Classification

STAT 471

September 28, 2021

Where we are

✓ **Unit 1:** Intro to modern data mining

Unit 2: Tuning predictive models

Unit 3: Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture 1: Model complexity

Lecture 2: Bias-variance trade-off

Lecture 3: Cross-validation

Lecture 4: Classification

Lecture 5: Unit review and quiz in class

Homework 1 due the following Monday.

Recall: Clinical decision support

A patient comes into the emergency room with stroke symptoms. Based on her CT scan, is the stroke ischemic or hemorrhagic?

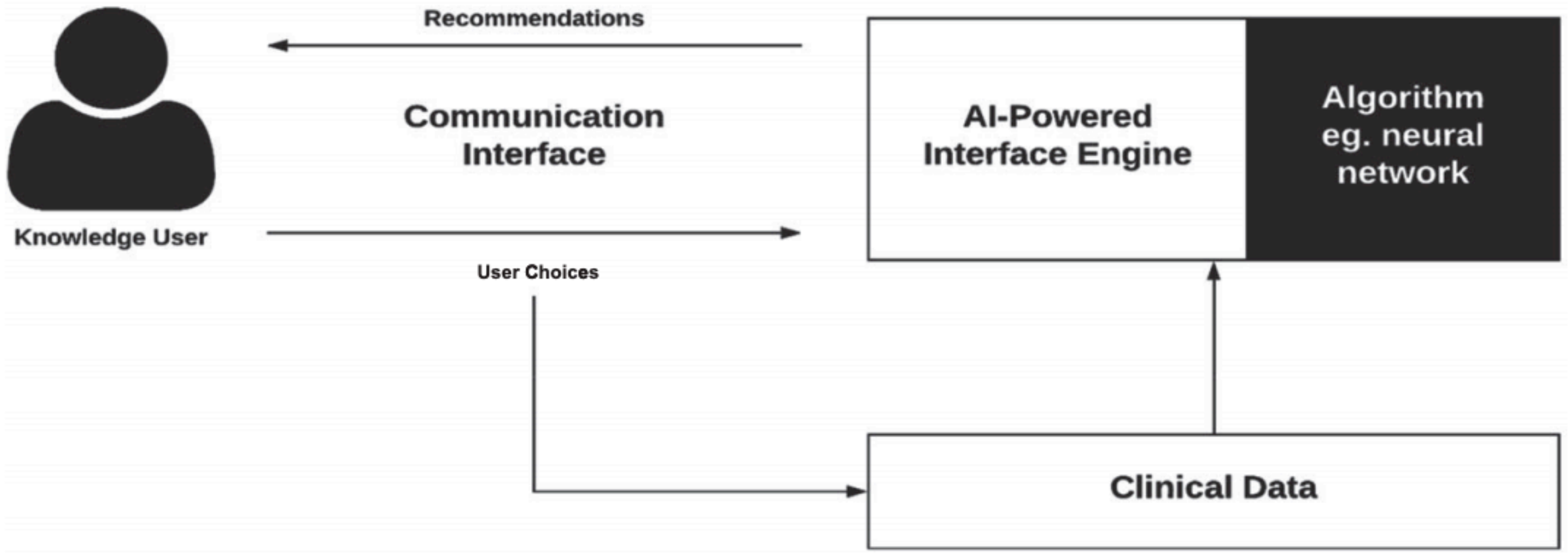


Image source: Sutton et al. 2020 (npj Digit. Med.)

This is a binary classification problem: $Y \in \{0,1\}$.

Given features $X = (X_1, \ldots, X_p)$, the goal is to guess a response $\widehat{Y} = \hat{f}(X)$ that is close to the true response, i.e. $\widehat{Y} \approx Y$. Measure of success is usually the

$$\text{test misclassification error} = \frac{1}{N}\sum_{i=1}^{N} I(Y_i^{\text{test}} \neq \hat{f}(X_i^{\text{test}})).$$

Classification via probability estimation

Suppose that the true relationship between Y and X is

$$\mathbb{P}[Y = 1 \mid X] = p(X), \quad \text{for some function } p.$$

Base line for classification problems

Then, the optimal classifier (called the Bayes classifier) is

$$\hat{f}^{\text{Bayes}}(X) = \begin{cases} 1, & \text{if } p(X) \geq 0.5; \\ 0 & \text{if } p(X) < 0.5. \end{cases}$$

p is the probability, and if p is > .5 then it is 1, else it is 0

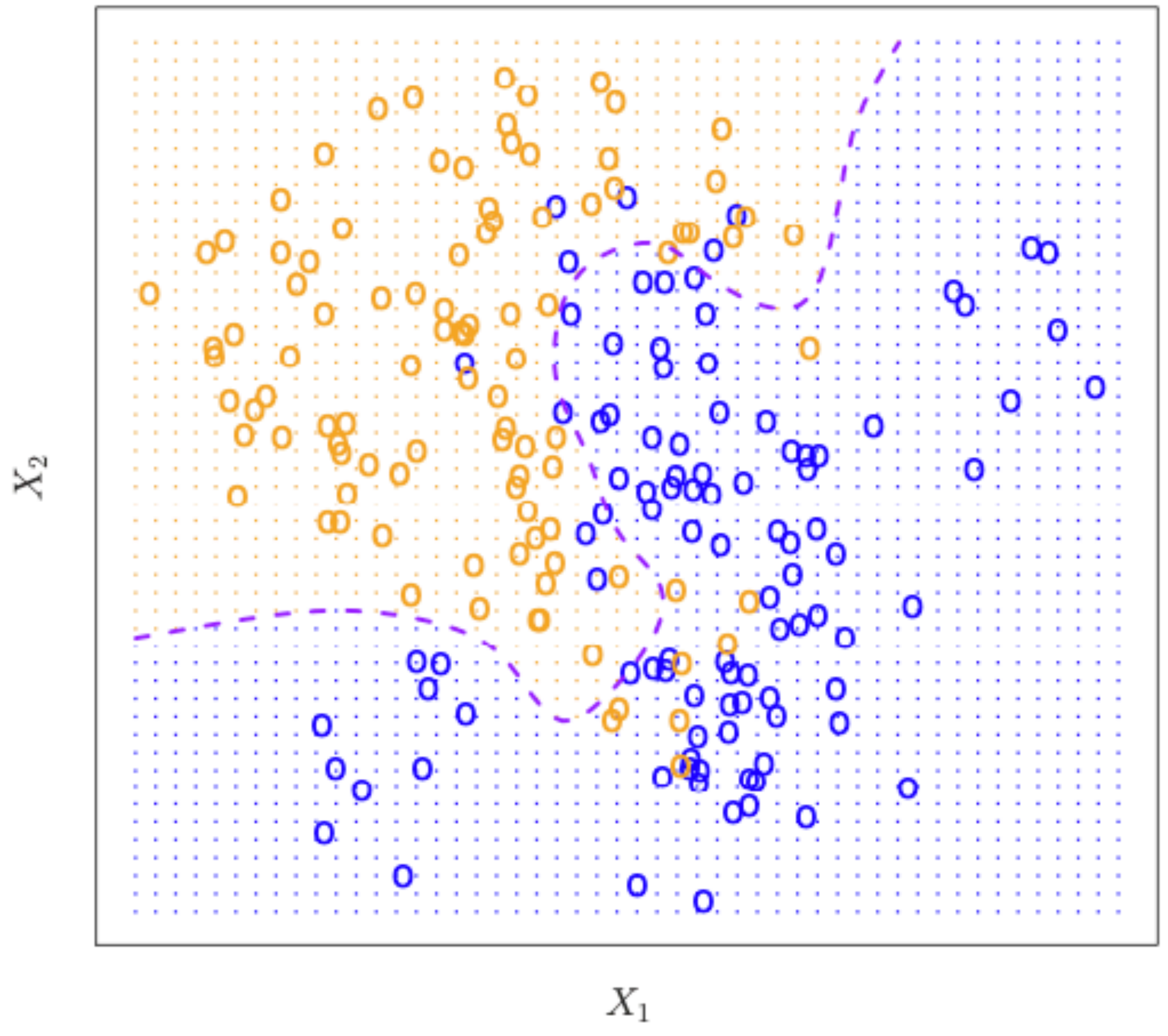
Classifiers usually build an approximation $\hat{p}(X) \approx \mathbb{P}[Y = 1 \mid X]$, and define

