

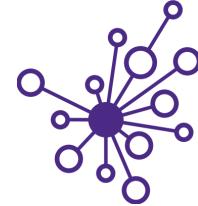


Knowledge and
solutions for a
changing world



Be boundless

Advancing data-
intensive discovery
in all fields



INTRODUCTION TO MACHINE LEARNING & KNN

UW DIRECT

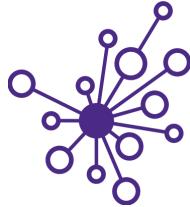
(Data Intensive Research Enabling Cutting-edge Tech)

<https://uwdirect.github.io>

Stéphanie Valleau

Chemical Engineering

Outline



Introduction to Machine Learning (ML)

- Statistical learning – inference and prediction
- Parametric, non-parametric models
- Supervised, unsupervised models
- Regression, classification
- Error: Variance and Bias

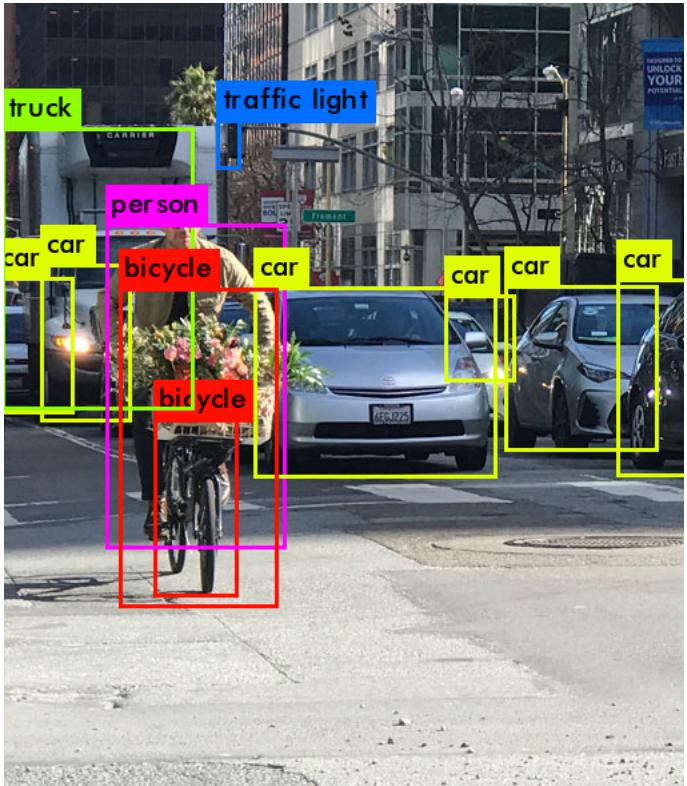
Classification methods

- K-nearest neighbors, KNN

Many figures and notation will follow “*An Introduction to Statistical Learning: with applications in R*” unless otherwise noted; see the syllabus for a free PDF of the book.

ML models can tackle many types of problems

Self-driving cars use trained ML algorithms to predict the objects that surround them



M. I. Jordan T.
M. Mitchel
Machine
learning:
Trends,
perspectives,
and prospects
Science 255-
260 (2015)

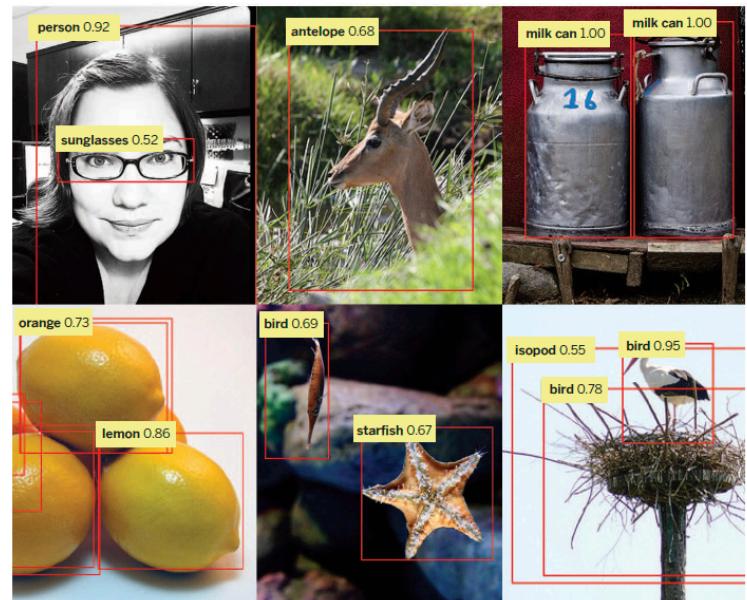
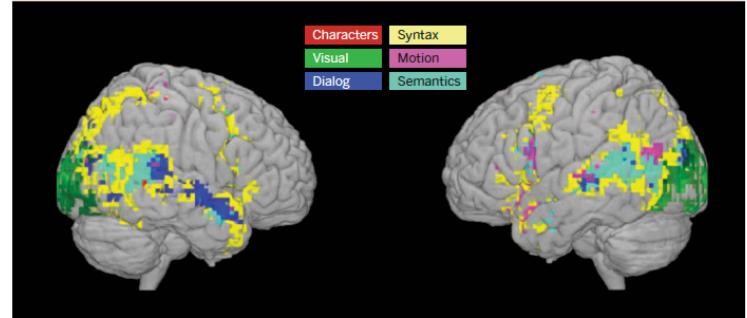
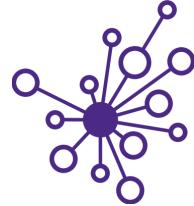


