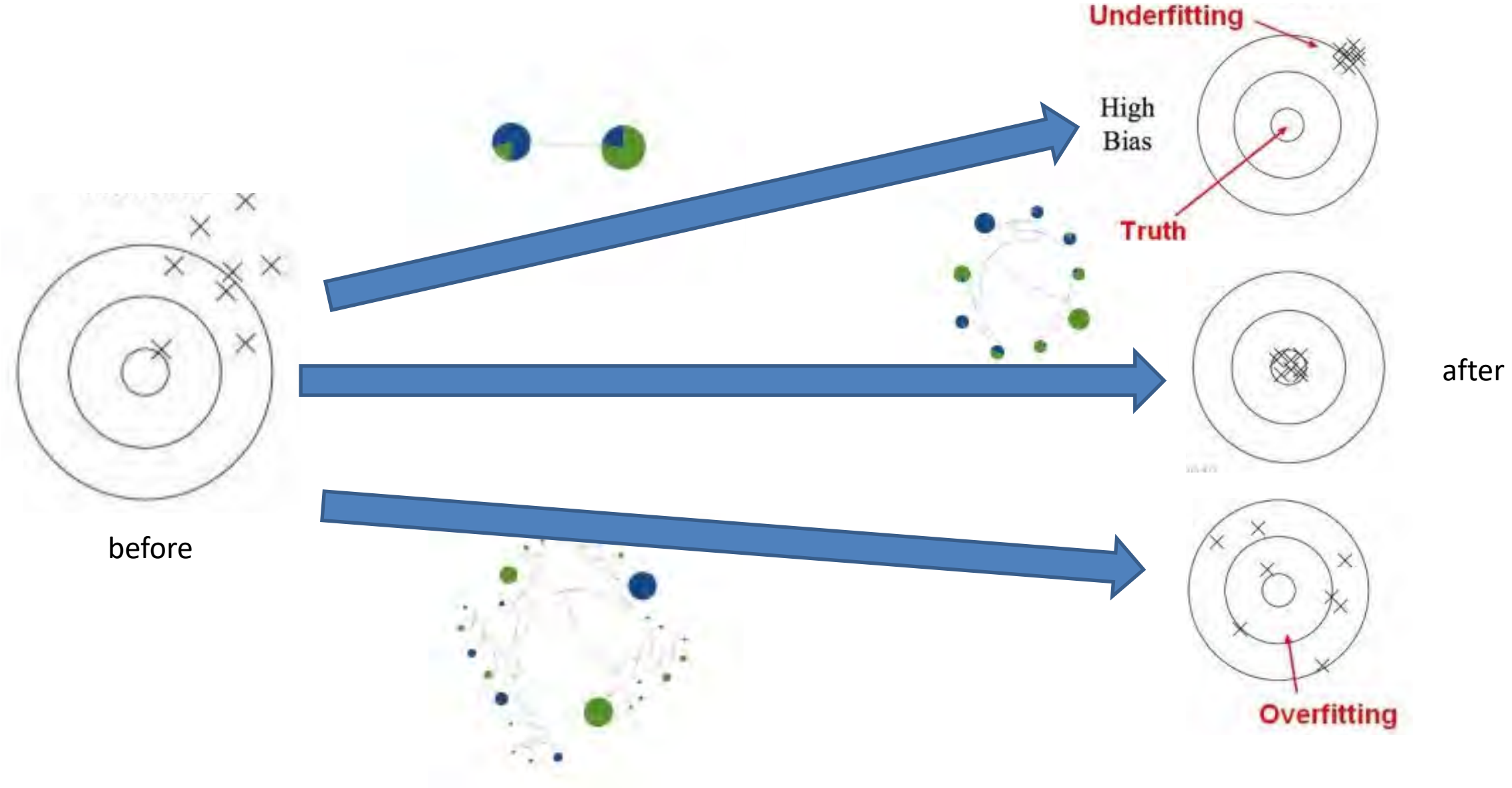
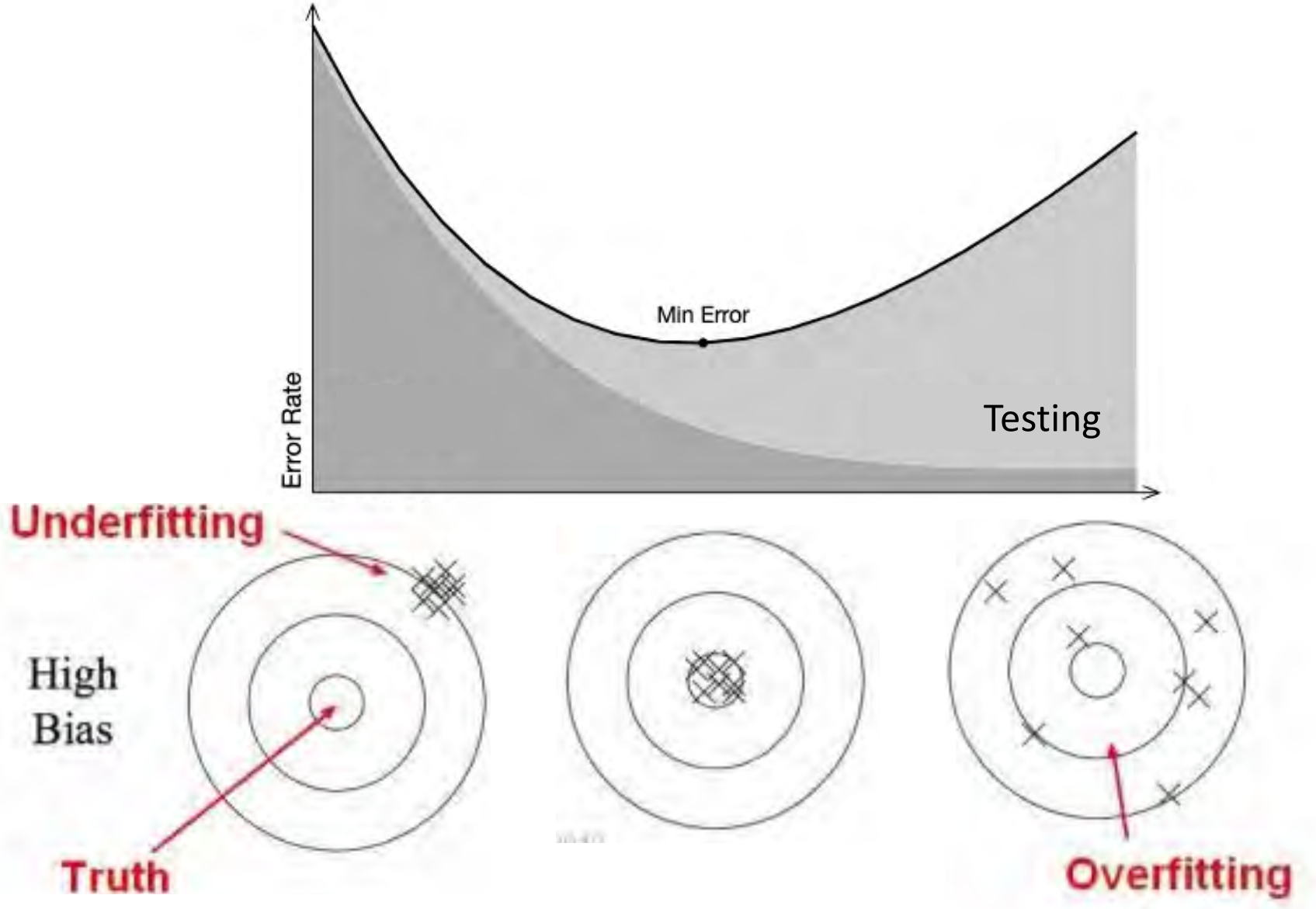


Some people think of it this way in ML



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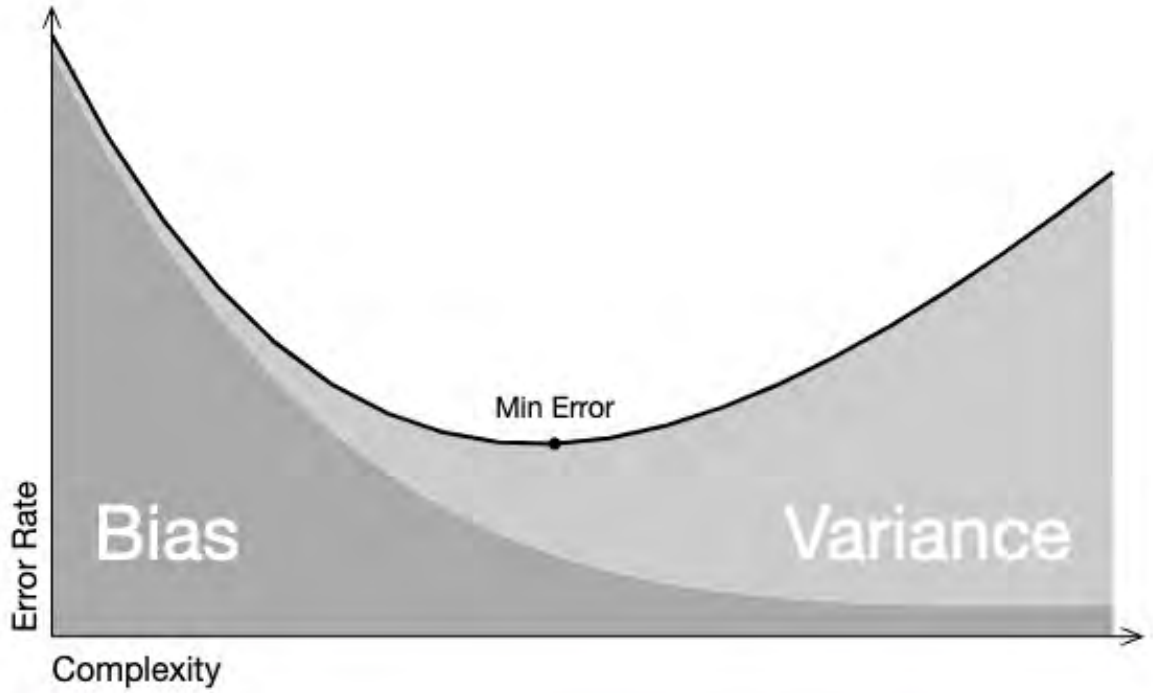
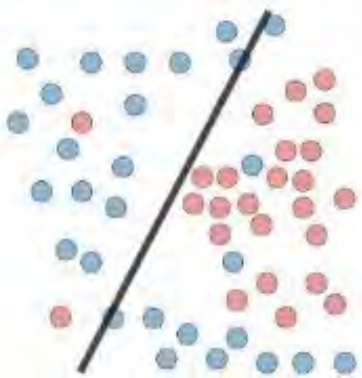
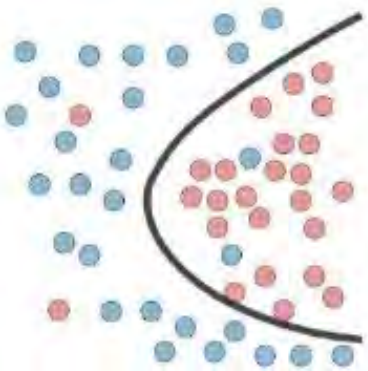
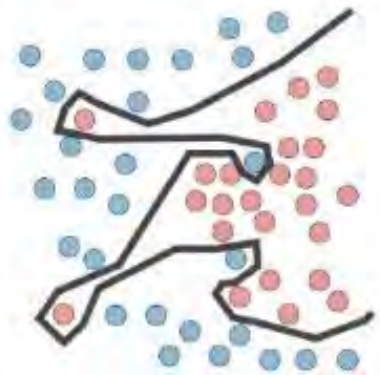
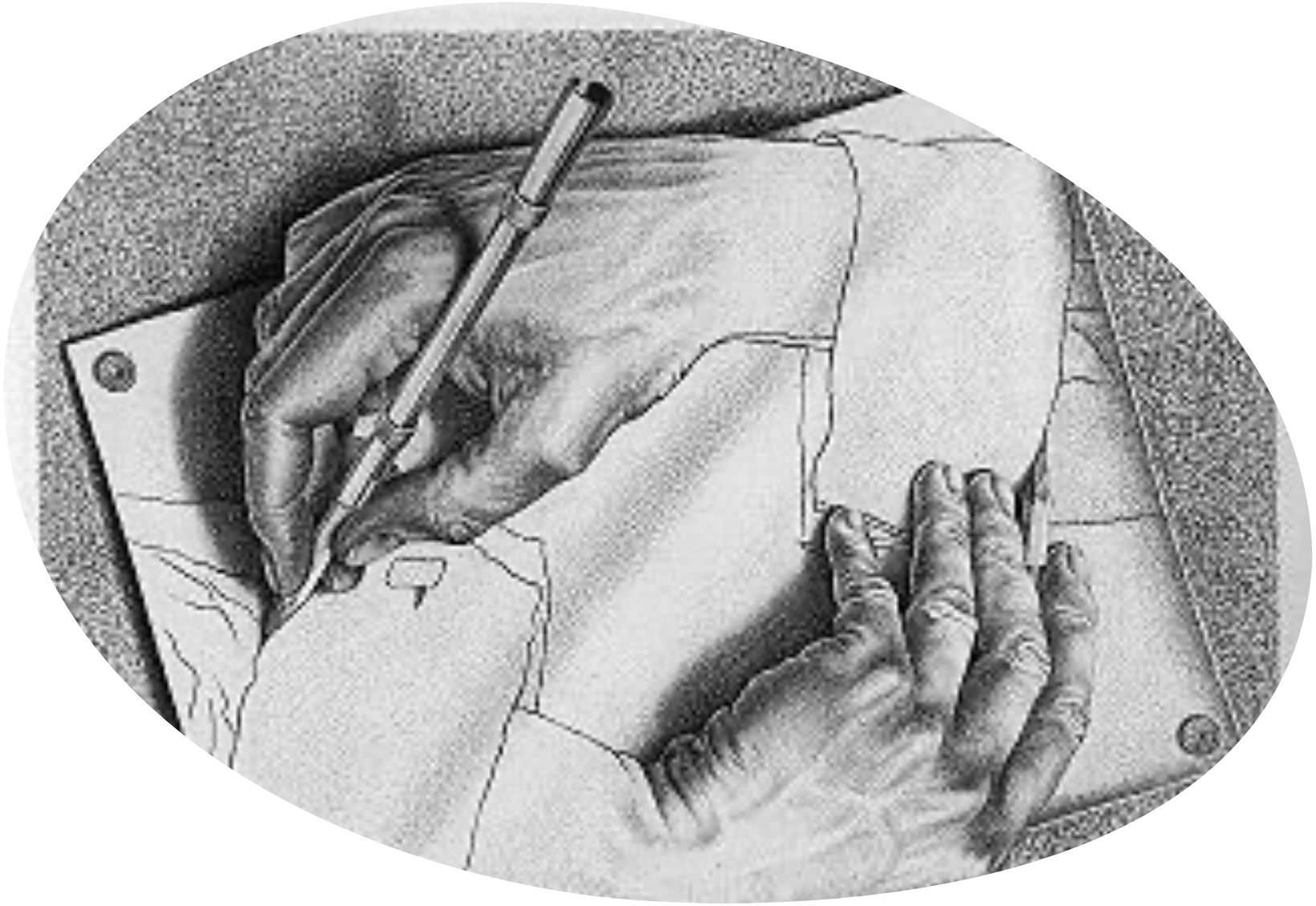