$$\hat{f}(X) = \begin{cases} 1, & \text{if } \hat{p}(X) \geq 0.5; \\ 0 & \text{if } \hat{p}(X) < 0.5. \end{cases}$$

What does it do? Classifies as 0 and 1

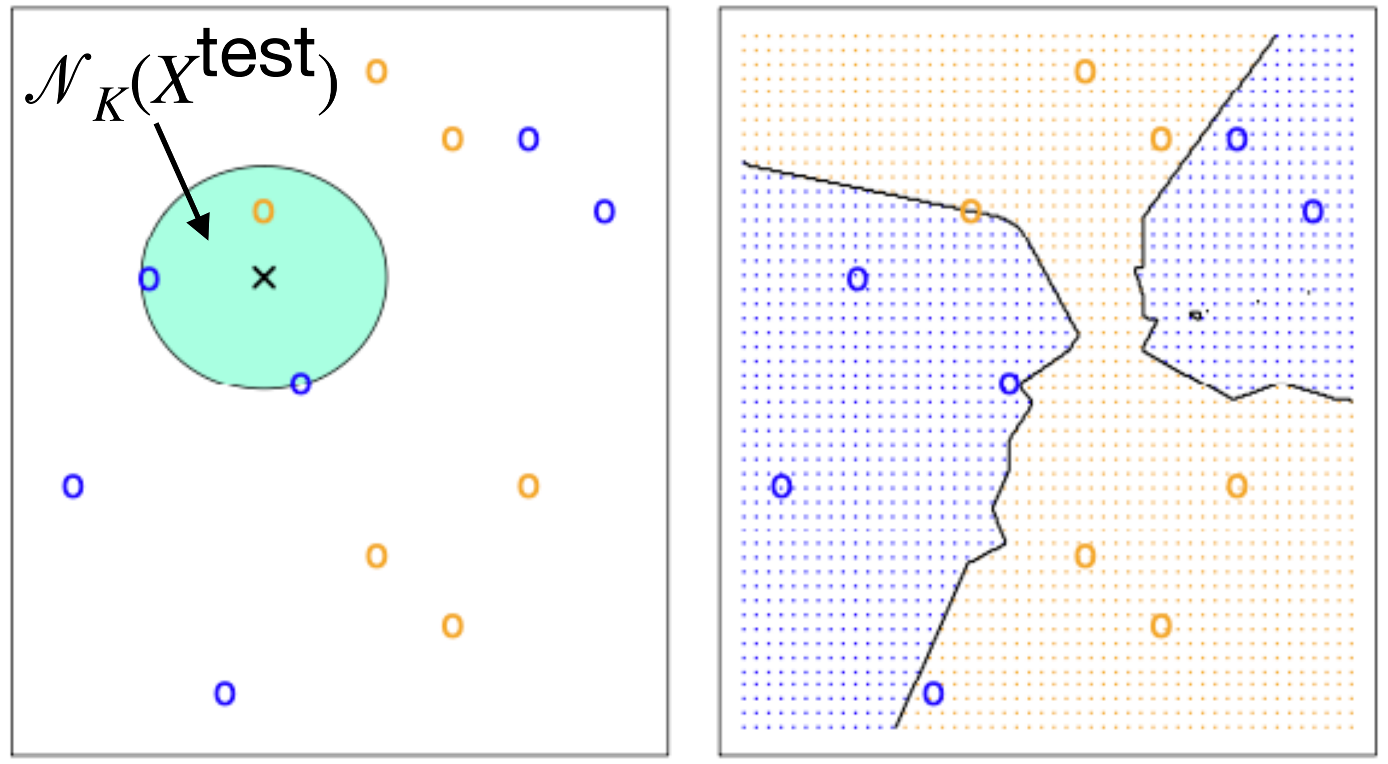
Does it make mistakes? Yes, 25% of the time because you minimizing the error

Example: K-nearest neighbors



Simulated binary classification data.
Bayes classifier in purple.
E.g., color = stroke type, (X_1, X_2) = CT image.

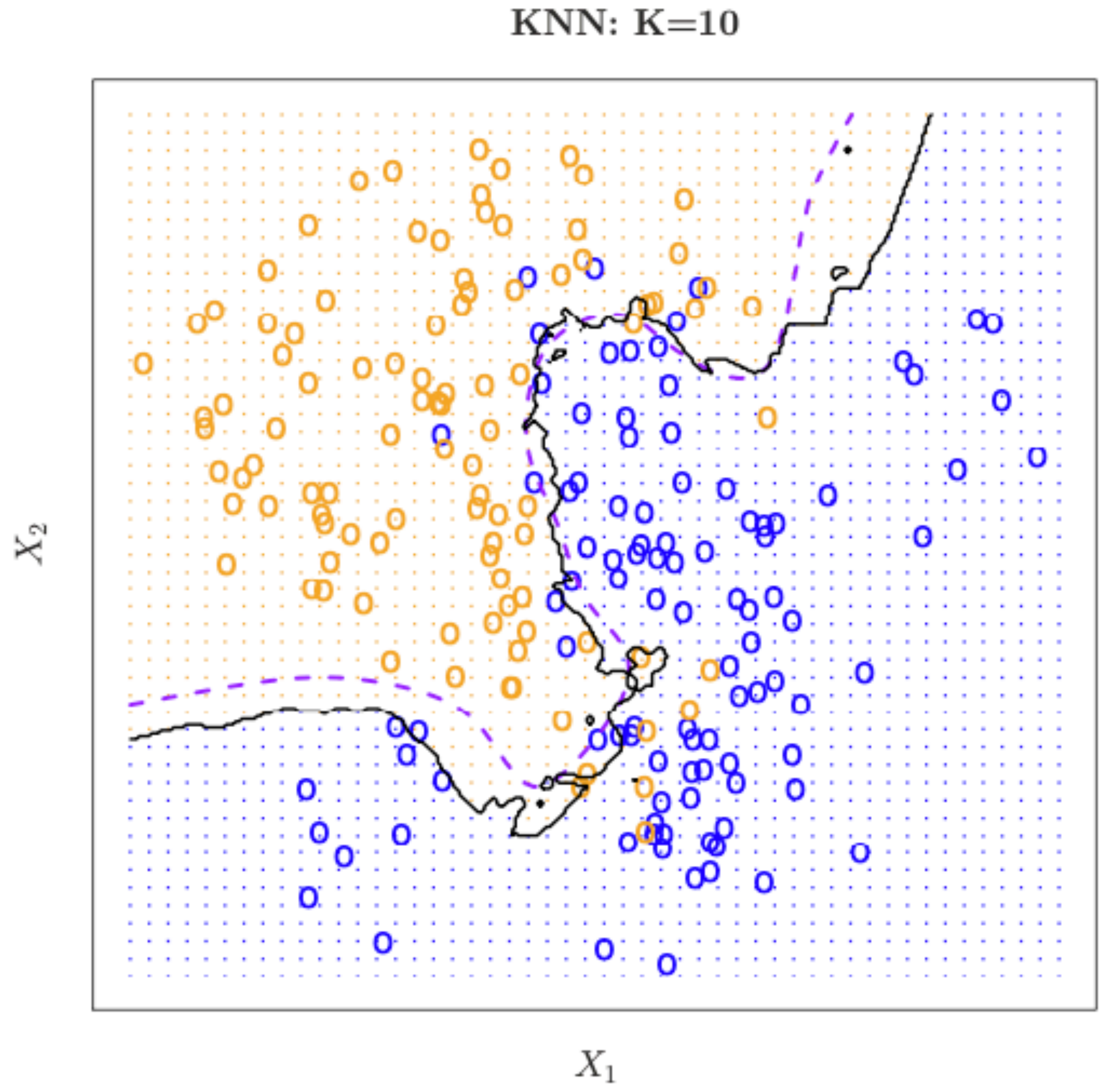
Line determines what the points are classified as