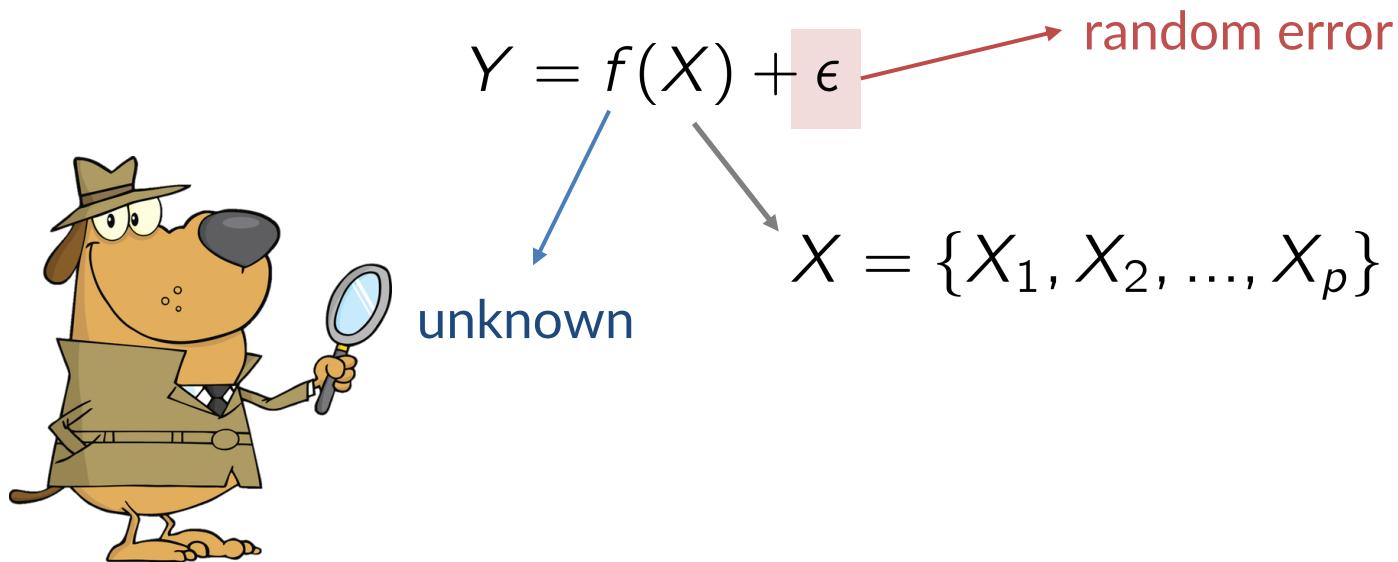
Fig. 1. Applications of machine learning. Machine learning is having a substantial effect on many areas of technology and science; examples of recent applied success stories include robotics and autonomous vehicle control (top left), speech processing and natural language processing (top right), neuroscience research (middle), and applications in computer vision (bottom). [The middle panel is adapted from (29). The images in the bottom panel are from the ImageNet database; object recognition annotation is by R. Girshick.]

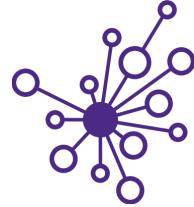


Statistical learning

Ansatz

Given an input vector, X , and output vector, Y ,
a function $f(X)$ exists such that





Why estimate f ?

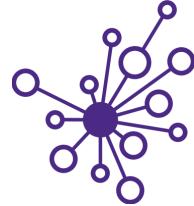
To predict the output Y (**prediction**)

e.g. *predict amount of fructose in an apple given its weight and type?*



To connect X to Y (**inference**) – how do changes in X influence Y ?

e.g. *if the cost of tropical fruit increases will the amount of fruit sold go down?*



Prediction

GOAL: estimate a function – an **estimator** - which gives the “best” prediction of Y given X in input

$$\hat{Y} = \hat{f}(X)$$

Hat symbol
denotes estimator

How do we find it? How do we measure the **error**?

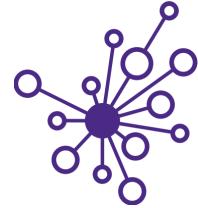
The **expected prediction error** of the estimator function is

$$E(Y, \hat{f}(x)) = E[(Y - \hat{f}(x))^2] = \underbrace{E[(f(x) - \hat{f}(x))^2]}_{\text{reducible error}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

E – stands for the expectation value or mean squared error

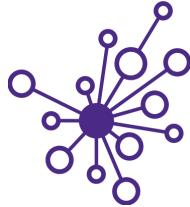
W

How to estimate f ?



Designed by Vecteezy

Parametric vs non-parametric ML models



Parametric models

Model defined by functional form over the entire range of input features, X_i

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

Parameters:

$$\{\beta_0, \beta_1, \dots, \beta_p\}$$

are found by minimizing the error between the model and exact values during training

Example: Linear regression

Non-parametric models

Do not assume a predefined functional form

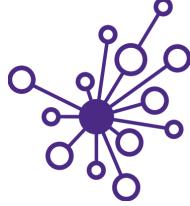
There is still a nonparametric model fitting procedure

Require much larger training datasets

Example: KNN classification

Flexibility vs interpretability

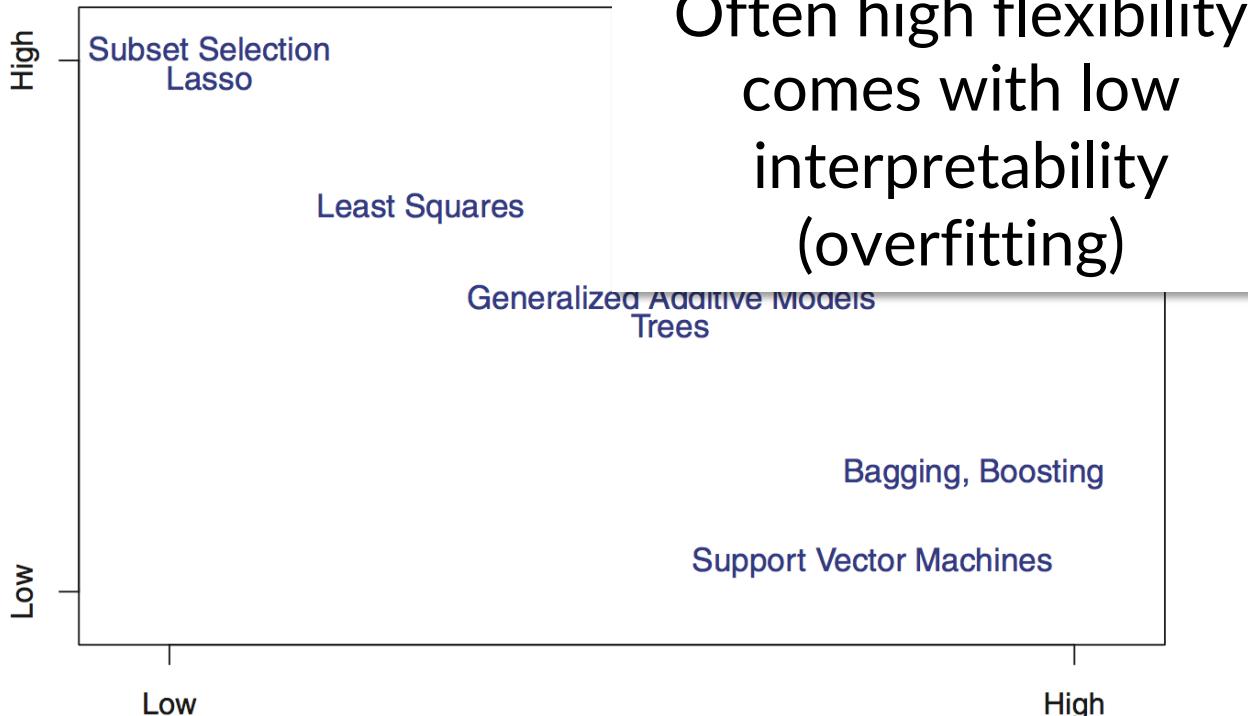
The tradeoff



It all makes
sense!