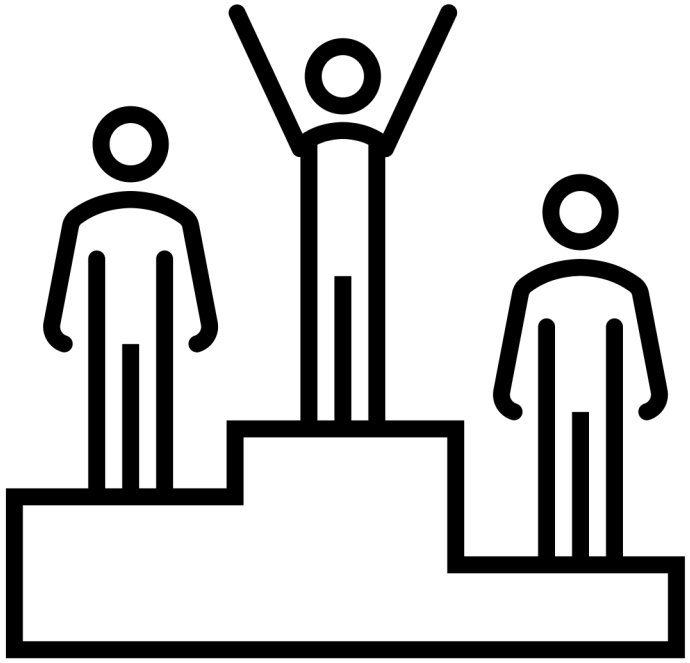
Some people think of it this way in ML

	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

Can **one** athlete be good at **many** sports?



If you train for the triathlon,

- you will not outrun a dedicated runner,
- you will not outswim a dedicated swimmer
- you will not cycle faster than a dedicated bicyclist

But you will finish the triathlon faster than any of them!

The bias-variance tradeoff

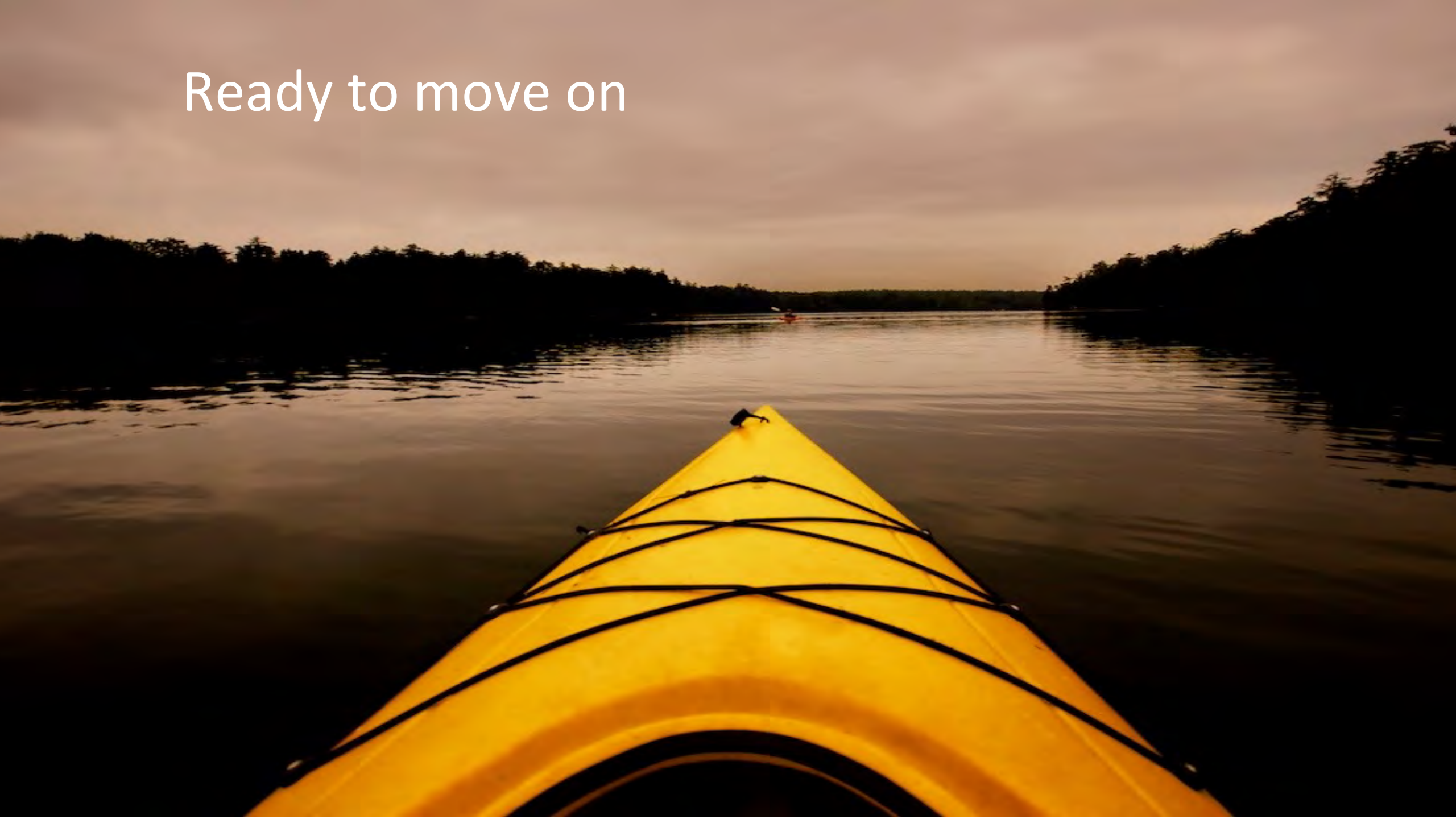
A **dedicated athlete** trains for a single sport, so

- performance is better (more biased) in that sport, but
- performance varies widely (more variance) across sports

vs.

A **triathlete** trains to reduce performance variance across sports, at the expense of bias for/against any one sport

Ready to move on



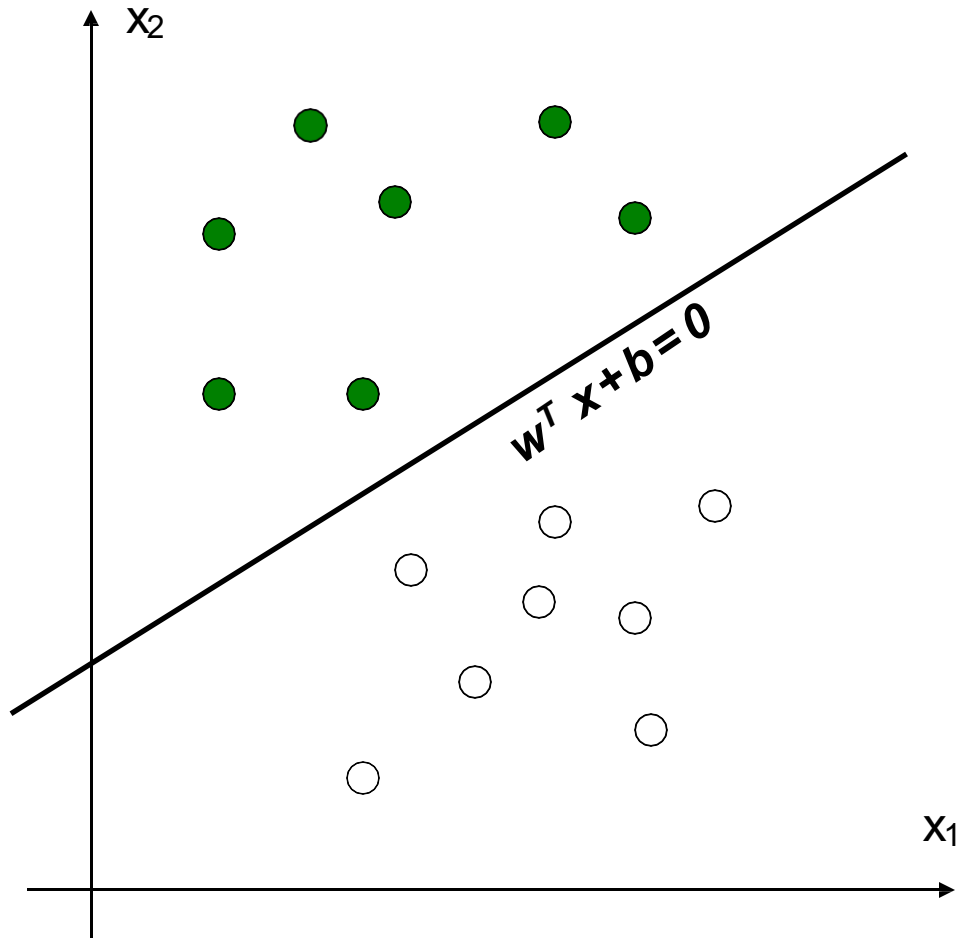
Remember Linear Discriminant Classifiers?