KNN illustration: Classify a test point based on majority vote among 3 nearest neighbors.

$$\hat{p}(X^{\text{test}}) = \frac{1}{K}\sum_{i\in\mathcal{N}_K} I(X_i^{\text{train}} = 1)\,.$$

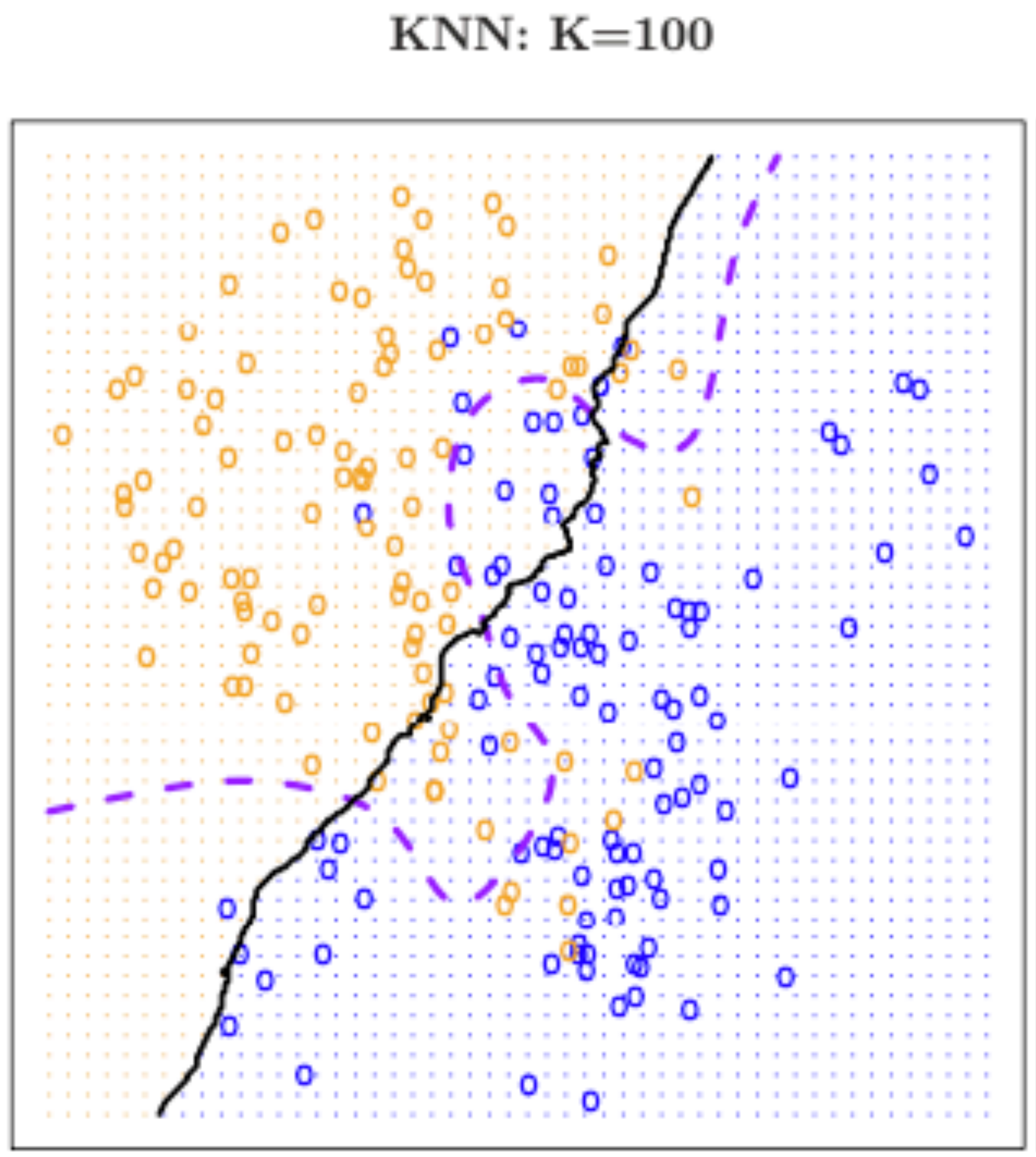
Estimate based on neighbors