INTERPRETABILITY

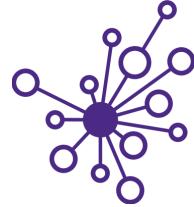
Very confused



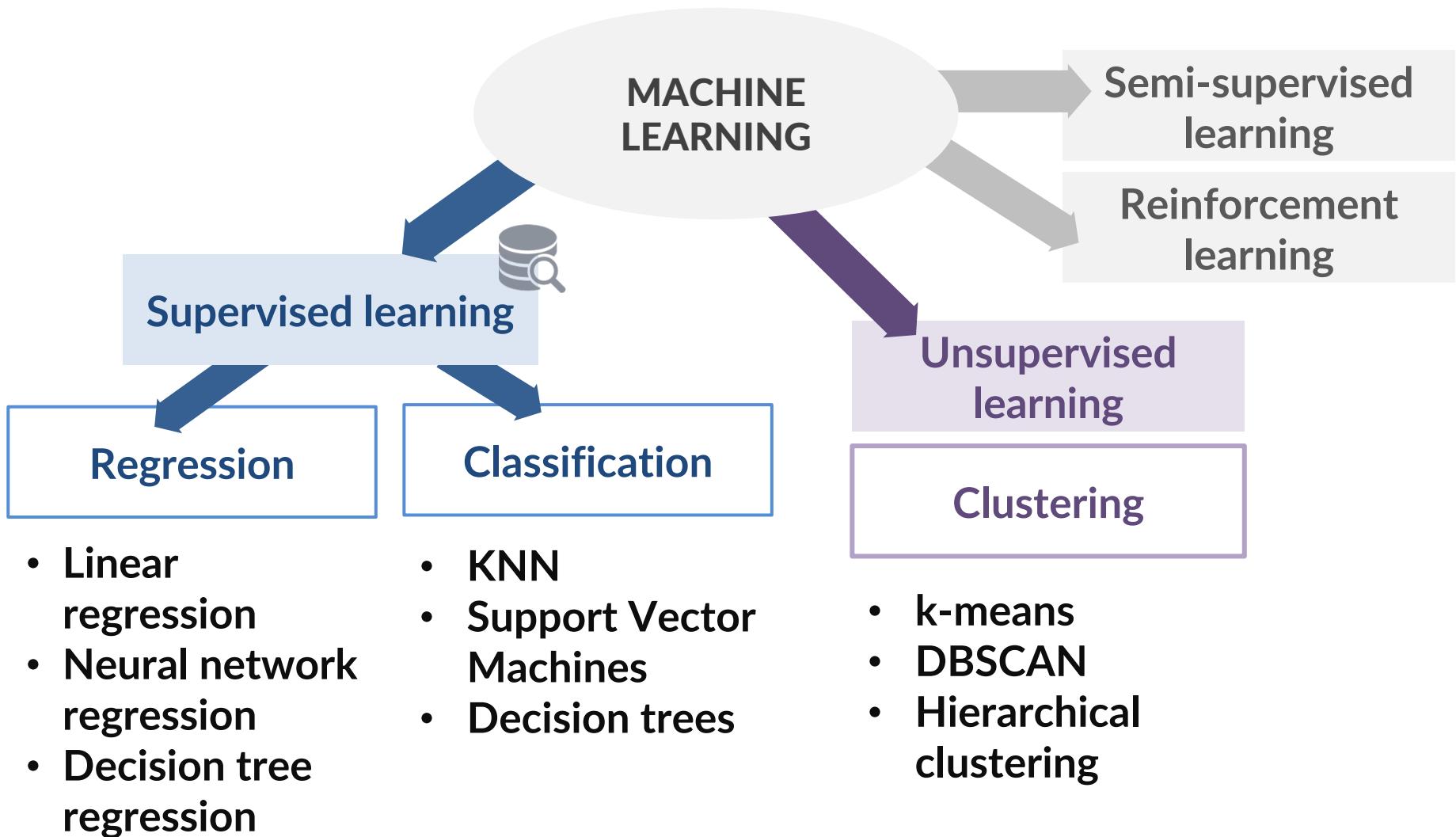
Eating apples
must follow a
linear trend
during the day

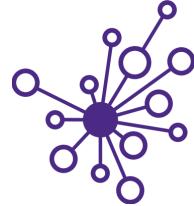
FLEXIBILITY

With 10 million
parameters I can predict
all apple shapes in the
world



Supervised vs Unsupervised





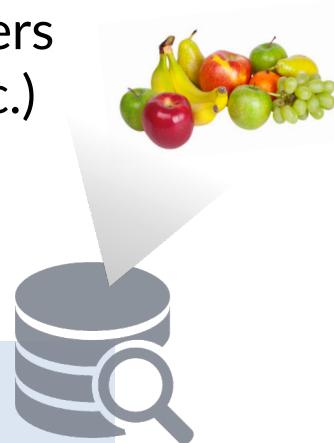
Supervised vs Unsupervised

X input feature/s –
independent variables
e.g. pictures, numbers
(weight / shape etc.)



SUPERVISED
ML models

PREDICT TARGET



target Y output
response / dependent variable
e.g. cost of fruit

Unlabeled X input feature/s
e.g. pictures, numbers
(weight / shape etc.)

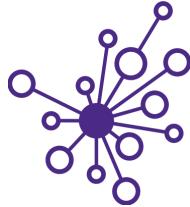


UNSUPERVISED
ML models

FIND PATTERNS

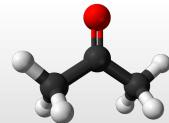
No predefined target Y !
e.g. find clusters in input data

Regression vs classification



Input: numeric or categorical

$$X = \{X_1, X_2, \dots, X_N\}$$



Organic compound (categorical)
Atom positions (numeric)

ML MODEL

Output

$$\hat{Y} = \hat{f}(X)$$

**quantitative
a.k.a. numerical**

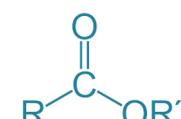
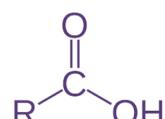
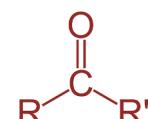
Regression

\hat{Y} numerical output:
e.g. weight, energy
(continuous)
 $m = 58.8 \text{ g/mol}$

**qualitative
a.k.a. categorical**

Classification

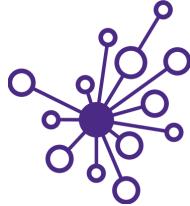
\hat{Y} categorical output:
category / class (discrete)
e.g. it is a **ketone**



Question

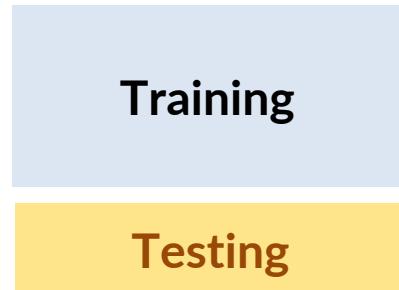
Think of an example of classification and / or regression & post it on the chat!