Linear Discriminant Classifier

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

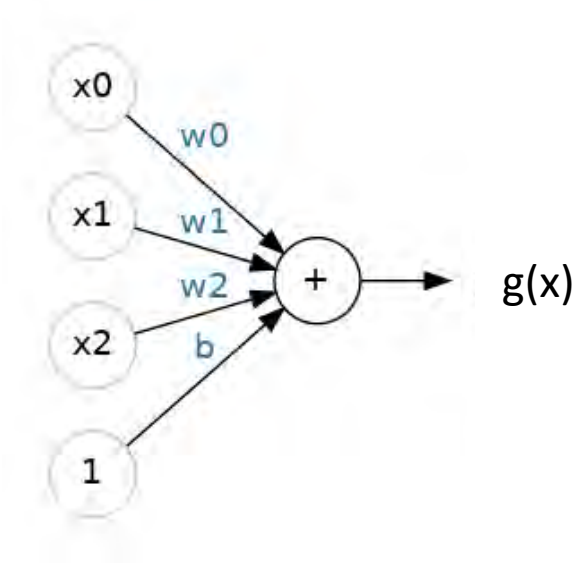
$$= \sum_{i \in SV} w_i\, x_i + b$$

Decision function = sign(x)

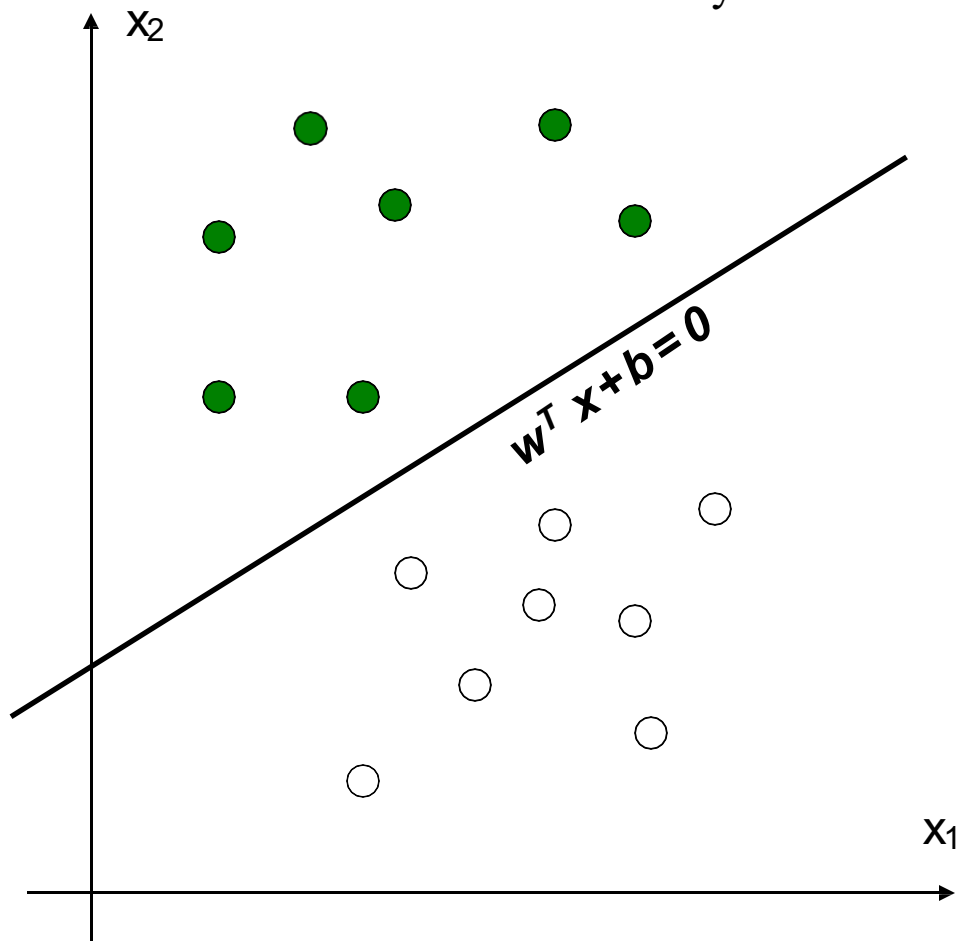


Linear units

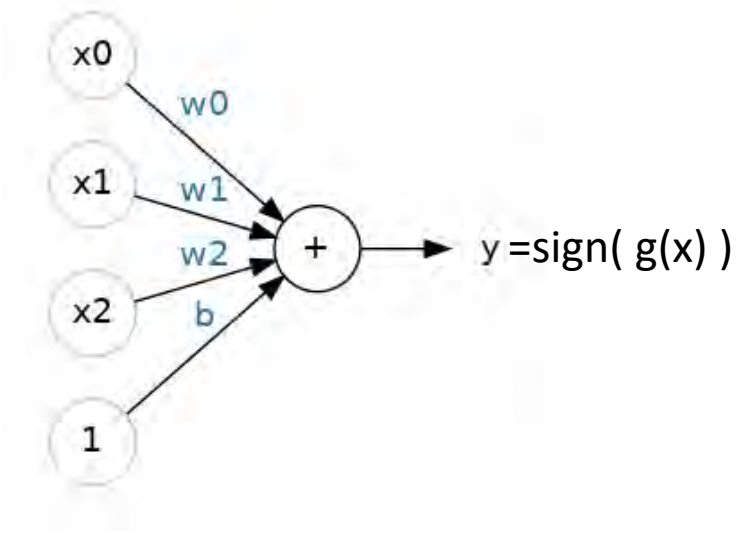
A linear unit:

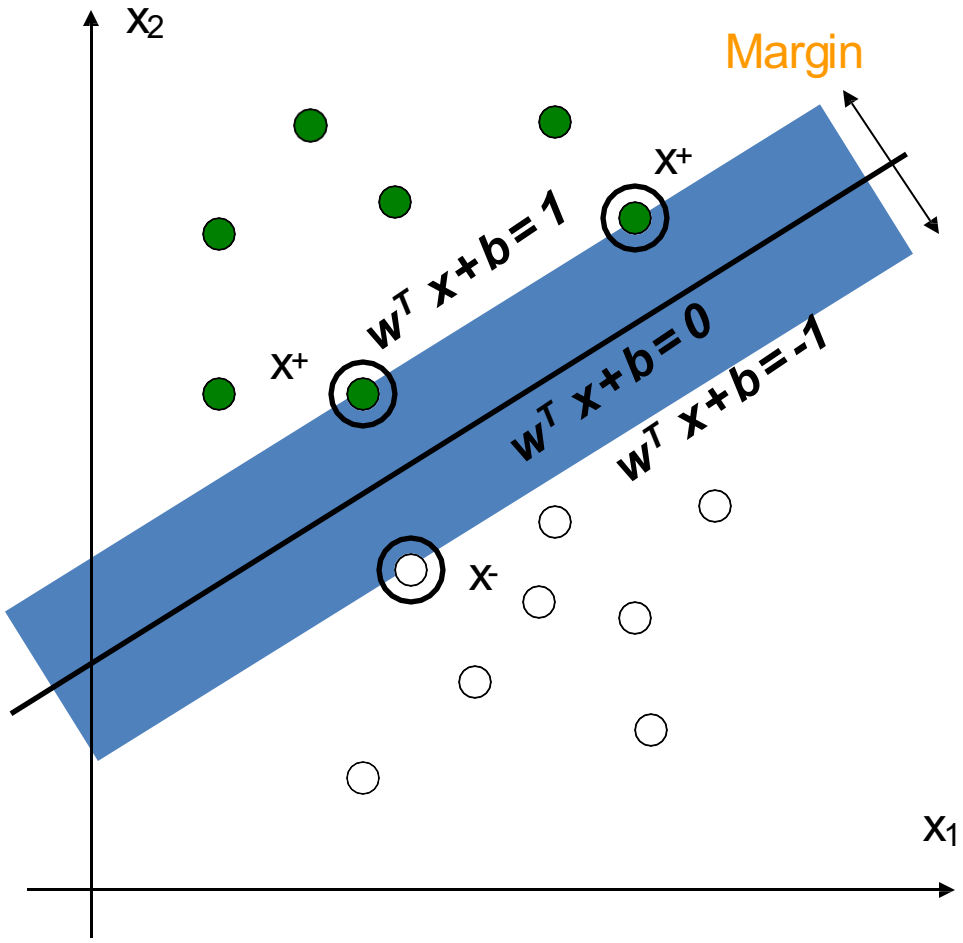


Decision Boundary



SVM: linear unit with largest margin + sign



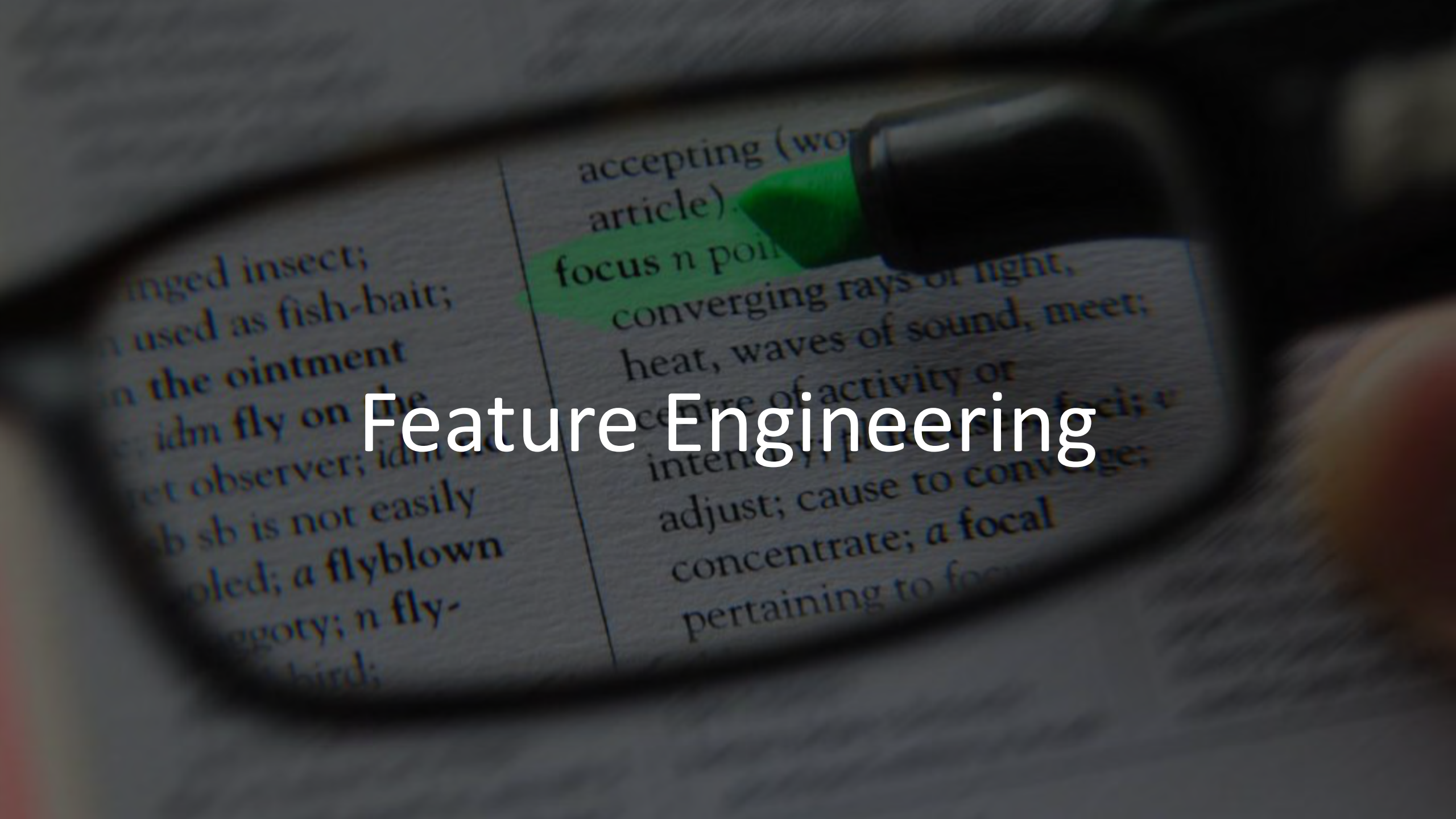


Speed vs. optimality

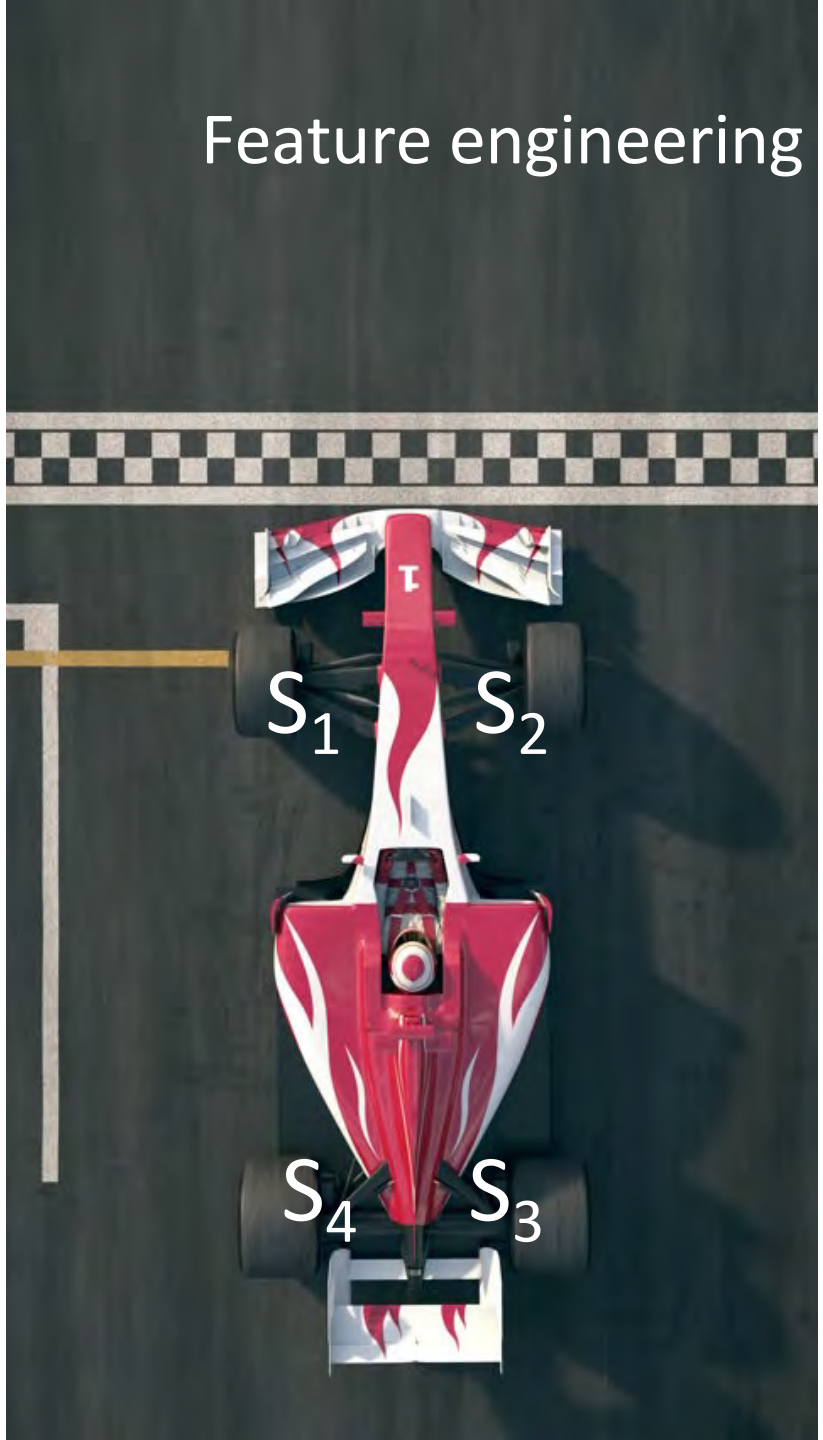
A 1080p digital image (most common screen size) comprises 1920 x 1080 pixels (1080 lines of vertical resolution) and three color channels (RGB): a total of more that 6 million variables!

- 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

Feature engineering example: domain knowledge



RAW DATA

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

FEATURES

$T_1 = (S_1 + S_2 + S_3 + S_4) / 4 = \frac{1}{4}S_1 + \frac{1}{4}S_2 + \frac{1}{4}S_3 + \frac{1}{4}S_4$

This is a more reliable indicator of car speed

$T_2 = \{ (\frac{S_1 + S_3 + S_4}{3}) - S_2\} / 2 = \frac{1}{6}S_1 - \frac{1}{2}S_2 + \frac{1}{6}S_3 + \frac{1}{6}S_4$

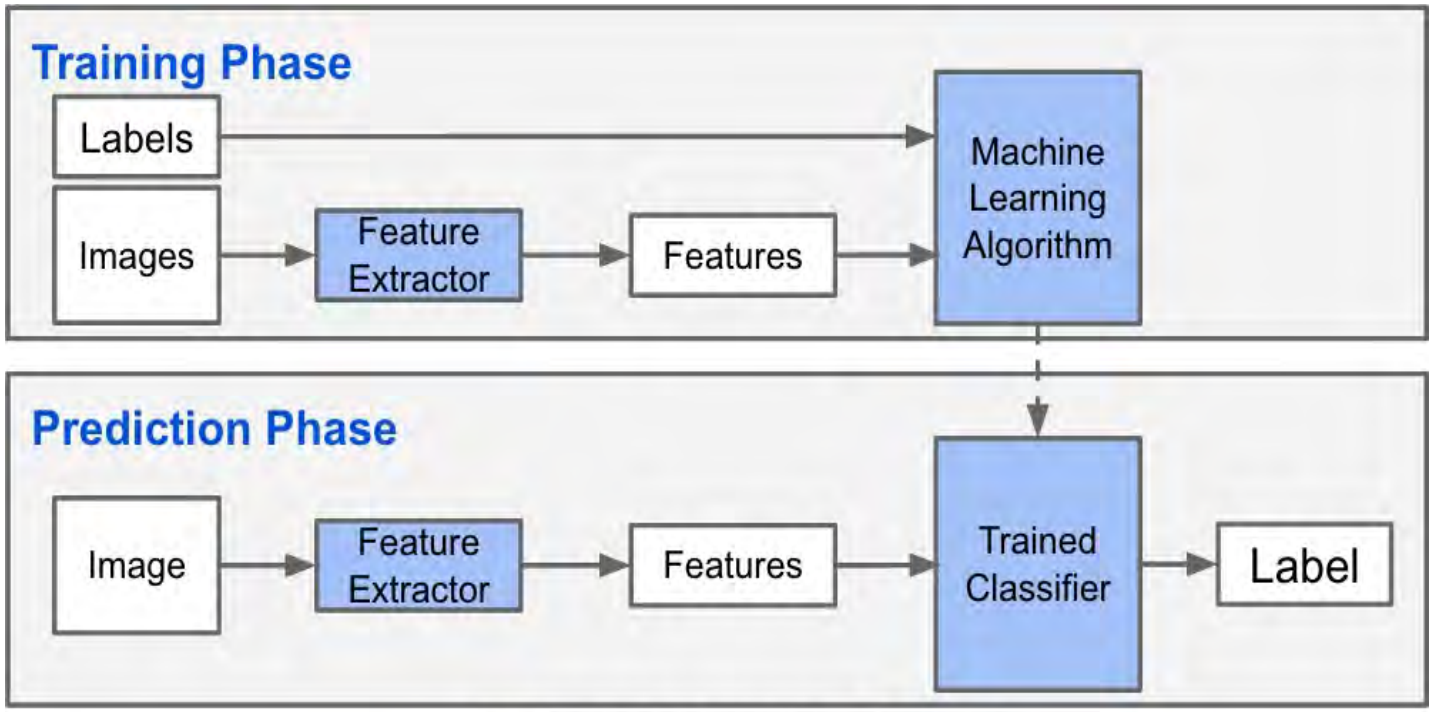
If this starts to veer away from zero, then tire #2 is spinning faster than the others (possible flat)

Similarly,

$T_3 = 0.5 \{ (\frac{S_1 + S_2 + S_4}{3}) - S_3 \}$

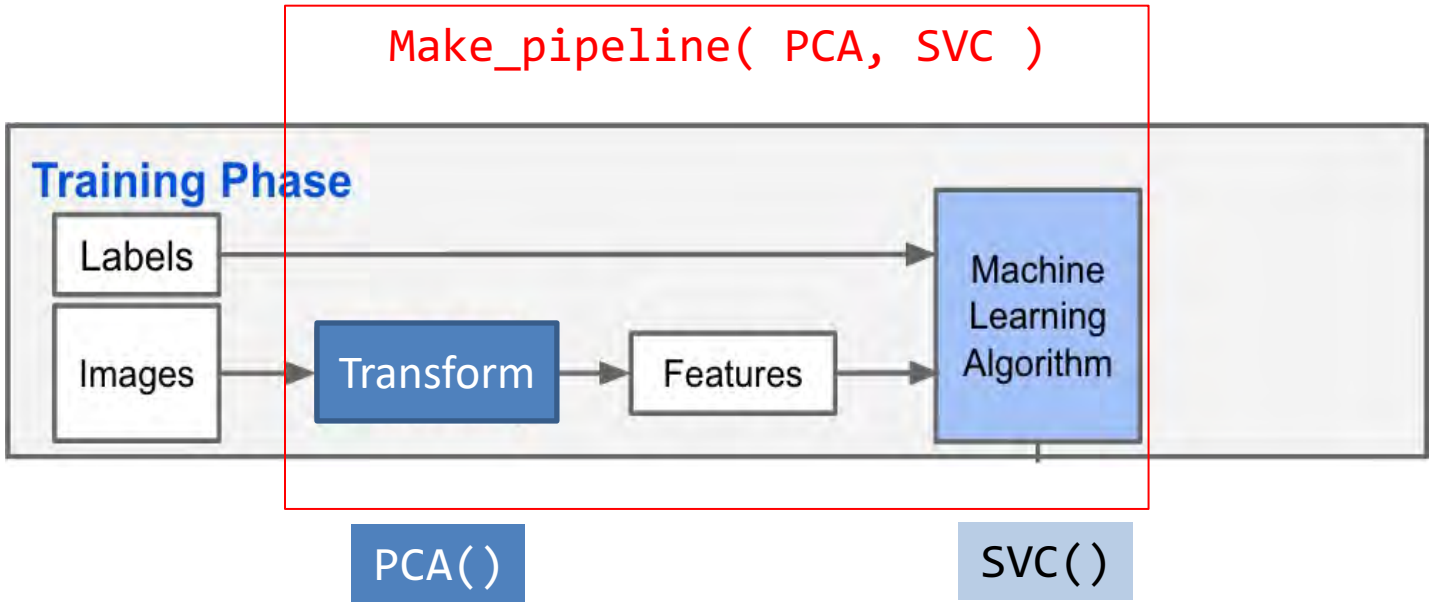
$T_4 = 0.5 \{ (\frac{S_1 + S_2 + S_3}{3}) - S_4 \}$

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

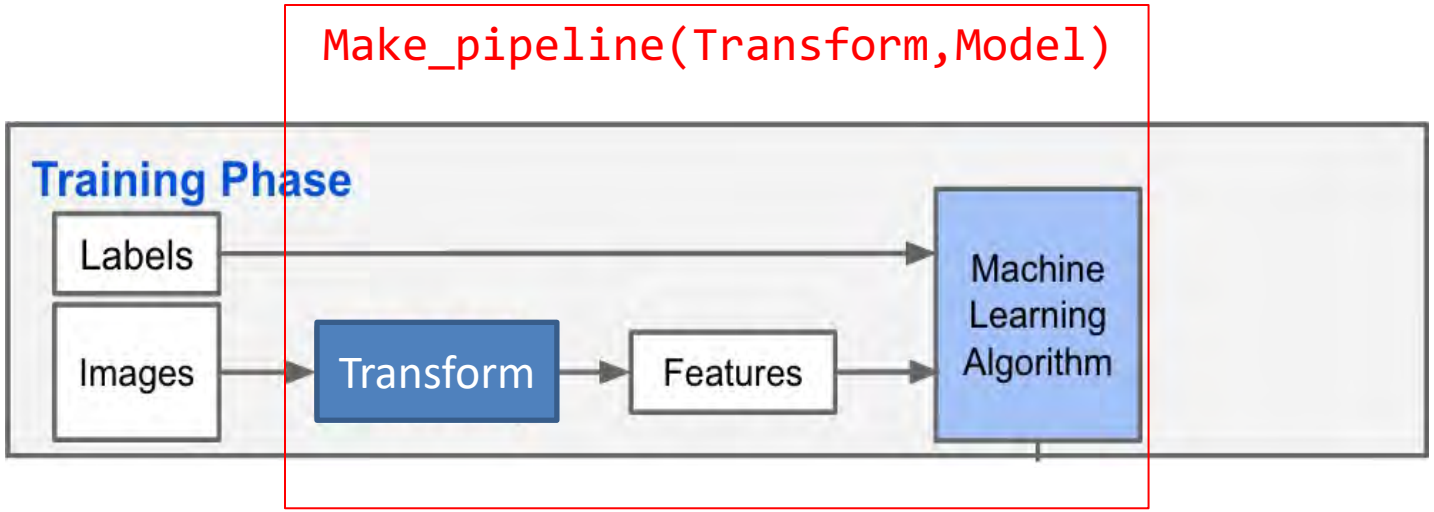


Machine Learning Phases

Feature engineering example: PCA



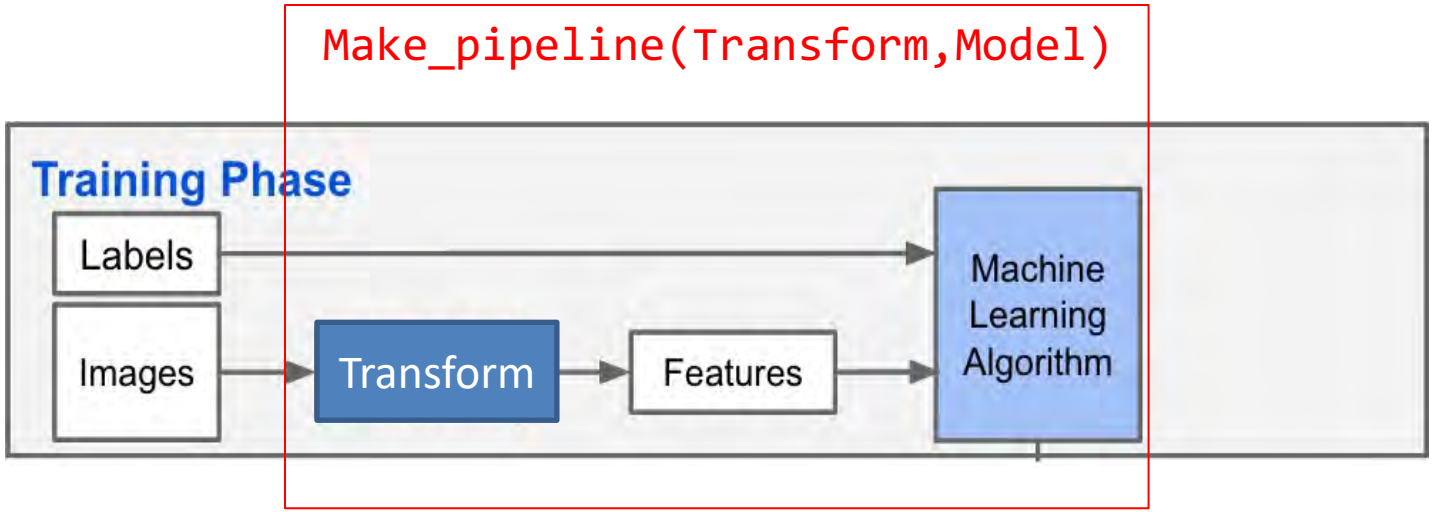
Feature engineering: a lot of possibilities