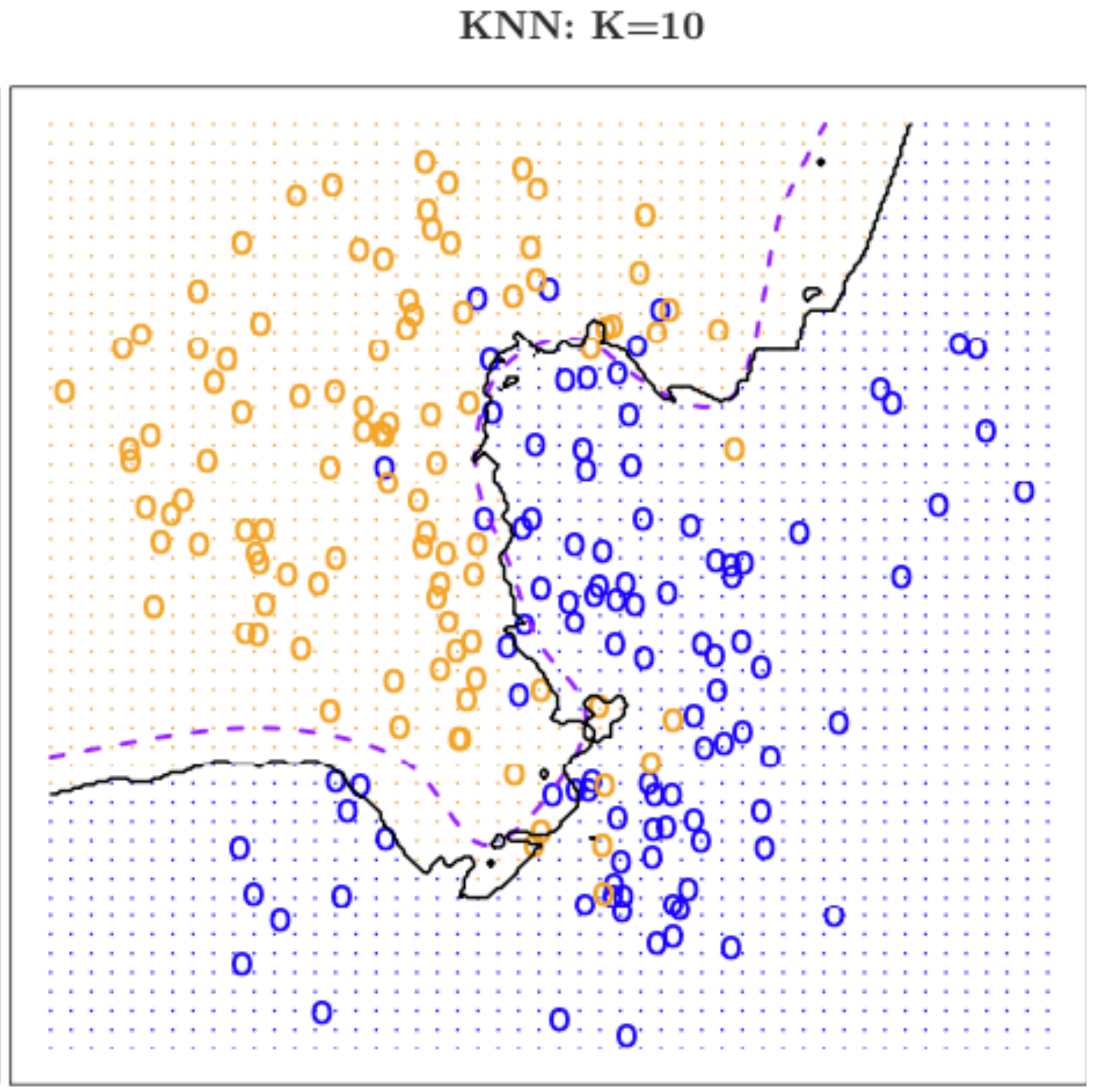
Applying KNN with K = 10 to simulated data.

Black line determines classification. Therefore, K = 10 looks pretty good

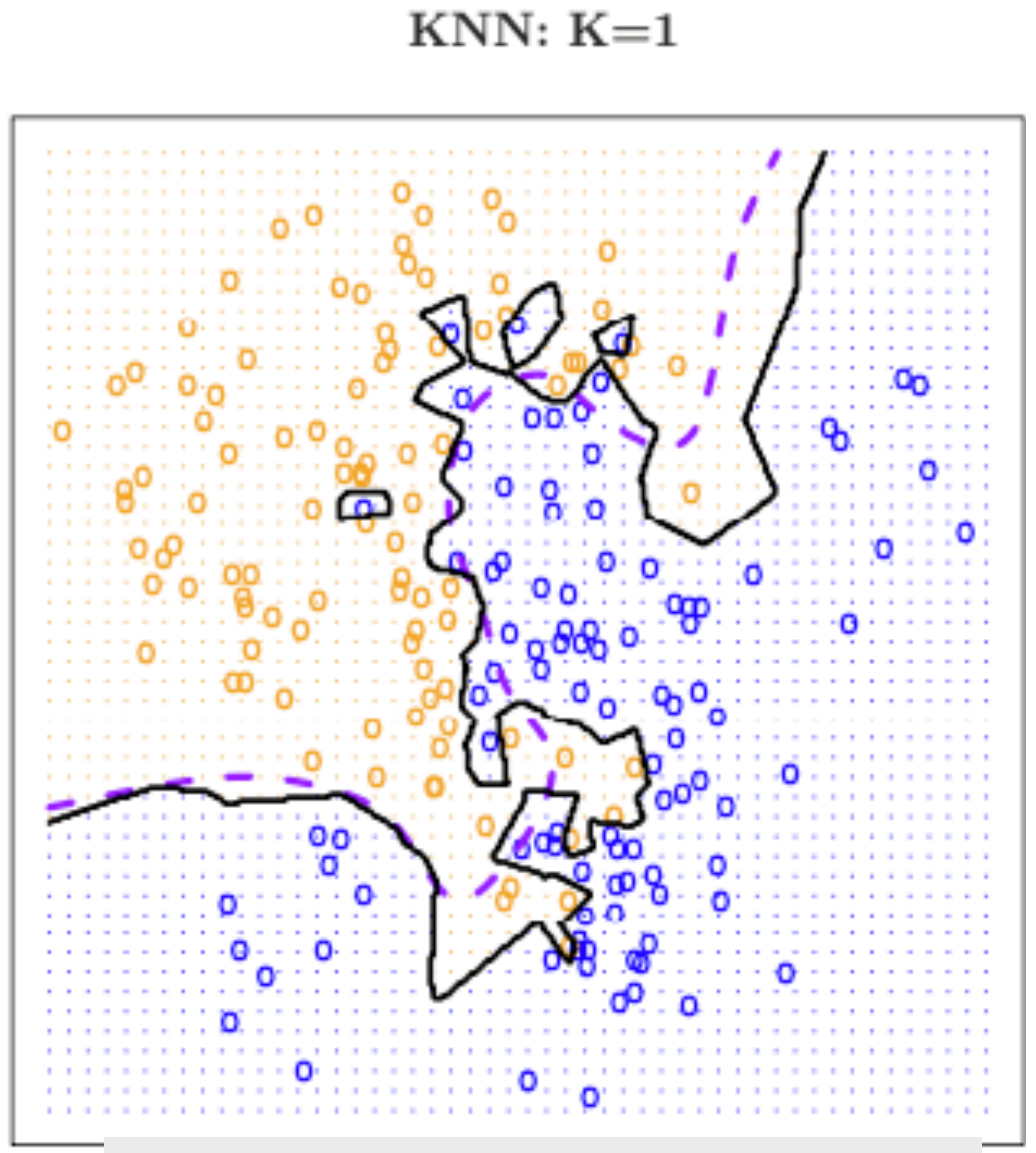
Model complexity and misclassification error