Think of questions for a minute or so and post what you thought of in the chat ☺



How accurate is my model?

Mean Squared Error (MSE) for regression



$$X_{train} = \{x_1, x_2, x_3, \dots, x_{N_{train}}\}$$

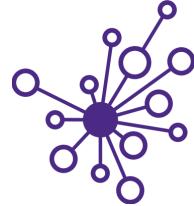
$$X_{test} = \{x_0, x_{N_{train}+1}, \dots, x_{N_{test}}\}$$

Recall

$$\mathbb{E} [(Y - \hat{f}(x))^2] = \underbrace{\mathbb{E} [(f(x) - \hat{f}(x))^2]}_{\text{reducible error}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

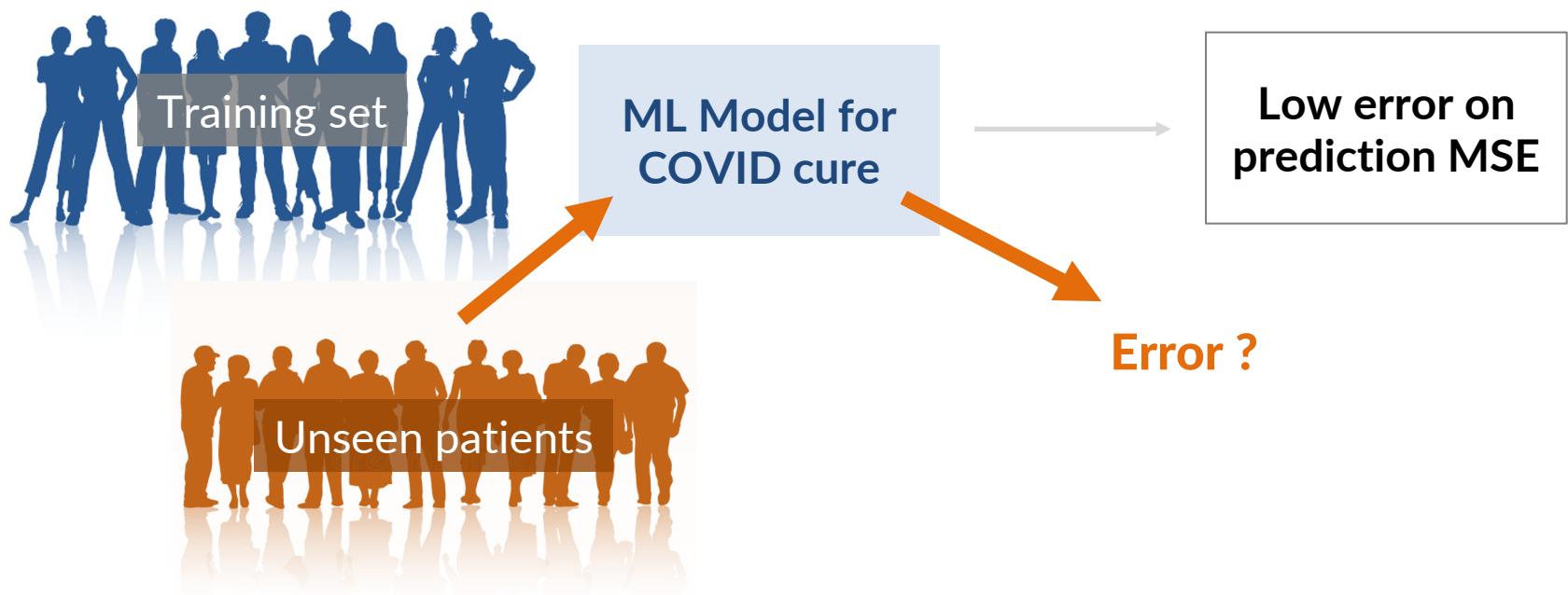
$$\text{MSE}_{test} = \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (Y_i - \hat{f}(x_i))^2 \equiv \frac{1}{N_{test}} \sum_{i=1}^{N_{test}} (Y_i - \hat{Y}_i)^2$$

Why the test set?



Assessing Model Accuracy

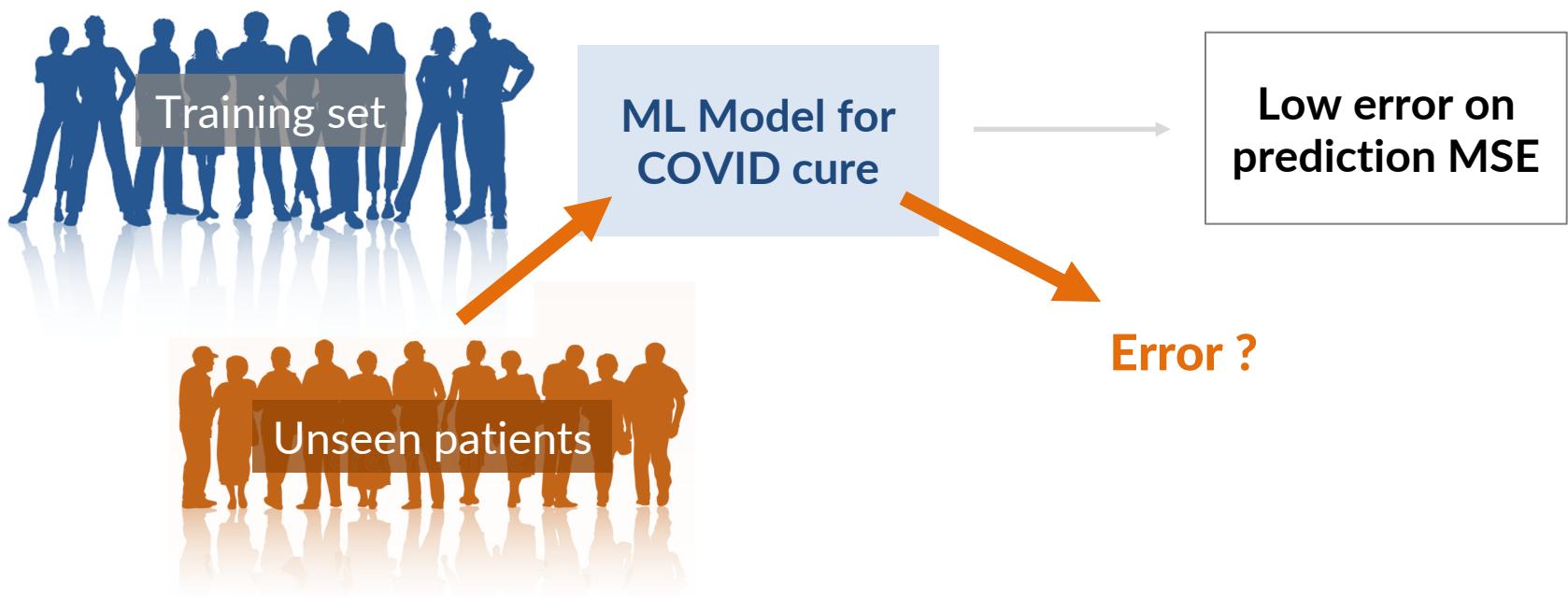
We always want to know how our model is doing “out in the real world” on some **test data** that the training process was blind to (validation) – We are not really interested in the training set.

