## Classification

**STAT 4710** 

#### Where we are



Unit 1: R for data mining

Unit 2: Prediction fundamentals

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

## 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?

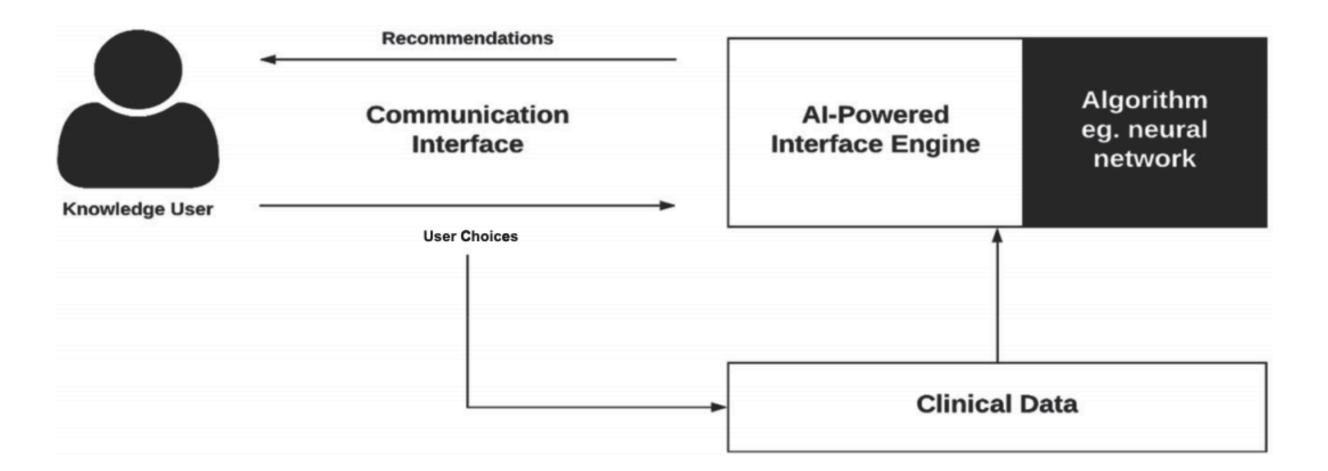


Image source: Sutton et al. 2020 (npj Digit. Med.)

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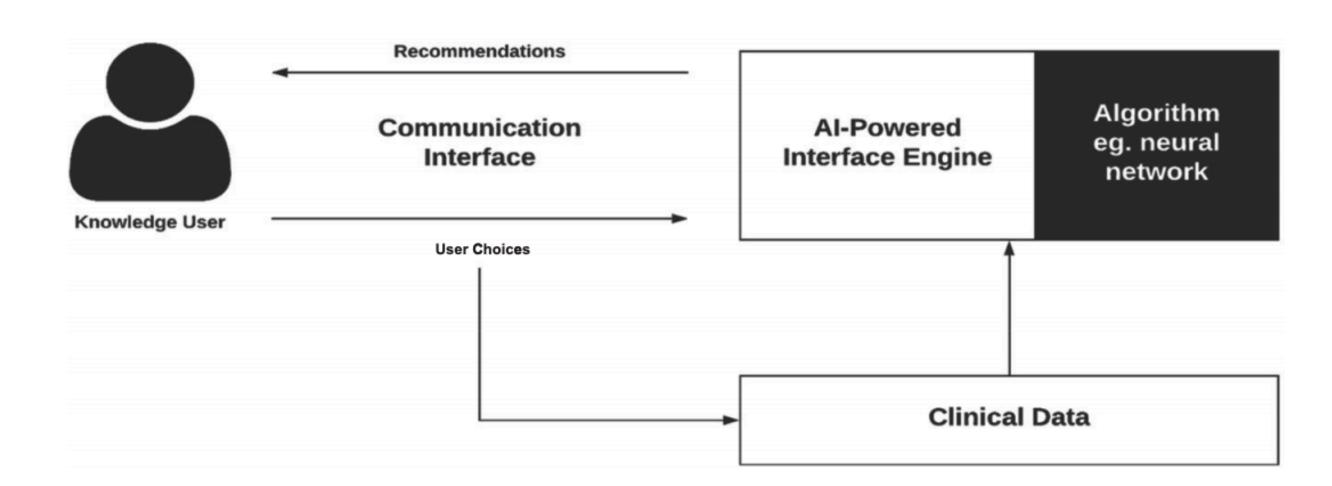


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This is a binary classification problem:  $Y \in \{0,1\}$ .

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

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

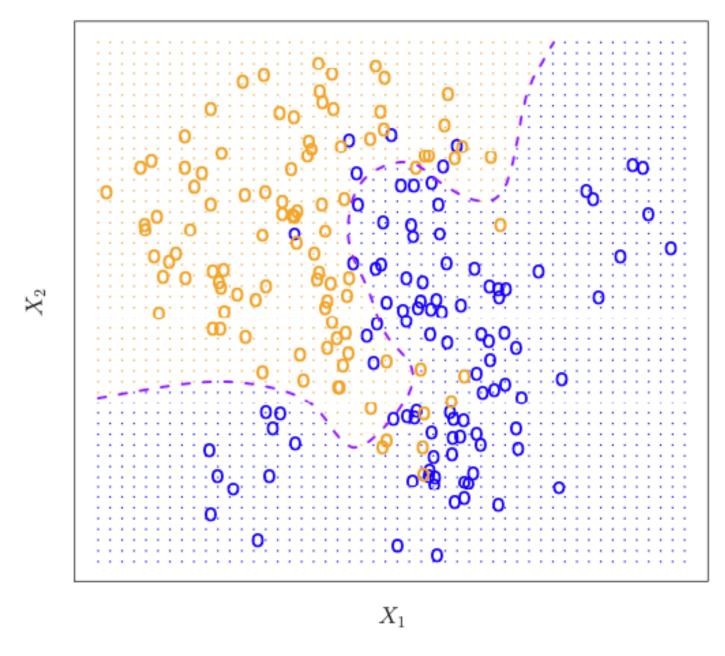
$$\mathbb{P}[Y=1 | X] = p(X)$$
, for some function  $p$ .