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

There are many other choices

Feature engineering: a lot of possibilities



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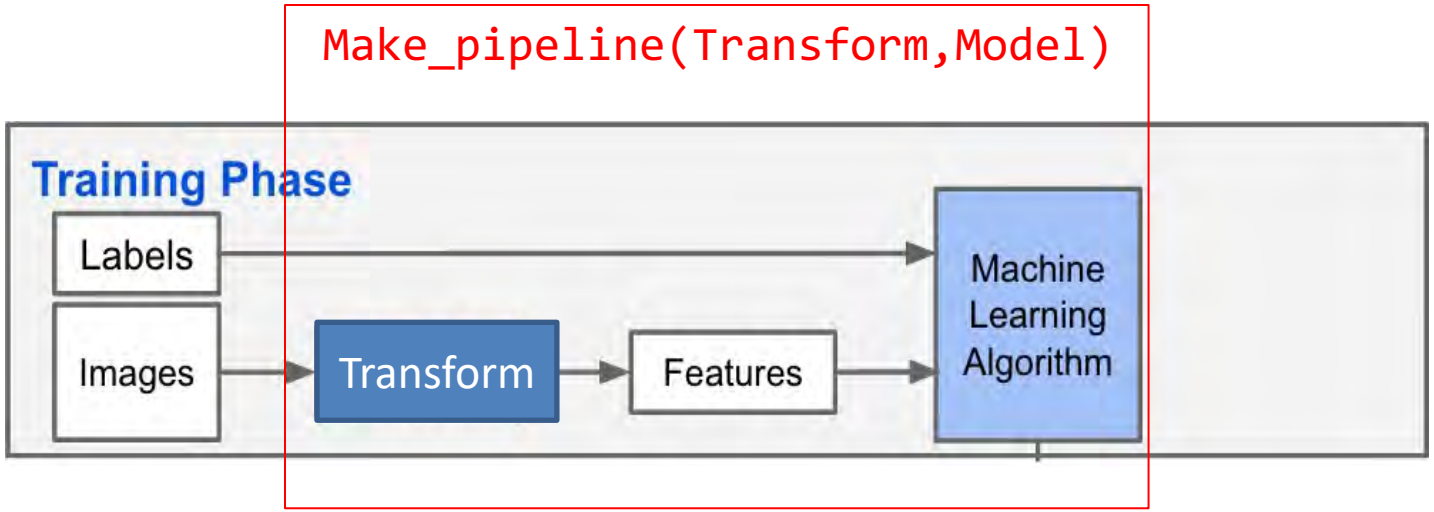
There are many other choices:
Fourier Transform: extract frequencies from wave signals

Feature engineering: a lot of possibilities



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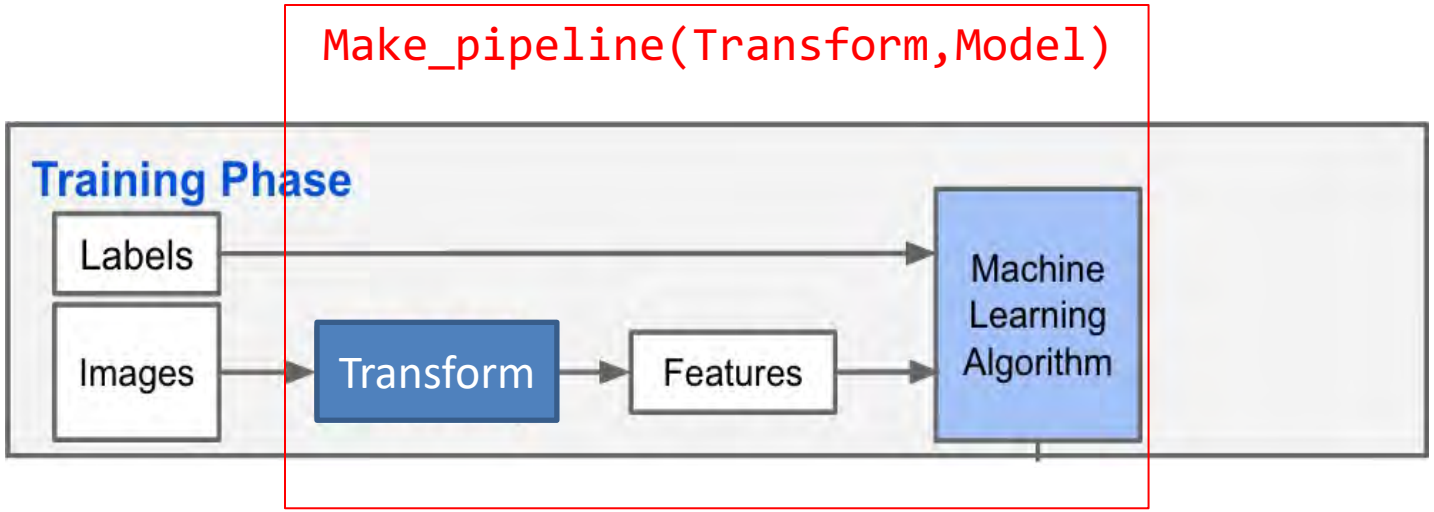
Fourier Transform: extract frequencies from wave signals
Wavelet Transform: extract levels of detail from images

Feature engineering: a lot of possibilities



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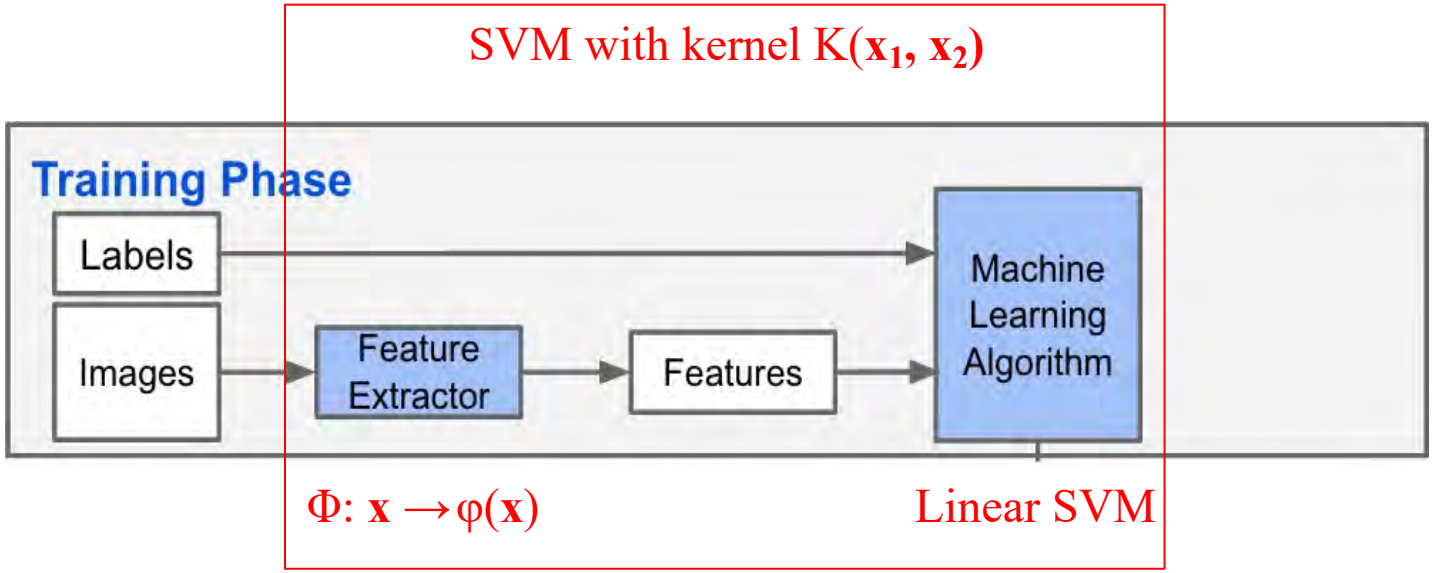
There are many other choices:
Fourier Transform: extract frequencies from wave signals
Wavelet Transform: extract levels of detail from images
Kernel Trick!

The kernel trick masks a data transform



Think of

```
SVC( kernel='rbf' )
```

as being the same as

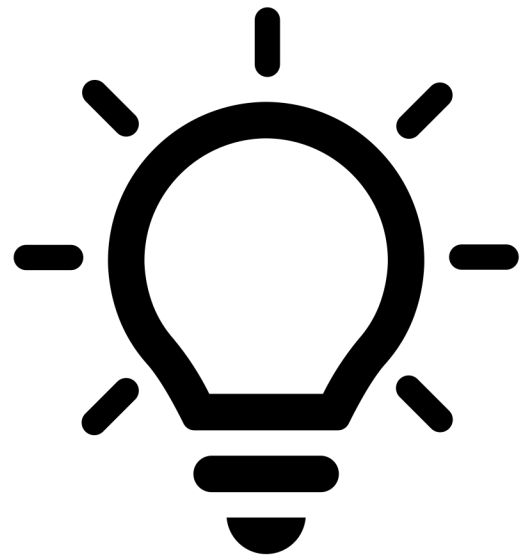
```
make_pipeline( rbfTransform, SVC )
```

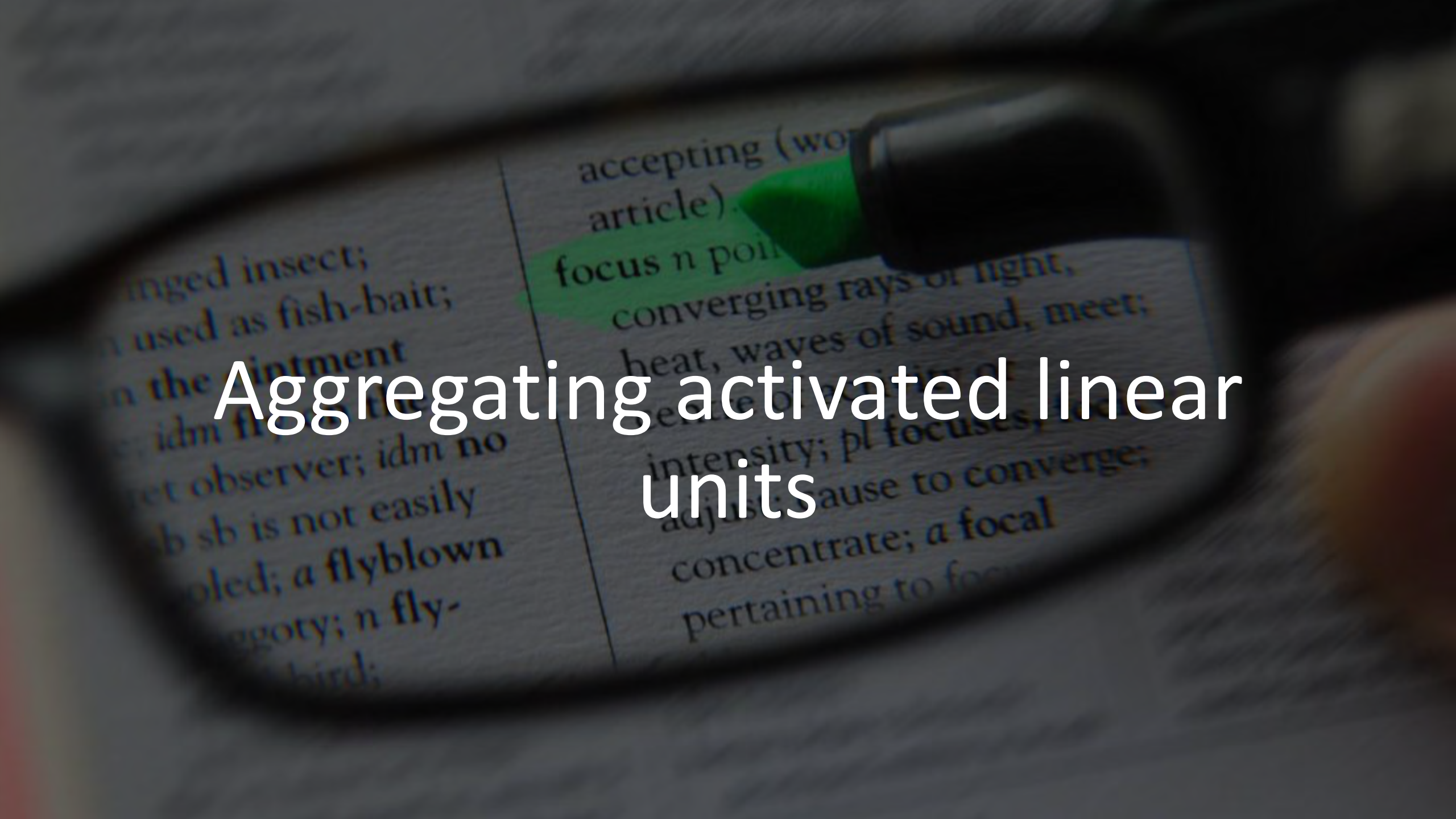
Feature engineering: speed vs. optimality

- Feature engineering is difficult, time-consuming, and requires domain expertise.
- Computing the optimal margin takes a lot of effort; can not always afford to update the model if new data came in. Train once and hope for the best.