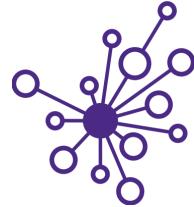


Think of questions for a minute or so and post what you thought of in the chat
😊

Question

When would you trust the model if you were an unseen patient? Is a low error on the training set enough?





Assessing Model Accuracy



Trained ML
Model for
COVID cure

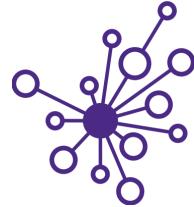
Low MSE on
training set

Minimize error on the test set

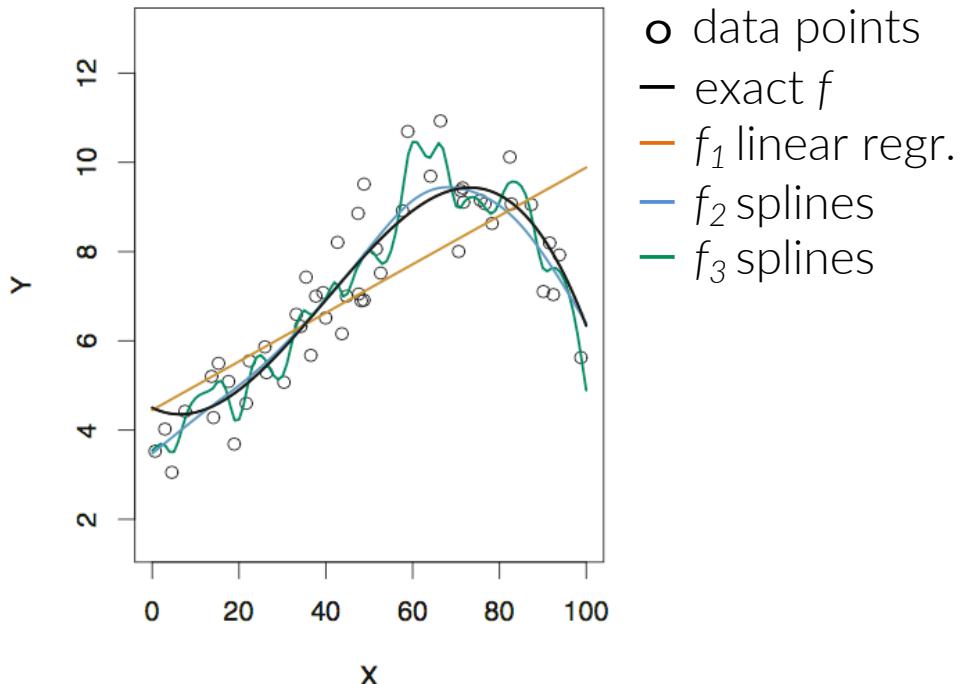


Unseen patients

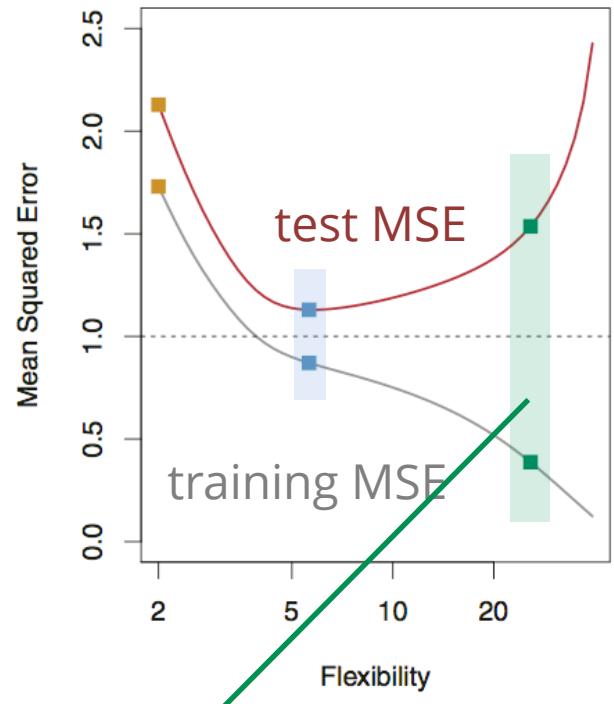
We need both a low training set error **AND** low test set error!!!



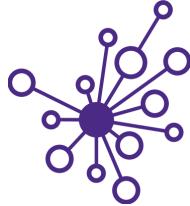
Assessing Model Accuracy



Hmm ... why is the test curve U-shaped?



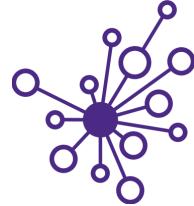
Overfitting!



Potential pitfalls

Test set is **not representative** – with a different test set a much larger MSE!

Cross-validation will come to the rescue! (estimate test MSE using training set)



Variance and bias

How does the error change as I change my test set? How does it change with the type of model?

$$\mathbb{E} \left[(Y - \hat{f}(x))^2 \right] = \underbrace{\mathbb{E} \left[(f(x) - \hat{f}(x))^2 \right]}_{\text{reducible error}} + \underbrace{\text{Var}(\epsilon)}_{\text{irreducible error}}$$

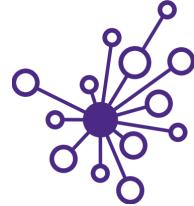
Average over training sets

$$\mathbb{E} (y_{\text{test}} - \hat{f}(x_{\text{test}}))^2 = \underbrace{\text{Var} (\hat{f}(x_{\text{test}}))}_{\text{Variance}} + \underbrace{(\text{Bias}(\hat{f}(x_{\text{test}})))^2}_{\text{Bias}} + \text{Var}(\epsilon)$$