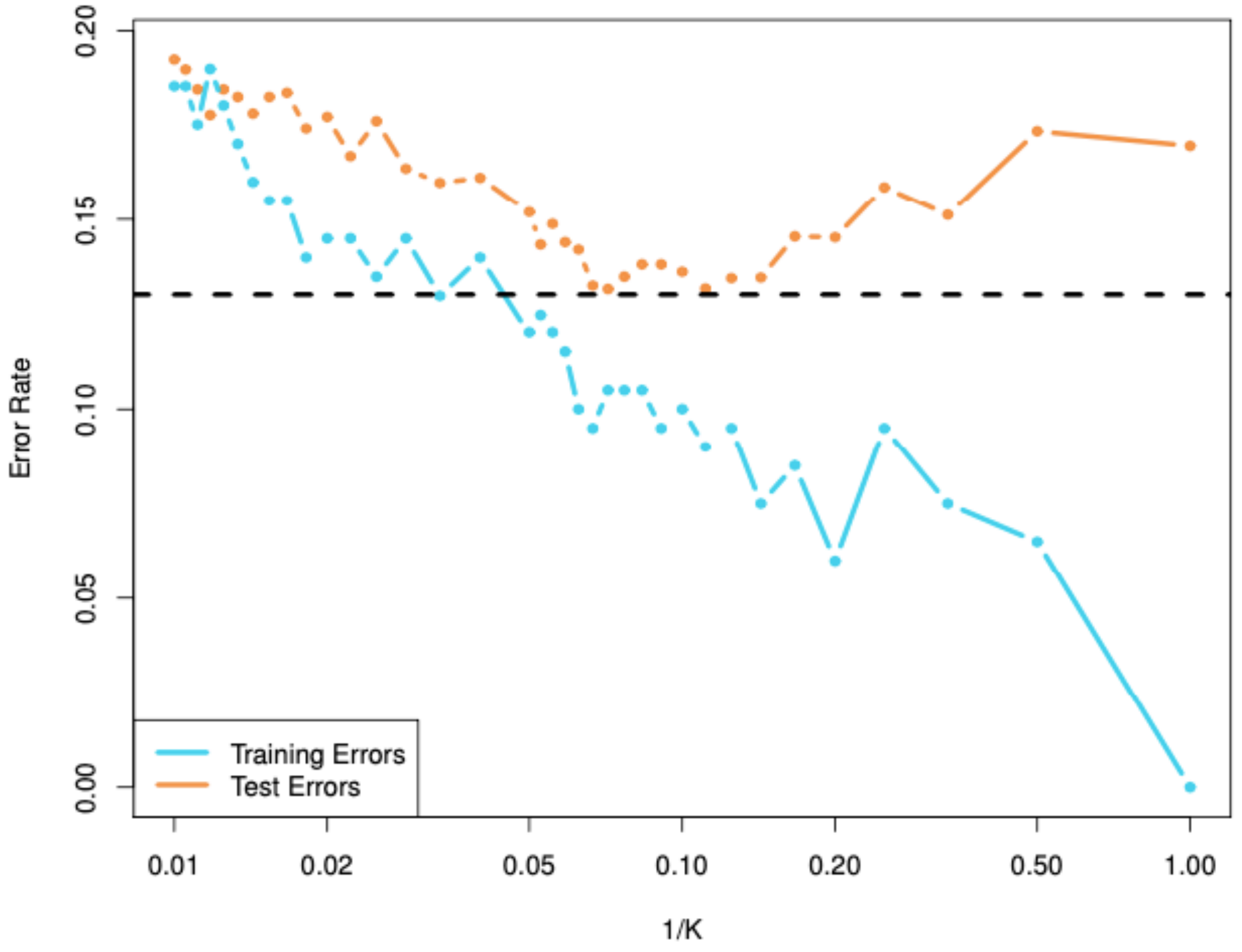
Not wiggly enough



Good balance of complexity



Adapting too much to the noise in the data

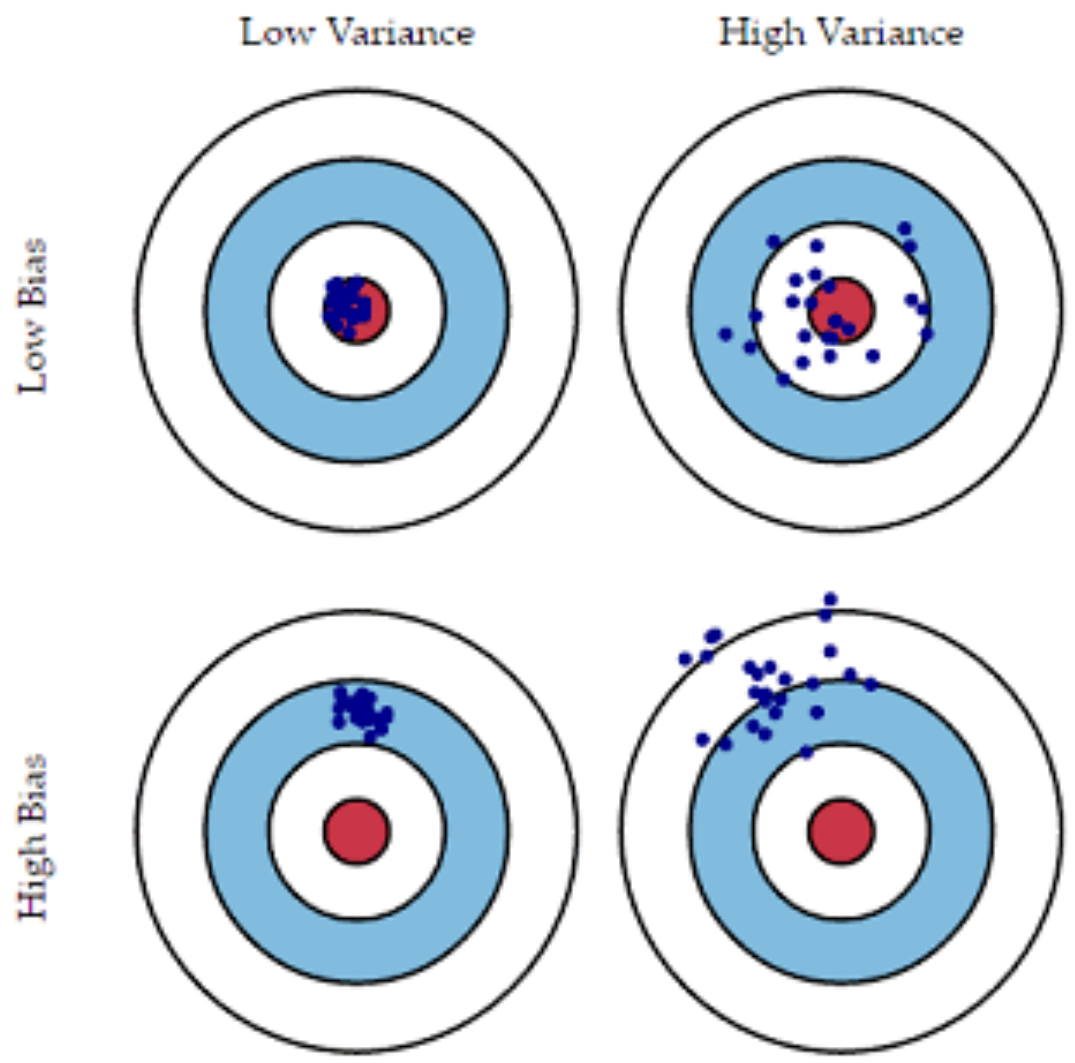


On training data, error decreases with increase in df while test error increases for test data

Same Goldilocks principle as in regression case:

- Too little complexity: Can’t capture the true trend in the data.
- Too much complexity: Too sensitive to noise in the training data (overfitting).

Bias-variance tradeoff



Mathematically: Applies only to continuous response variables and MSE.