Can we try something different?

First Idea:
Ensemble SVC



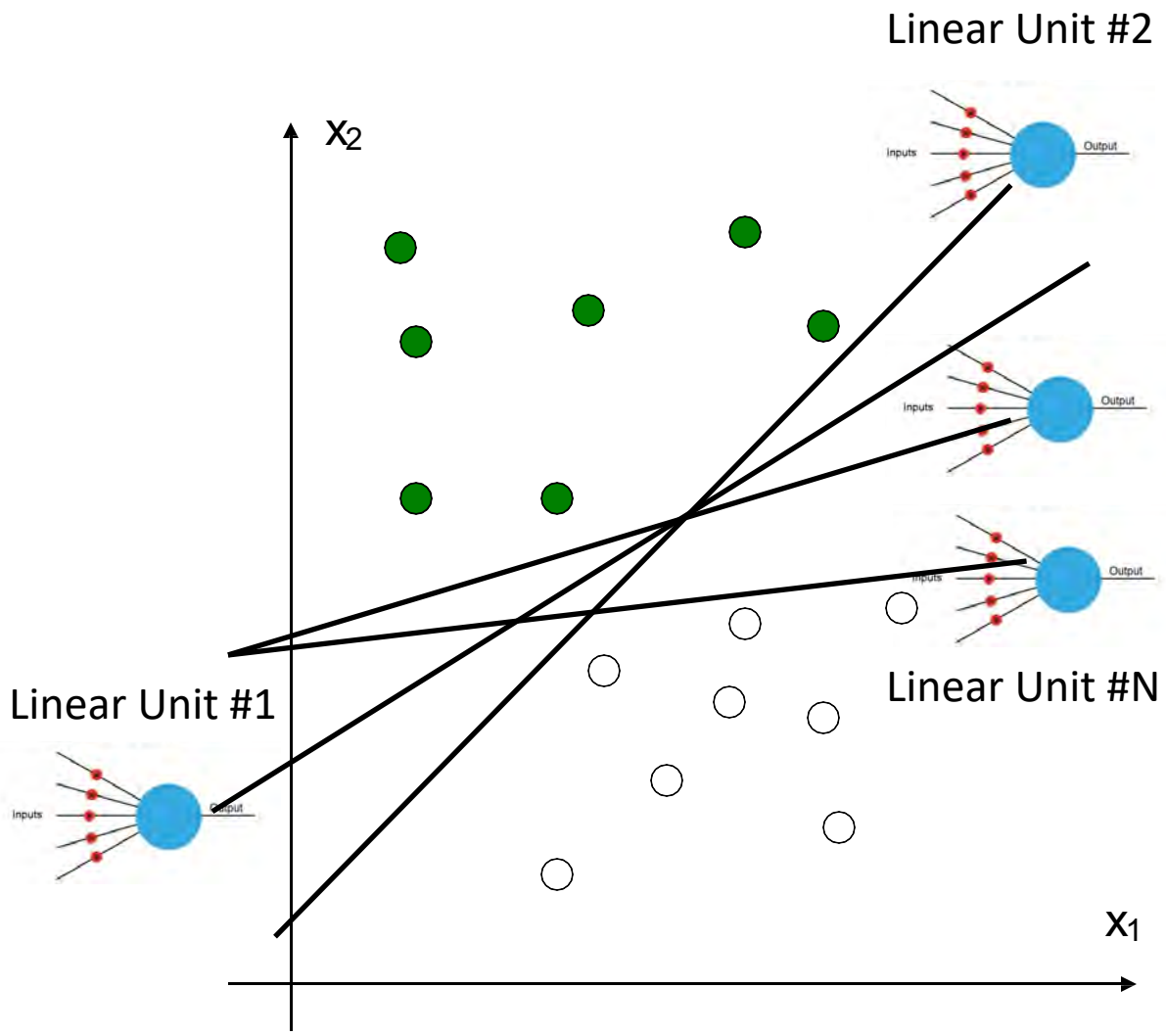


Aggregating activated linear units

Linear units

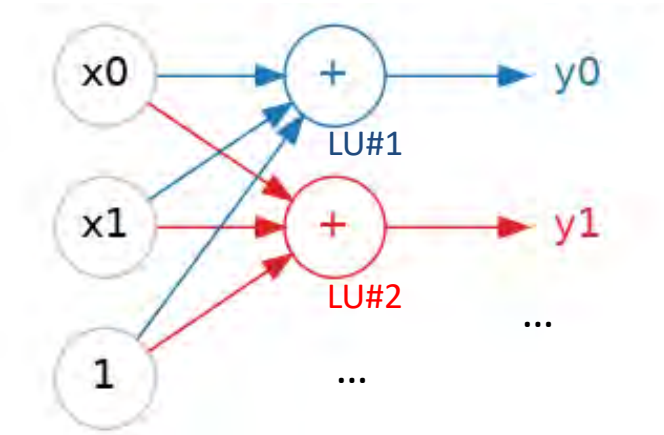
Different hyperplanes correspond to different linear units

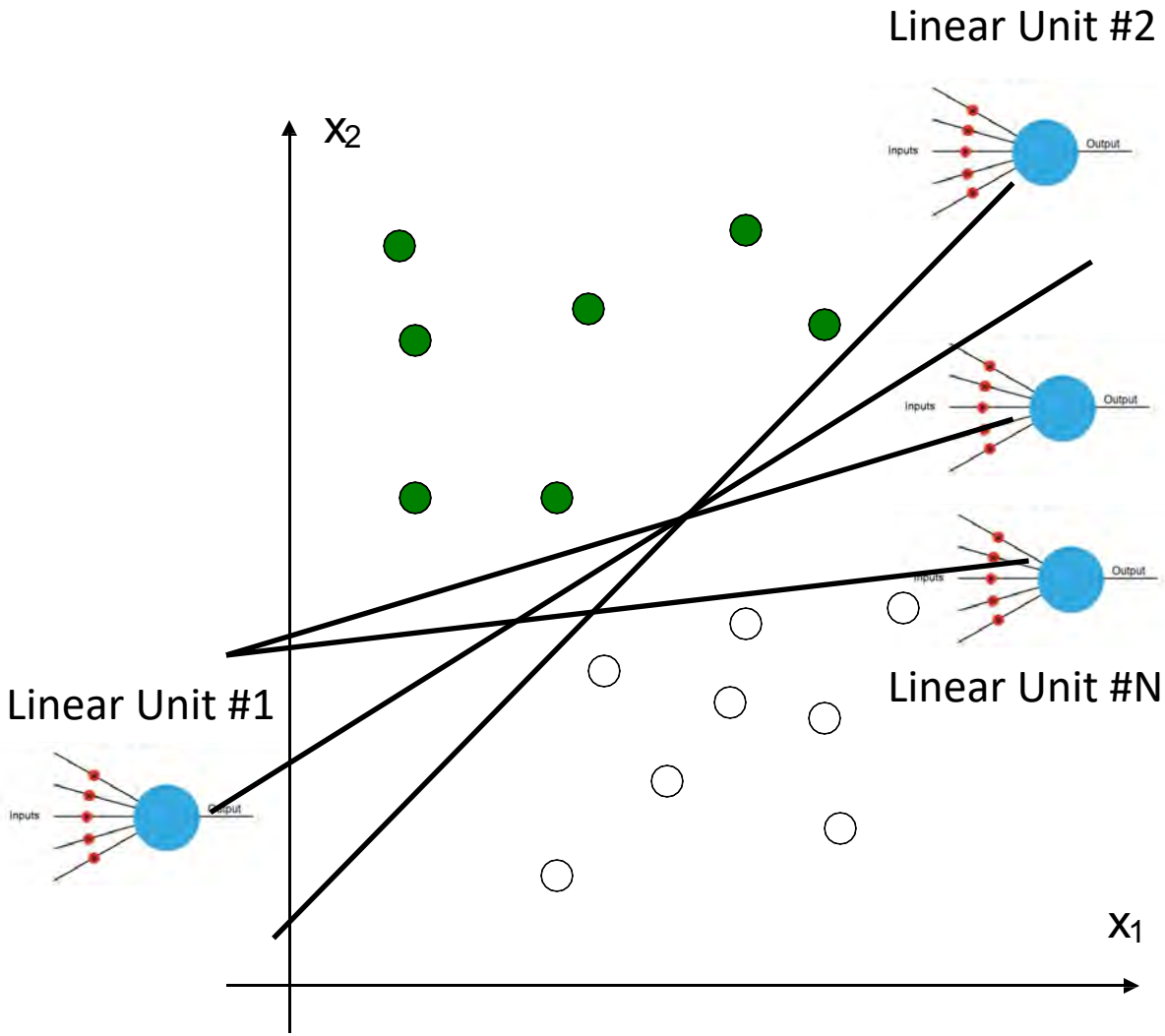
They all classify the training set correctly, but are slightly suboptimal



Linear units

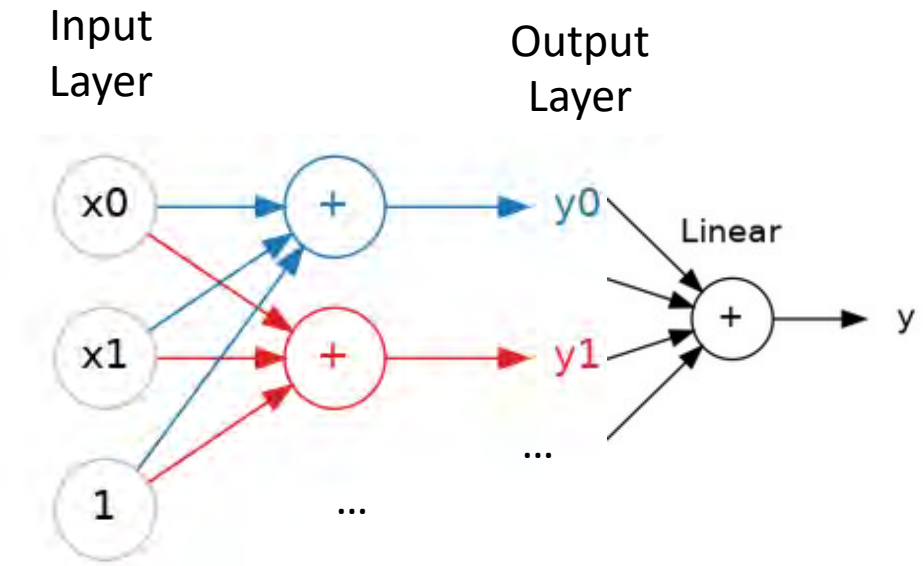
Aggregated as a group, their performance can be close to the SVM