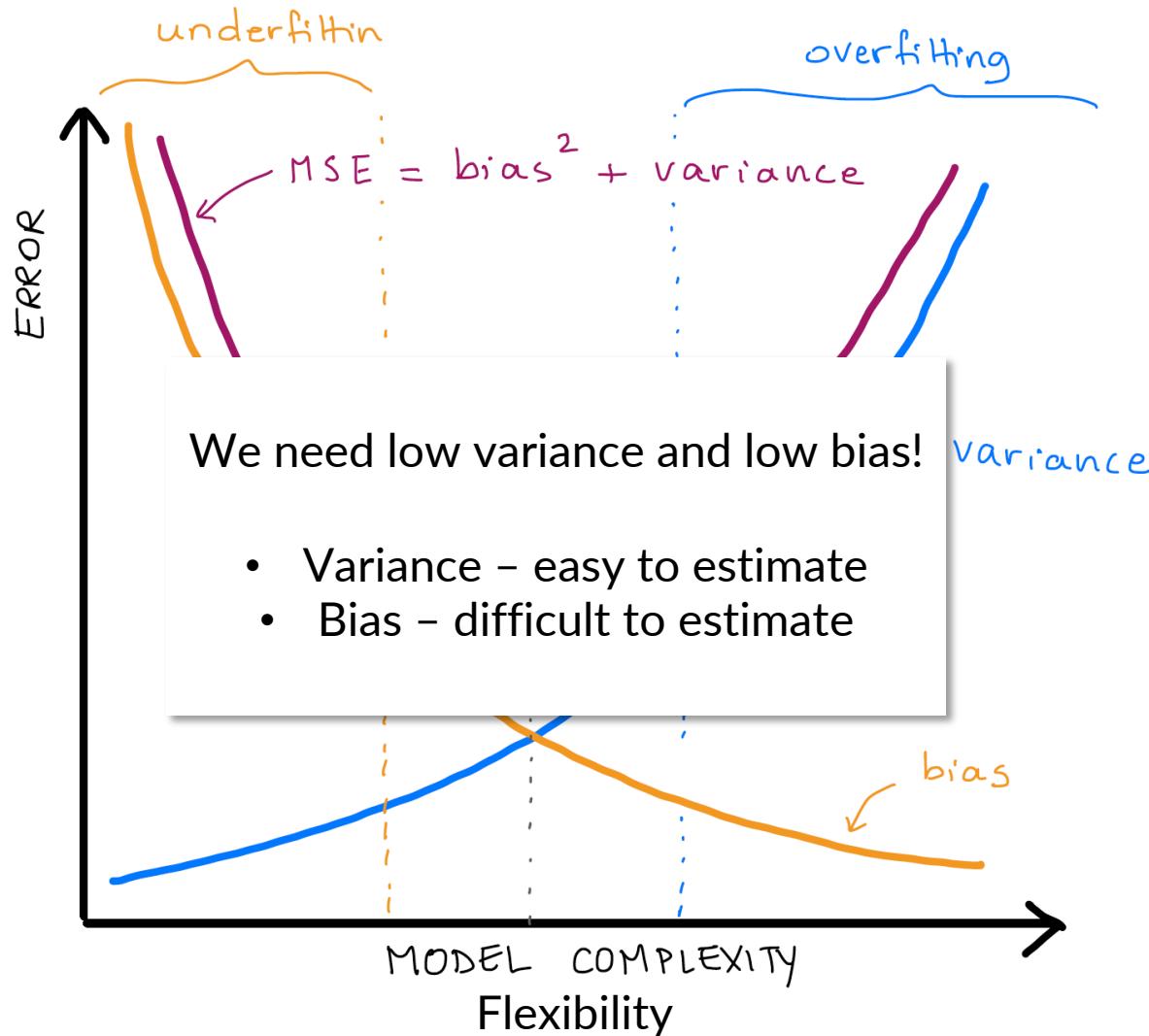
$$\begin{aligned} 2 &> -3 \\ \infty &\approx 3.14 \\ \sqrt{2} &\approx 1.41 \\ 5^{(2+2)} &\approx 25 \\ 101_2 &= 5_{10} \end{aligned}$$

Variance: quantifies how the choice of the **training set** influences \hat{f}

Bias: quantifies how the choice of the **model function** respect to the true f



Bias variance tradeoff



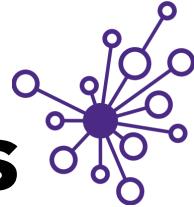
Question

Can the total error be zero?

Can I use MSE for classification?

Think of questions for
a minute or so and
post what you
thought of in the chat





Errors in classification problems

We are making qualitative predictions - how to assess the model accuracy?

We could look at the frequency of incorrect classification

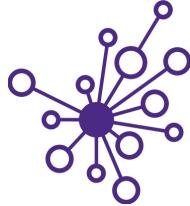
$$\text{training error rate} = \frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} I(y_i \neq \hat{y}_i)$$

0 if the two terms are equal;
1 otherwise

How can we use the test set? We want to minimize the error on the test set:

$$E(I(y_{i,\text{test}} \neq \hat{y}_{i,\text{test}}))$$

Estimating irreducible error in classification: Bayes classifier



*Test error is minimized by the **Bayes classifier** that assigns each observation to most likely class given its predictor values*

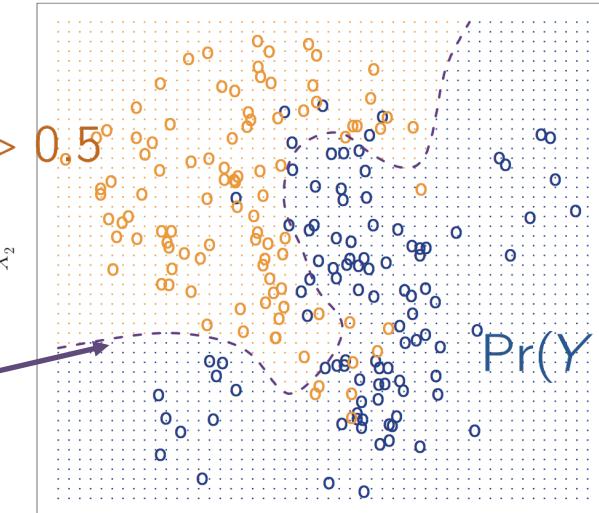
Probability that Y
belongs to class j
given x_{test}

$$\Pr(Y = j | X = x_{\text{test}})$$

Observed
predictor
vector

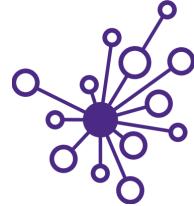
$$\Pr(Y = \text{orange} | X = x_{\text{test}}) > 0.5$$

Bayes decision
boundary $\Pr = 0.5$



$$\Pr(Y = \text{orange} | X = x_{\text{test}}) < 0.5$$

$$\text{bayes error rate} = 1 - E \left(\max_j \Pr(Y = j | X) \right)$$



One issue ...

For real data we do not know the **conditional probability distribution** of Y given X !



Classification methods



Two types of classification methods

- ***k* Nearest Neighbors (often KNN)** – Making a map of parameter space and estimating the class membership based on *locality respect to other members of the class*
- **Logistic regression** – Making a mathematic guess about the *likelihood of class membership* using a simplified mathematical model (the logistic function)

$$\Pr(Y = j \mid X = x_{\text{test}})$$



KNN on Jupyter!