Intuitively: Applies to any prediction problem, including classification. Does not matter if classification or not

For the estimate $\widehat{p}(X)$

- Bias: $\mathbb{E}[\widehat{p}(X)] - p(X)$ $\longrightarrow$

Bias does not always increase error. If true p is .9, and you always say .8, then you could still be getting a good classification

- Variance: $\text{Var}[\widehat{p}(X)]$ $\longrightarrow$

A little different than sigma ^2 term we see with rejection, but there is always going to be some error

This is due to the fact that you will always have things in the minority class

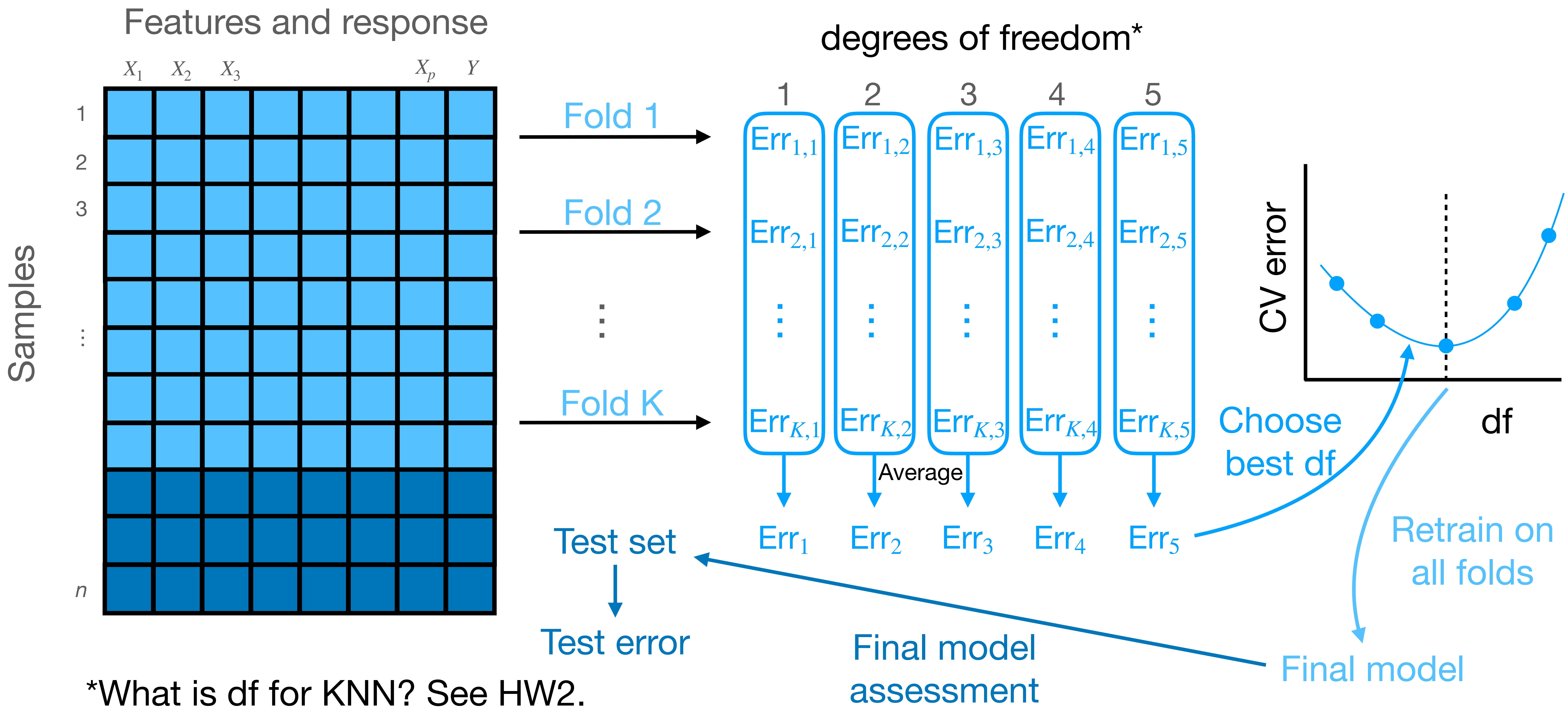
For classifying $\widehat{Y} = I(p(X) \geq 0.5)$

- Bias: Predict wrong class on average, to the extent $\widehat{p}$ on wrong side of 0.5
- Variance: Prediction varies with training set, to the extent $\widehat{p}$ fluctuates above or below 0.5
- Irreducible error (AKA Bayes error): Error incurred by Bayes classifier because $0 < \mathbb{P}[Y = 1 \,|\, X] < 1$.

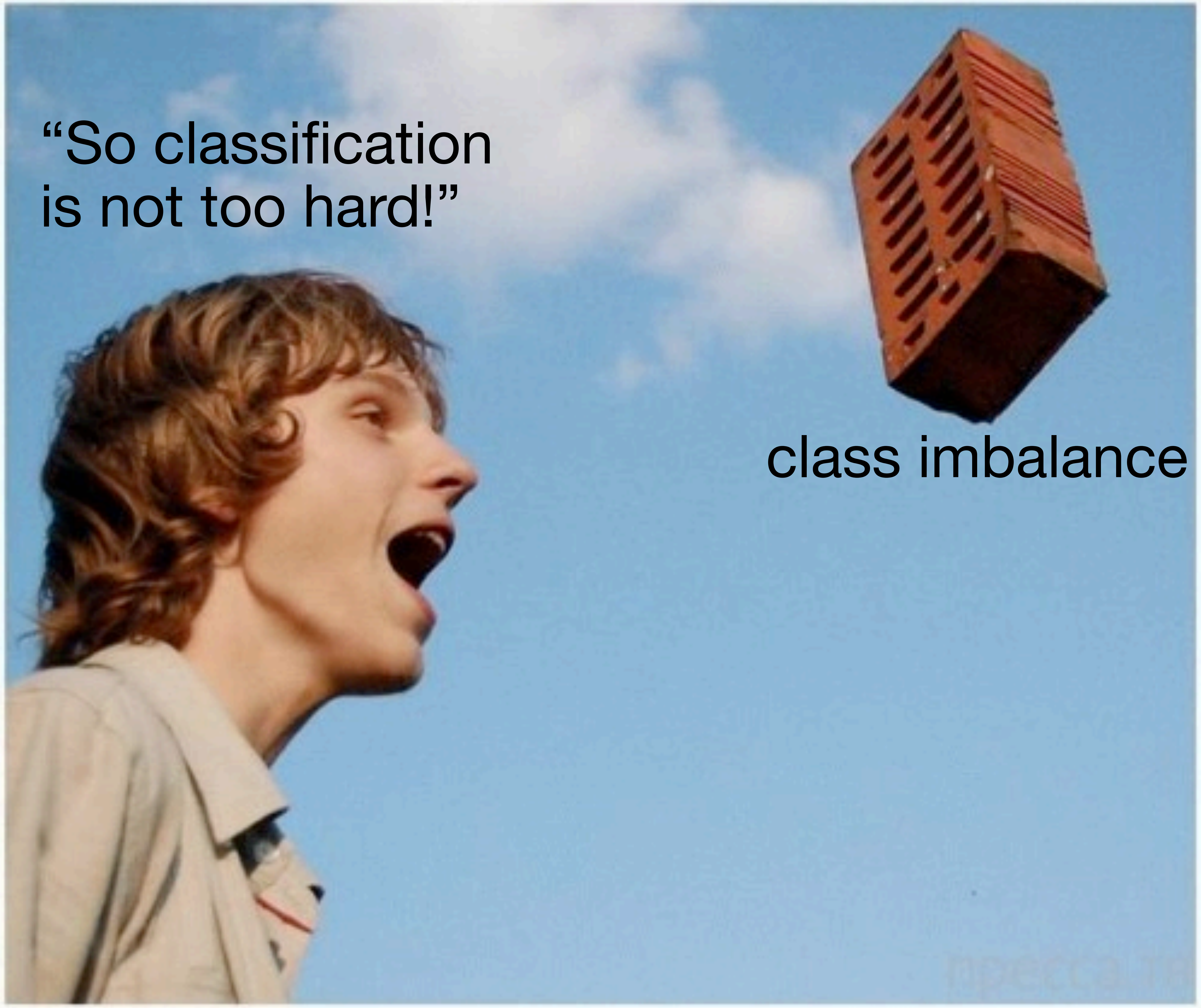
Cross-validation based on misclassification error

(otherwise same as before)

Not much needs to change for cross validation to accommodate classification problems



*What is df for KNN? See HW2.