A simple ensemble

Decision function: Add the outcome of each unit to aggregate



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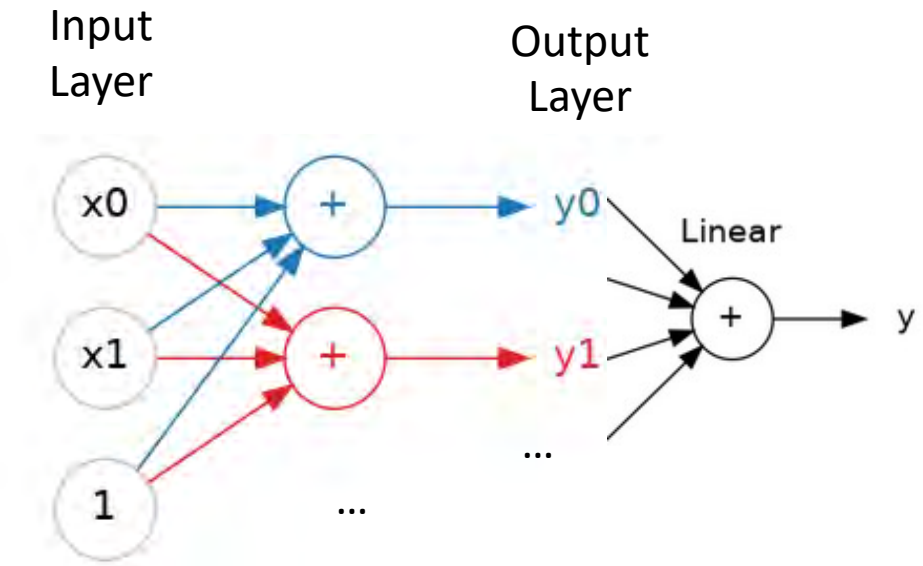
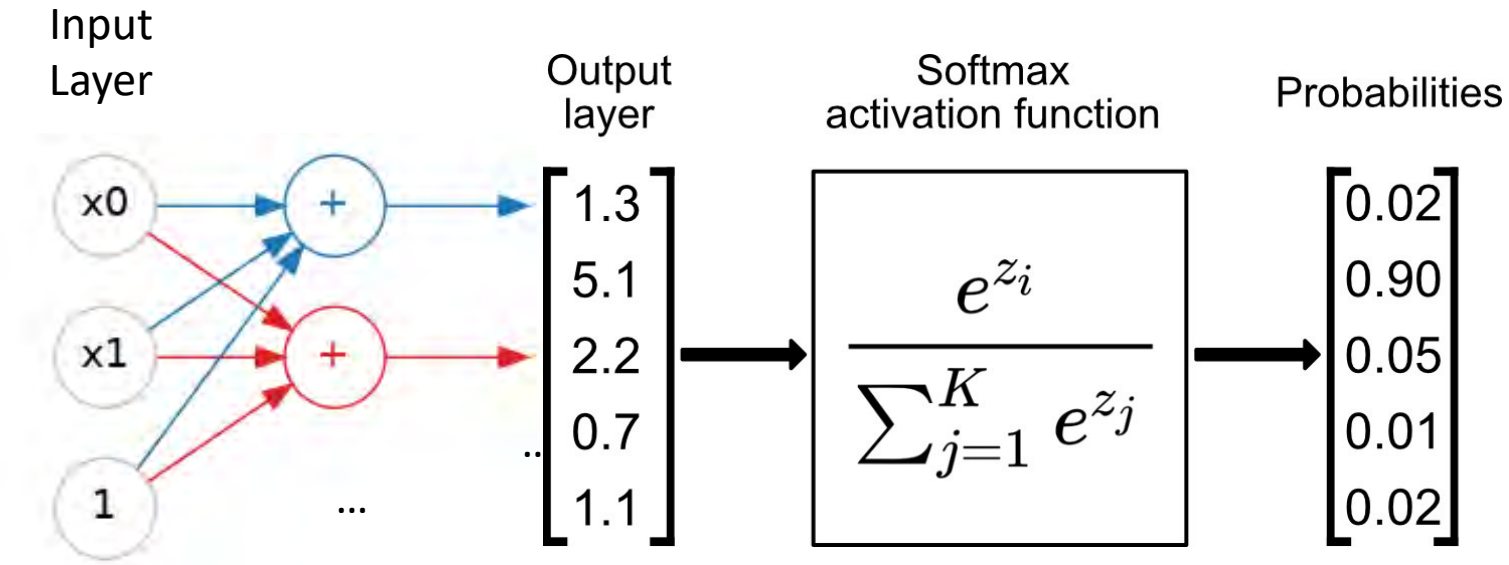


The final (output) layer is also a linear unit.
That makes this network appropriate to a regression task, where we are trying to predict some arbitrary numeric value.

A simple ensemble

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

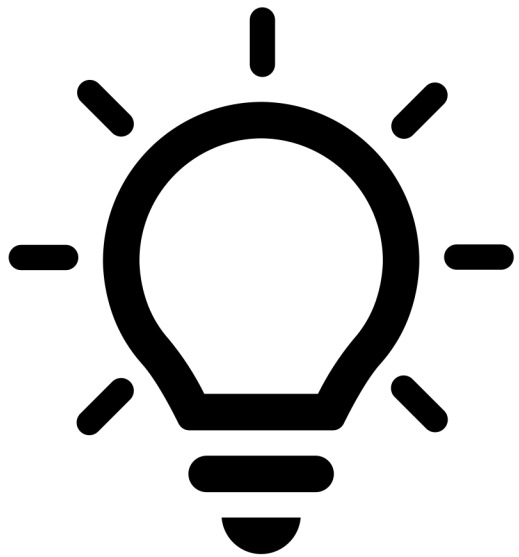


SoftMax is the most common for classification

Added benefit: online learning

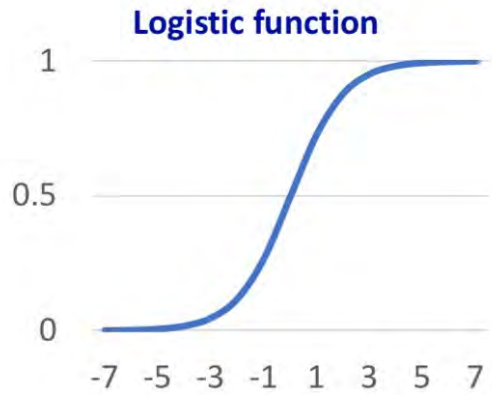
More data vs. More sophistication

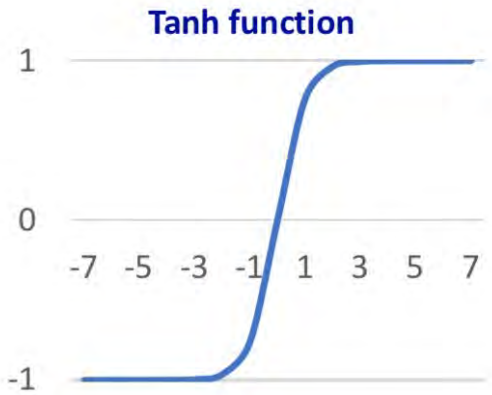
- No need to wait for all the training data to come in so you can find the optimal solution.
- Instead, process the data points in batches, and update the weights as newer training data arrives.
- Thus the same classifier can be modified (increased sophistication) over time.

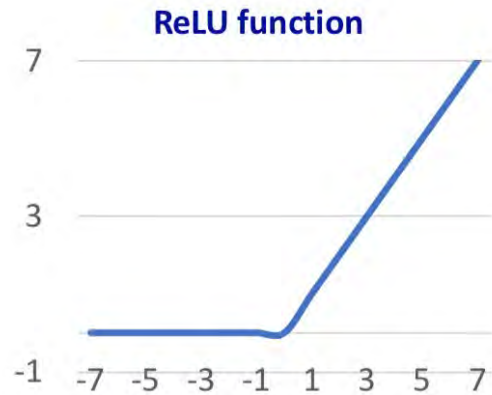


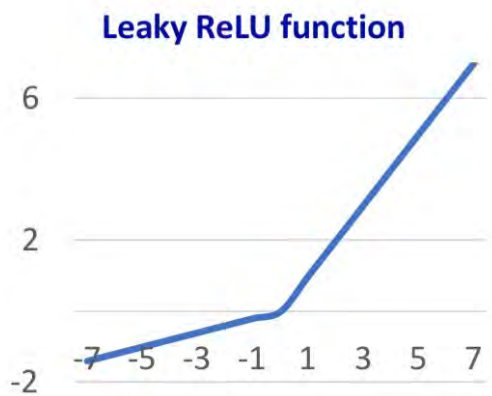
Second Idea:
sign, logit, … ?

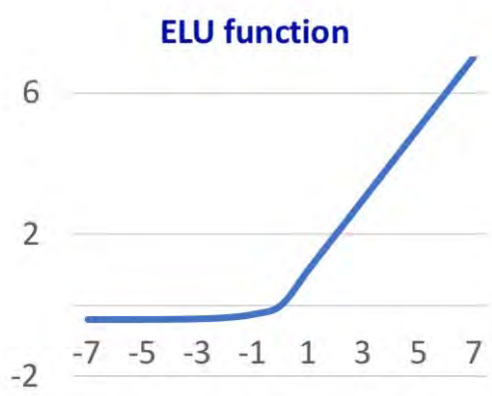
Many choices for the activation function

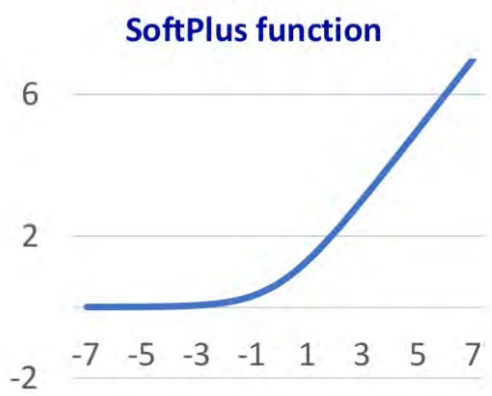




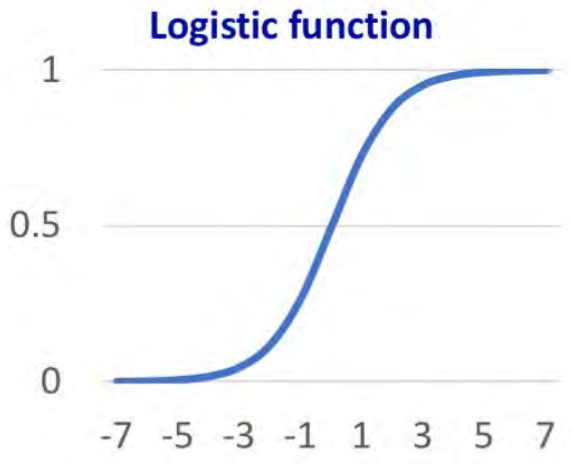






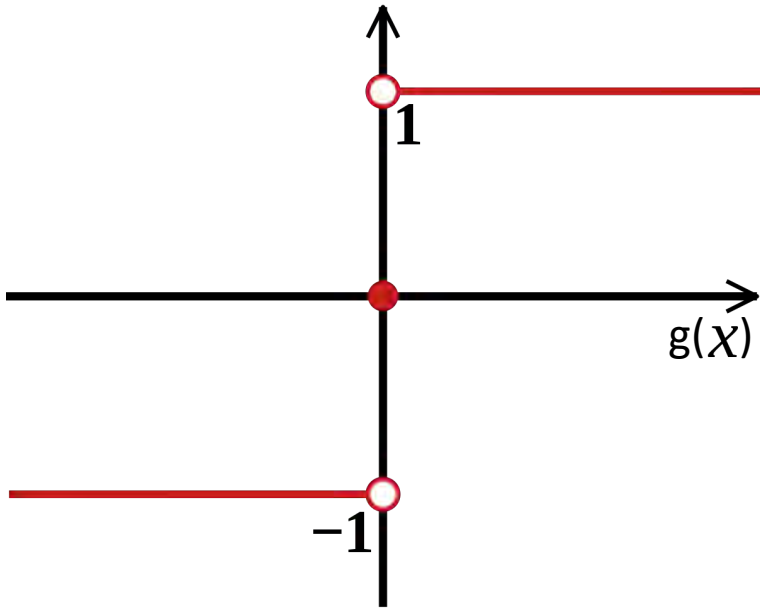


Logistic Regression: activate using the logistic function



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

SVC: activate using the sign function

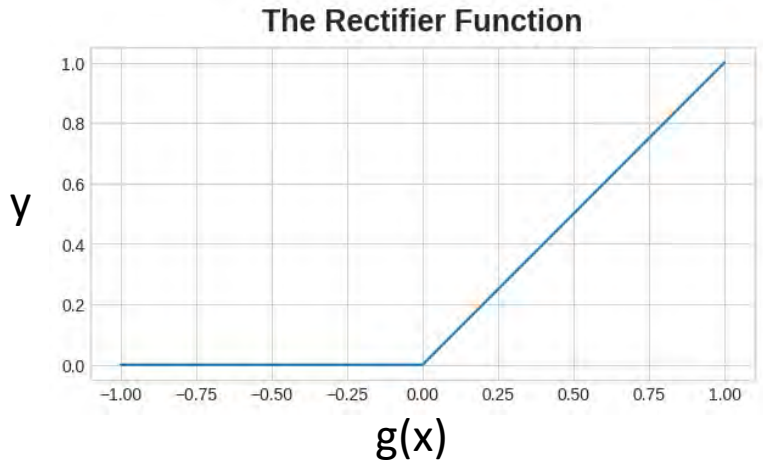


The output is sign(g(x))