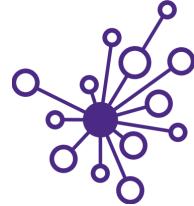
```
curl -O  
https://raw.githubusercontent.com/UWDIRRECT/UWDIRRECT.github.io/master/Wi21\_content/DSMCER/L6\_Intro\_ML\_KNN.ipynb
```



More on KNN



After you have gone through the notebook **read the next few slides** – these provide information on the role of K



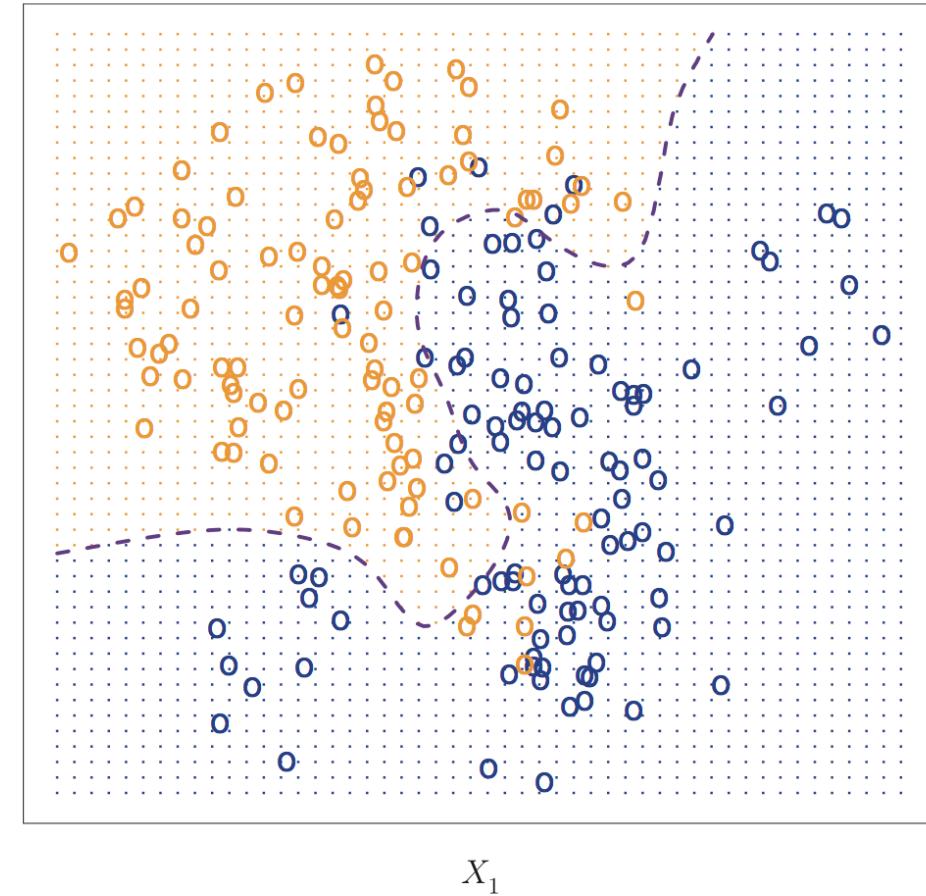
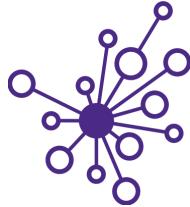
K-nearest neighbors (KNN)

The KNN classifier works on assigning the probability of membership in a class based on **distance** to other members in a class

- Our selection is based only on K – the number of neighbors we consider
- What are the possible ranges of K?
- Recall the KNN classifier

$$\Pr(Y = j \mid X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j)$$

A note about distances and identifying who is “nearest” ?



- The data in each dimension of X should be scaled similarly!
- We are concerned with relative distances in the parameter space, not absolute distances in the underlying units
- Otherwise, units, dimensionality, etc. can drastically favor closeness in arbitrary dimensions of X

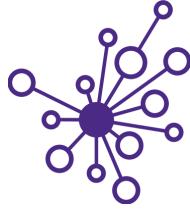
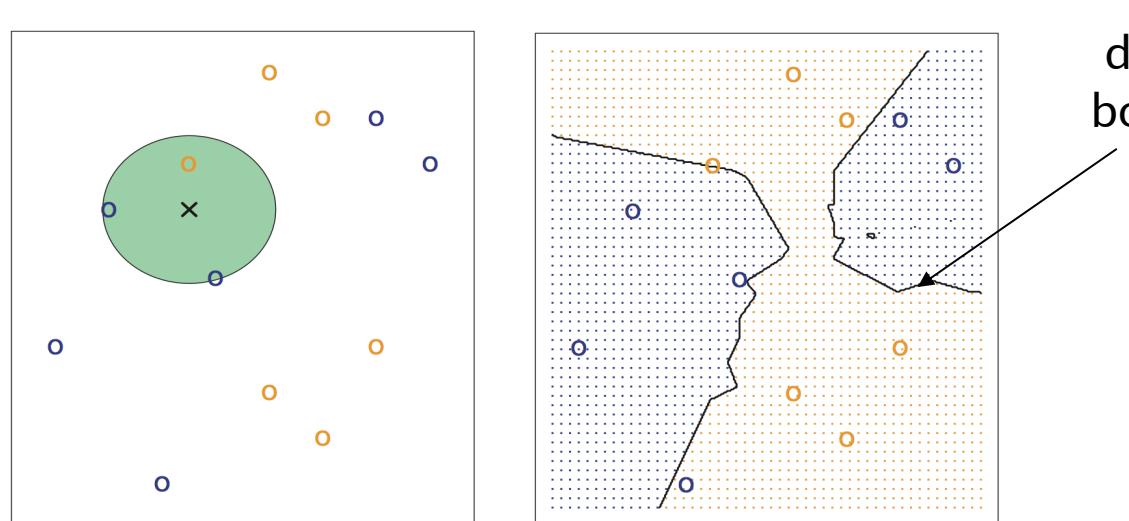


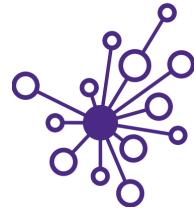
Illustration of KNN

$$\Pr(Y = j \mid X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j)$$



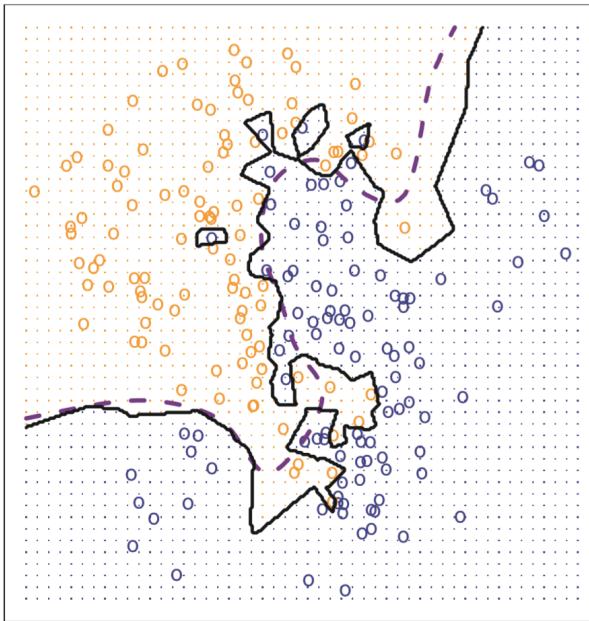
KNN
decision
boundary

FIGURE 2.14. The KNN approach, using $K = 3$, is illustrated in a simple situation with six blue observations and six orange observations. Left: a test observation at which a predicted class label is desired is shown as a black cross. The three closest points to the test observation are identified, and it is predicted that the test observation belongs to the most commonly-occurring class, in this case blue. Right: The KNN decision boundary for this example is shown in black. The blue grid indicates the region in which a test observation will be assigned to the blue class, and the orange grid indicates the region in which it will be assigned to the orange class.