"So classification is not too hard!"
class imbalance

Class imbalance

Cost of misclassification are also asymmetric

E.g. a non-fraudulent credit card charge that is classified as fraudulent charge

E.g. COVID test false positive rates

In many real-world classification problems, one class (say $Y = 1$) is significantly less frequent than the other. For example:

- Credit card transaction classification: normal versus fraudulent
- COVID testing: negative versus positive

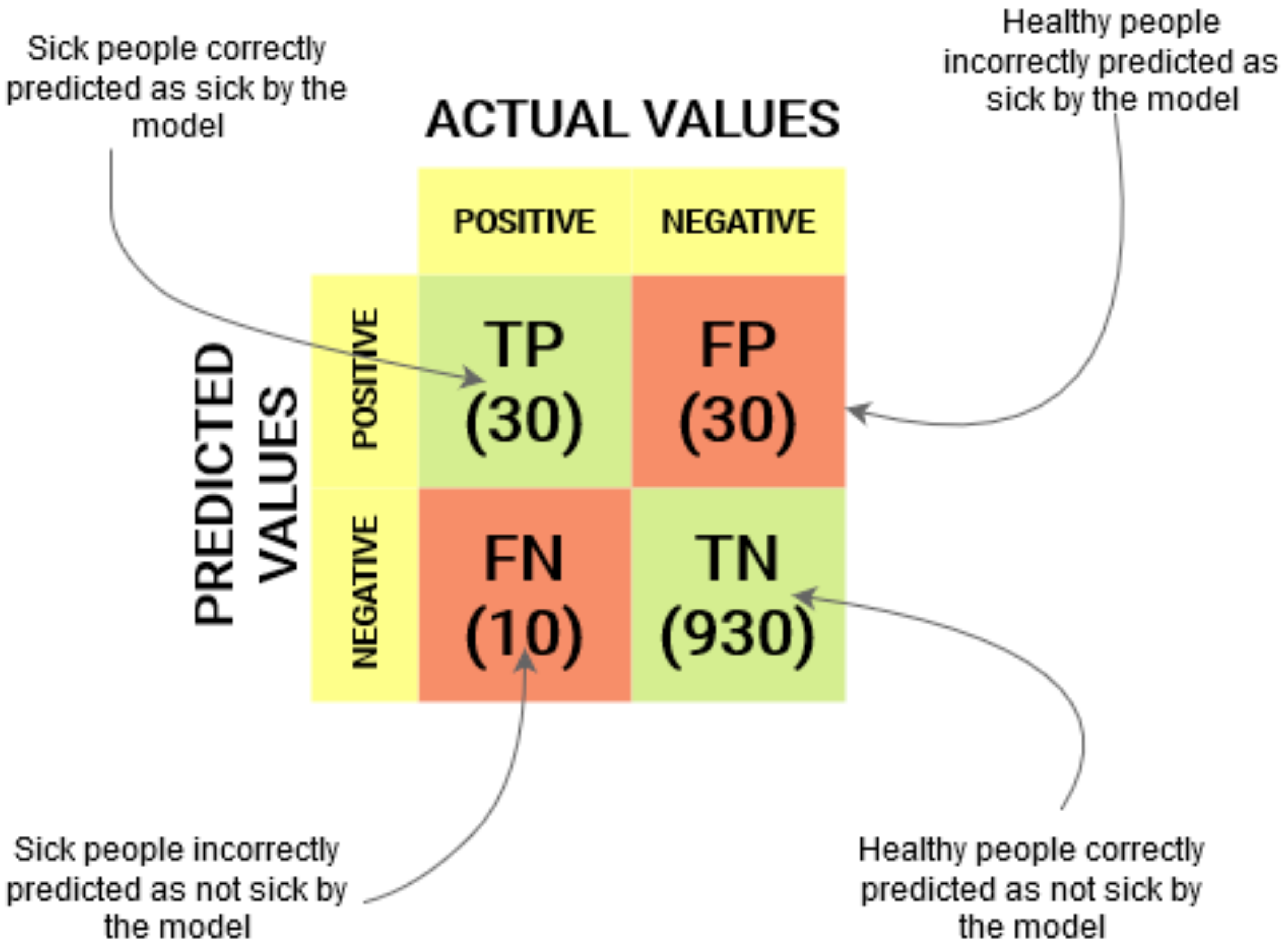
Often in these cases, the costs of misclassification are also asymmetric, i.e. the misclassification error is not the right metric.

Let's say 1% of credit card transactions are fraudulent. Then, the classifier that always predicts "not fraudulent" will have a misclassification error of only 1%.

Cross-validation based on misclassification error leads to overly simple models that ignore the minority class.

A more wholistic picture of a classifier

Confusion matrix



		ACTUAL VALUES	
		POSITIVE	NEGATIVE
PREDICTED VALUES	POSITIVE	TP (30)	FP (30)
	NEGATIVE	FN (10)	TN (930)

Sick people correctly predicted as sick by the model
Healthy people incorrectly predicted as sick by the model
Sick people incorrectly predicted as not sick by the model
Healthy people correctly predicted as not sick by the model

Image source: https://www.analyticsvidhya.com/blog/2020/04/confusion-matrix-machine-learning/

Summaries of confusion matrix

$$\text{False positive rate} = \frac{\text{number false positives}}{\text{total actual negatives}}$$

Actual value is negative, but said positive

$$\text{False negative rate} = \frac{\text{number false negatives}}{\text{total actual positives}}$$

Actual value is positive, but said negative

E.g. for COVID, we want to minimize false negatives more than positive

Thinking about misclassification costs

The cost of a false negative might be much greater than a false positive:

- Undetected fraudulent credit card transaction (false negative)
  → drained bank account. Cost: $C_{\text{FN}} = \$10{,}000$.
- False alarm of fraud (false positive)
  → annoying text message and/or replaced credit card. Cost: $C_{\text{FP}} = \$10$.