decision = +1 if g(x) > 0

decision = -1 if g(x) < 0

New: activate using the rectifier function

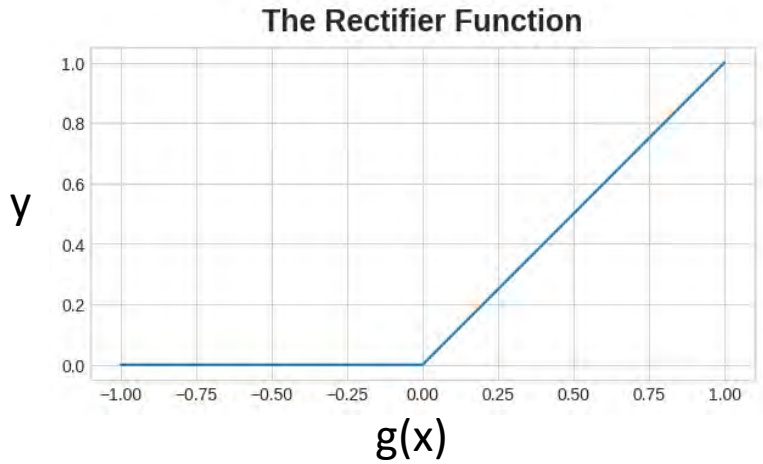


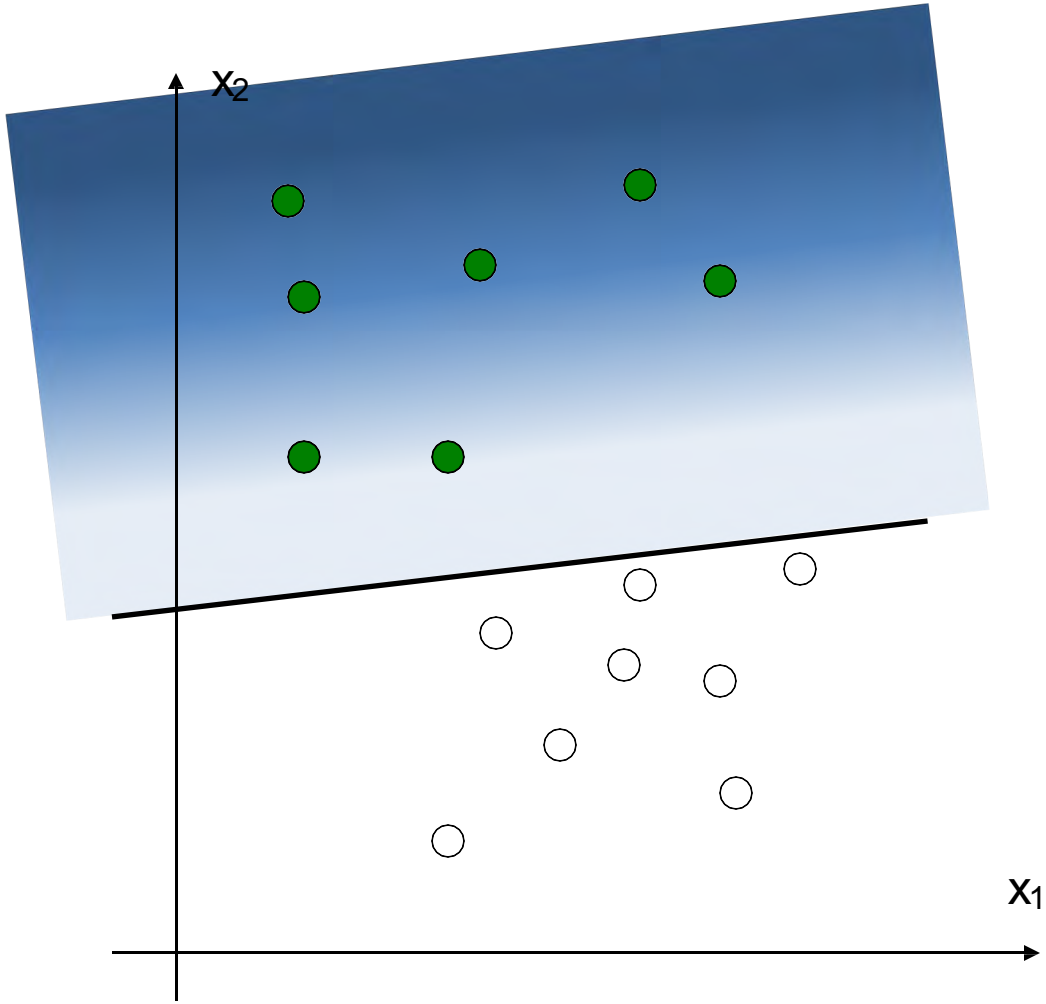
Instead of strict binary sign(g(x)), the output is max(0, g(x))

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

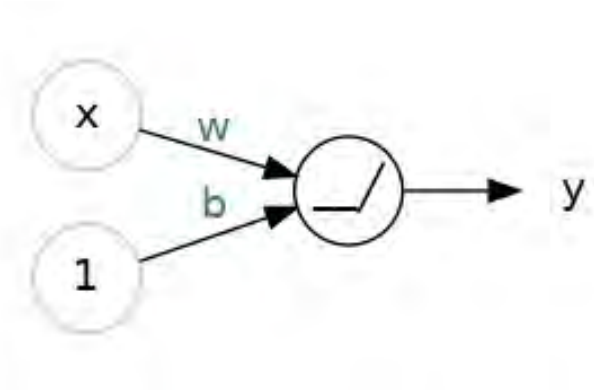
$y = 0$ if $g(x) < 0$

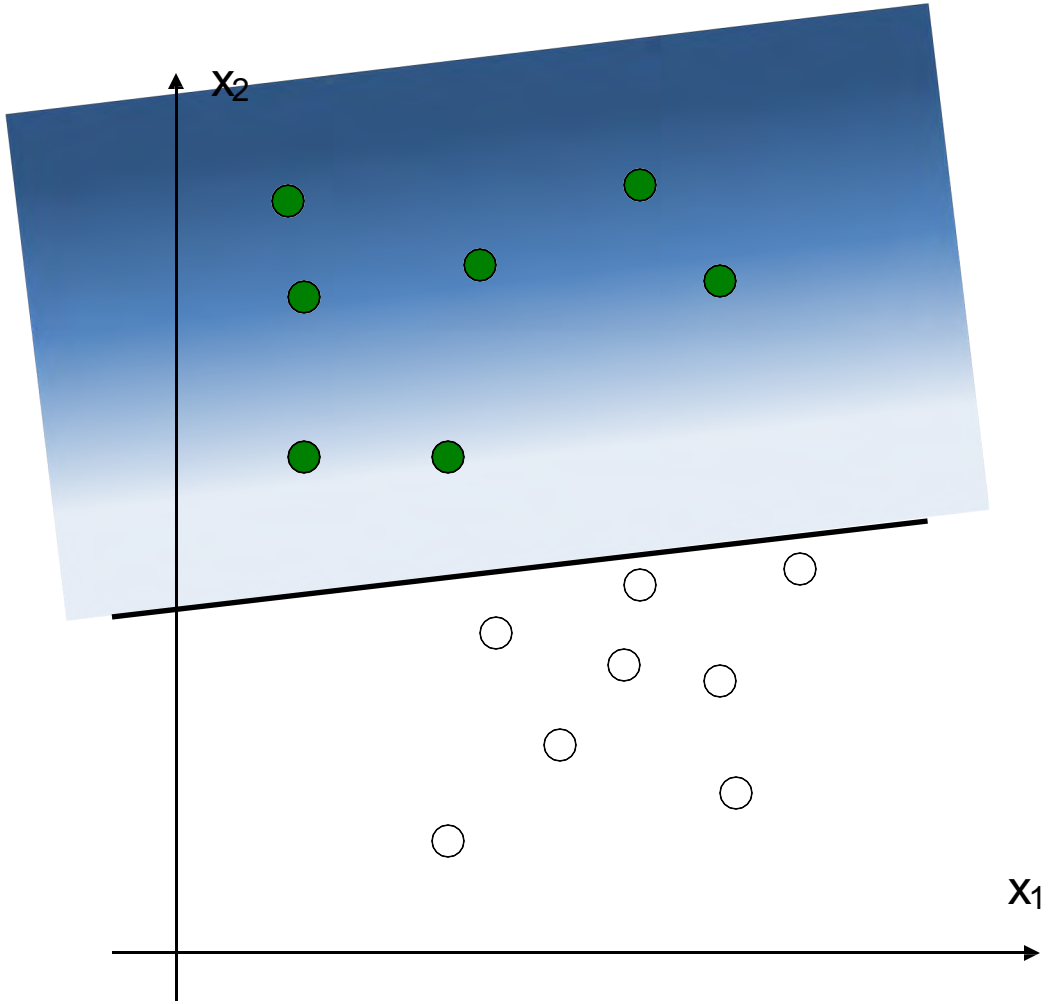
New: activate using the rectifier function





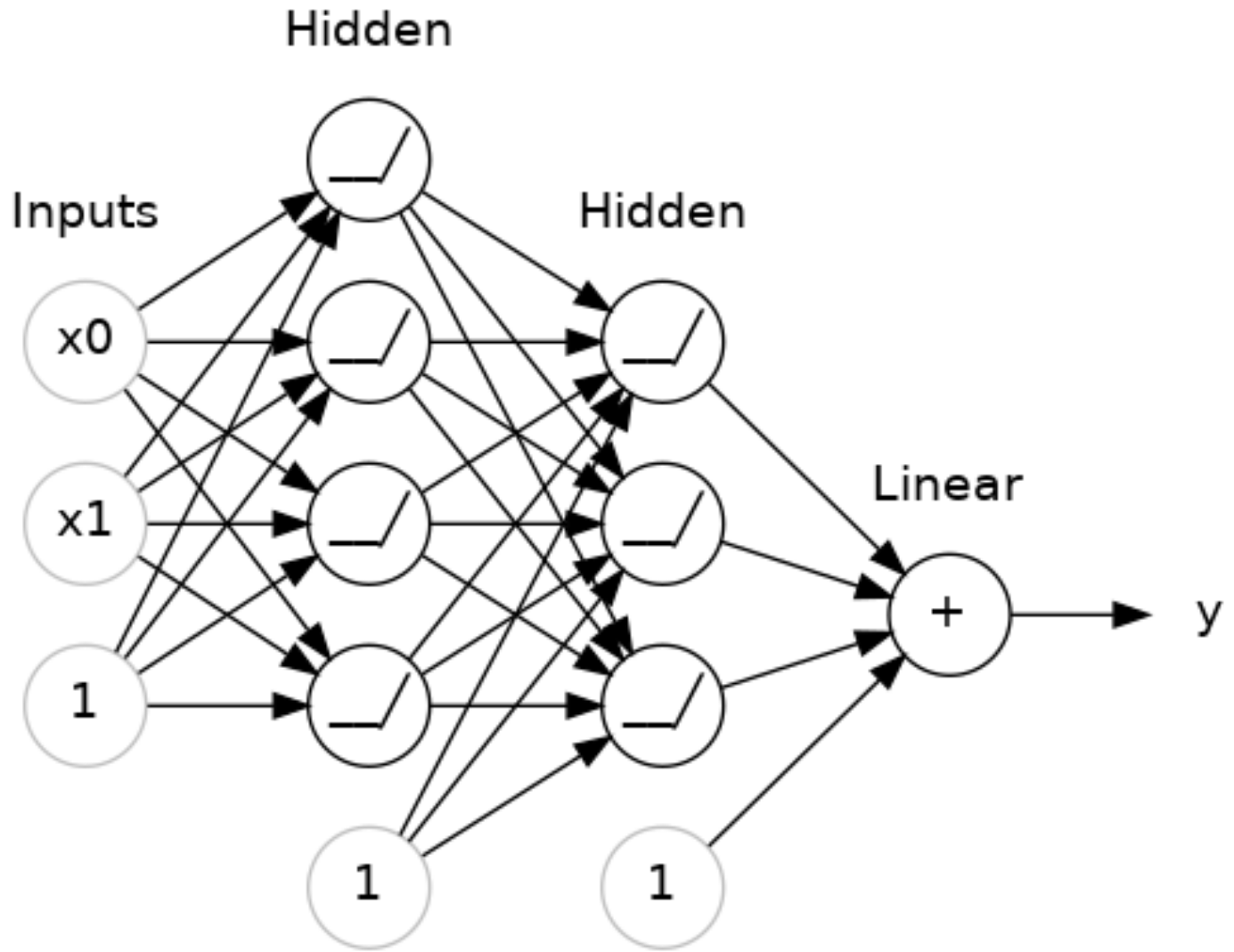
ReLU: a Linear Unit activated using the rectifier function





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/