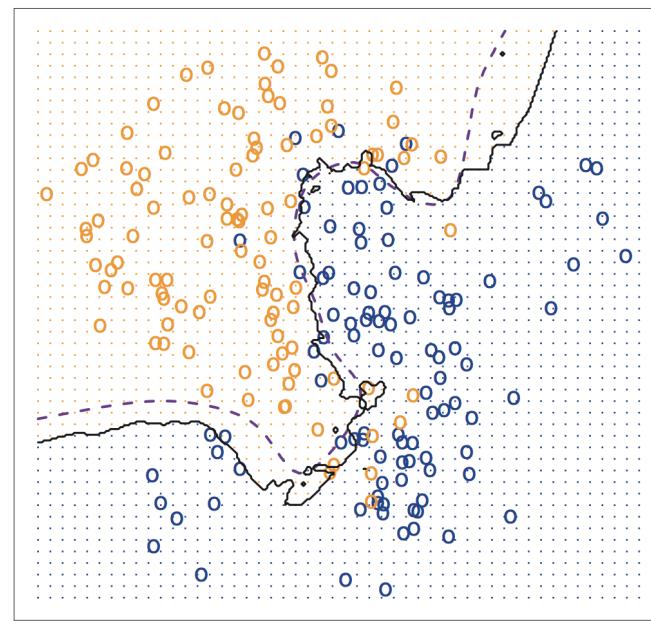


Effect of K on boundary

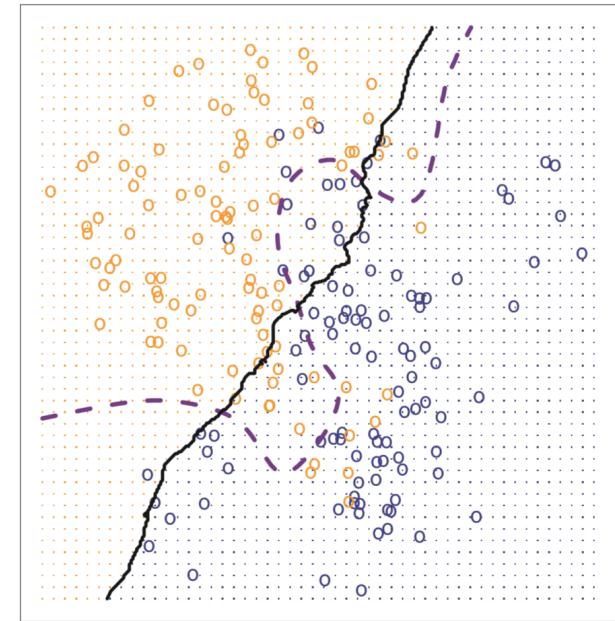
K=1



K=10



K=100



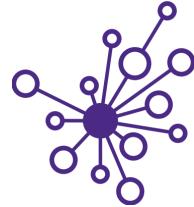
High flexibility



Low bias

Low flexibility

Low variance



Effect of K on accuracy

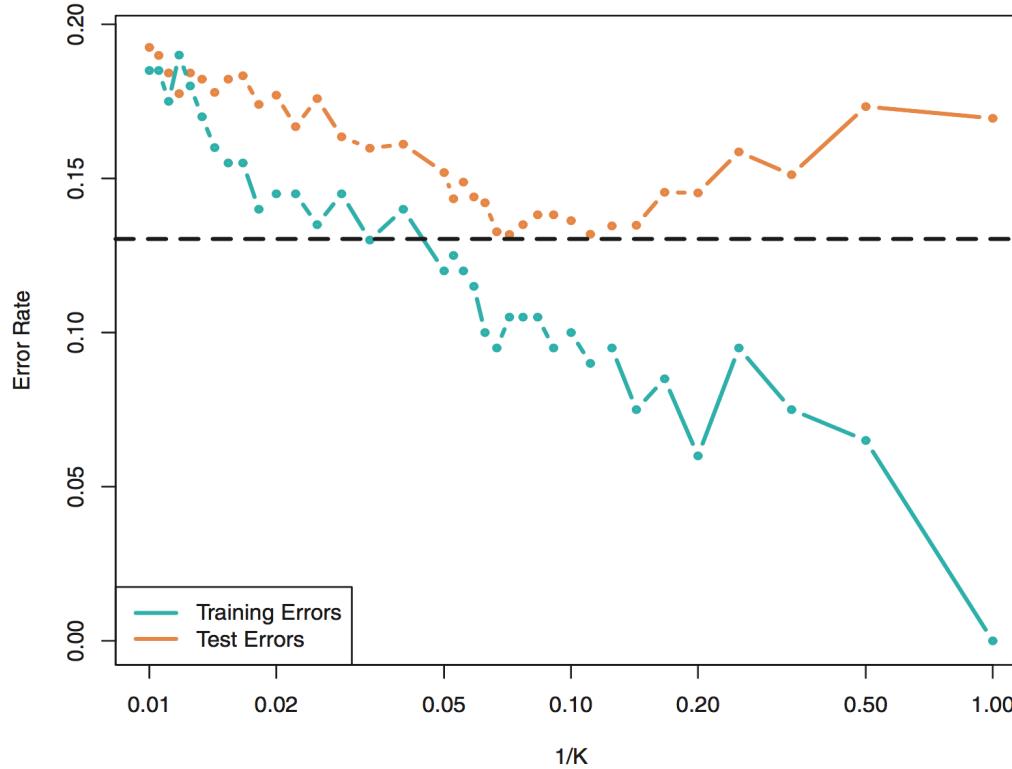


FIGURE 2.17. The KNN training error rate (blue, 200 observations) and test error rate (orange, 5,000 observations) on the data from Figure 2.13, as the level of flexibility (assessed using $1/K$) increases, or equivalently as the number of neighbors K decreases. The black dashed line indicates the Bayes error rate. The jumpiness of the curves is due to the small size of the training data set.