Weighted misclassification error:

If have handle on what issues might be, can better tune classifiers

$$\frac{1}{N}\sum_{i=1}^{N} C_{\text{FP}} \cdot I(\widehat{Y}_i^{\text{test}} = 1, Y_i^{\text{test}} = 0) + C_{\text{FN}} \cdot I(\widehat{Y}_i^{\text{test}} = 0, Y_i^{\text{test}} = 1).$$

Building misclassification costs into training

If going to down sample, should downsample to make representation of class match the cost of making the corresponding mistake

There may be two issues with

$$\hat{f}(X) = \begin{cases} 1, & \text{if } \widehat{p}(X) \geq 0.5; \\ 0 & \text{if } \widehat{p}(X) < 0.5. \end{cases}$$

1. The minority class is poorly captured by the probability model $\widehat{p}(X)$.
2. The probability threshold of 0.5 is suboptimal.

To fix these, a variety of strategies can be employed:

- Downsample the majority class by a factor $C_{\text{FP}}/C_{\text{FN}}$.

People do not like because feels like you are wasting data

- Choose the probability threshold $C_{\text{FP}}/(C_{\text{FN}} + C_{\text{FP}})$ instead of 0.5.

Otherwise, you can just tune the threshold to reflect costs

- Build cost directly into the objective function when training.

Example: KNN with $K = \infty$

Suppose we apply KNN with $K = \infty$ (each data point has the same prediction); class 0 costs $10 to misclassify and class 1 costs $1000 to misclassify.

Computing expected weighted misclassification error

Let $\hat{c}$ be the class predicted for each data point. Then, we have

$$10 \cdot \mathbb{P}[\hat{Y} = 1, Y = 0] + 1000 \cdot \mathbb{P}[\hat{Y} = 0, Y = 1] = \begin{cases} 10 \cdot \mathbb{P}[Y = 0], & \text{if } \hat{c} = 0; \\ 1000 \cdot \mathbb{P}[Y = 1], & \text{if } \hat{c} = 1. \end{cases}$$

Therefore, we should set

Notes that this formula might not be correct

$$\hat{c} = \begin{cases} 1 & \text{if } \mathbb{P}[Y = 1] \geq \dfrac{10}{10 + 1000}; \\ 0 & \text{if } \mathbb{P}[Y = 1] < \dfrac{10}{10 + 1000}. \end{cases}$$

We can recover this prediction rule from KNN via downsampling, threshold adjustment, or cost-sensitive training (in general these three strategies can give different answers).

Evaluating classification errors on a test set

Given C_{FN} and C_{FP}, best single number to summarize classification performance is the weighted misclassification error on the test set.

There are other ways of assessing classification performance without quantifying these costs:

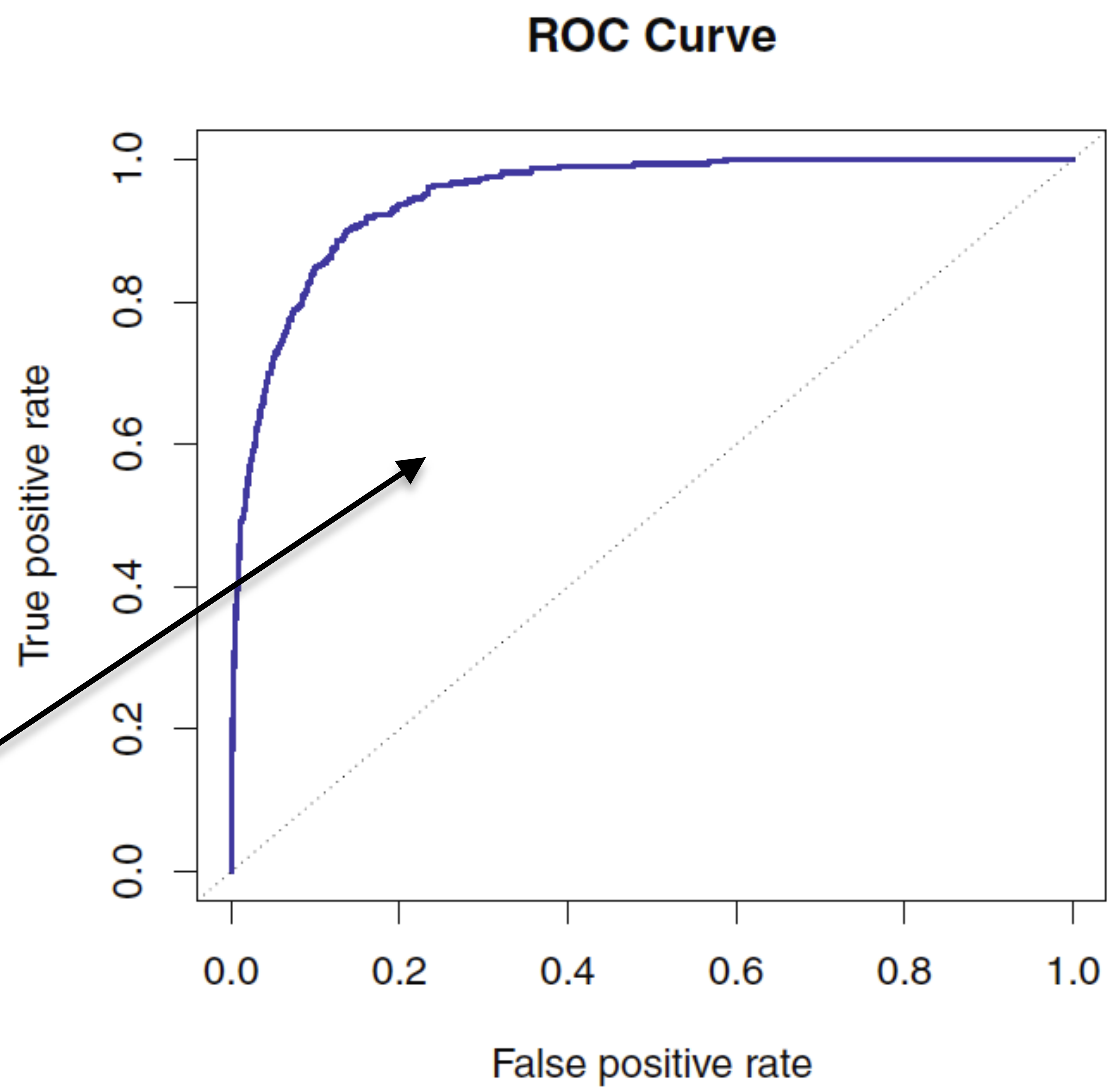
- Confusion matrix
- False positive rate and false negative rate
- Receiver operating characteristic (ROC) curve; area under the curve (AUC)

ROC curve

Helps us determine what threshold to include

Quantifies how well we are doing on the negative cases and how well are doing on the positives

- The ROC curve plots the true positive rate (one minus the false negative rate) versus the false positive rate, as the threshold is varied from 0 to 1.
- We want the curve to get as close to the upper left-hand corner as possible.
- Area under the curve (AUC) is another measure of the quality of a classifier.



Want to maximize the area under the ROC curve

Summary

- Classification problem is similar in some ways to regression; different in others.
- Classification typically done by estimating $\mathbb{P}[Y = 1 \,|\, X]$, thresholding at 0.5 (e.g. KNN).
- The bias-variance tradeoff carries over intuitively, but not mathematically, to classification.
- The misclassification error is not a good metric for problems when different misclassifications have different costs; often the case when classes are imbalanced.
- Other metrics for classifiers include the weighted misclassification error, false positive and false negative rates (based on the confusion matrix), and ROC curve.
- Class imbalance can be remedied through downsampling, threshold adjustment, or cost-sensitive training.