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

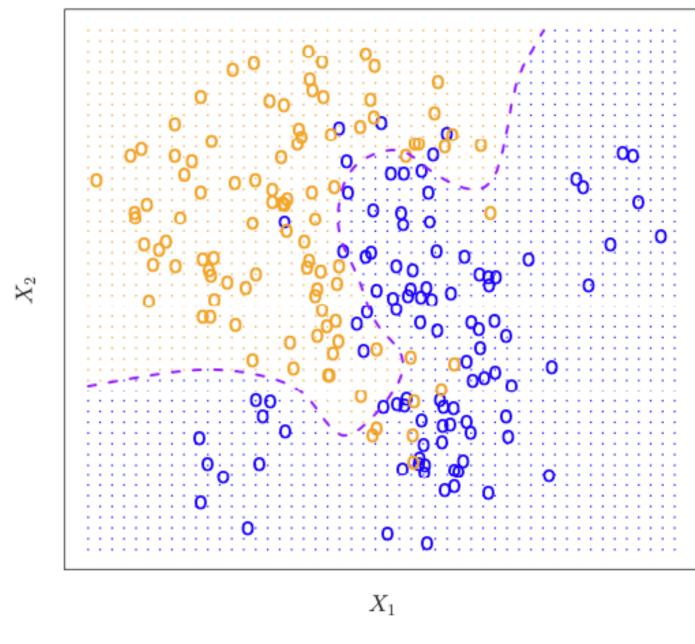
$$\hat{f}^{\text{Bayes}}(X) = \begin{cases} 1, & \text{if } p(X) \ge 0.5; \\ 0 & \text{if } p(X) < 0.5. \end{cases}$$

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

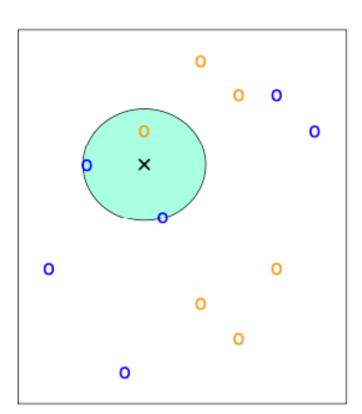
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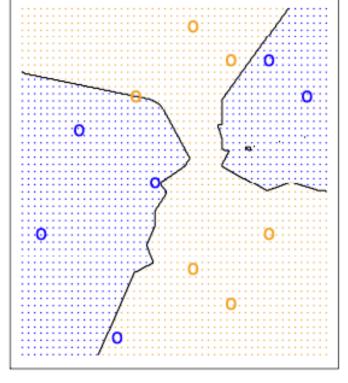


Simulated binary classification data. Bayes classifier in purple.

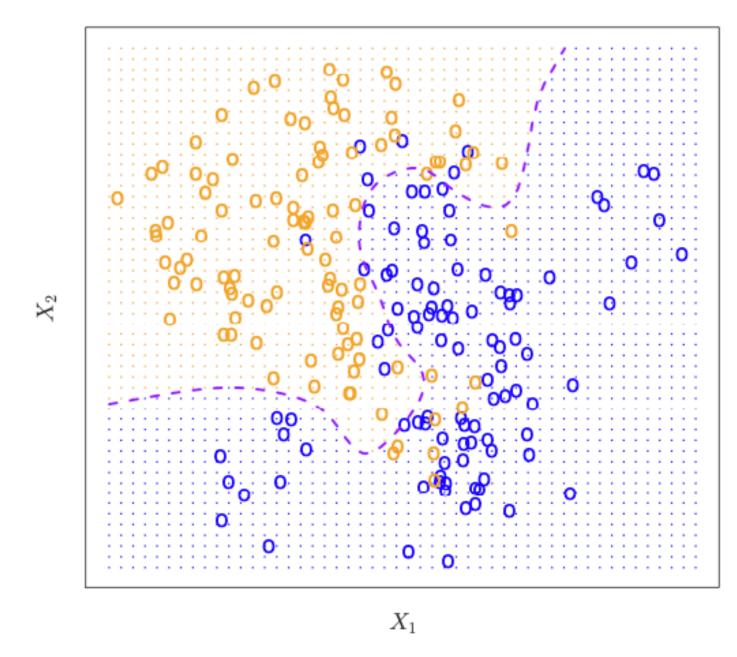


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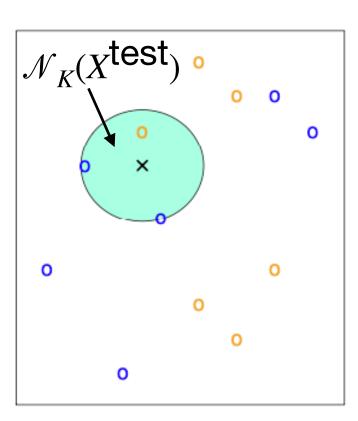


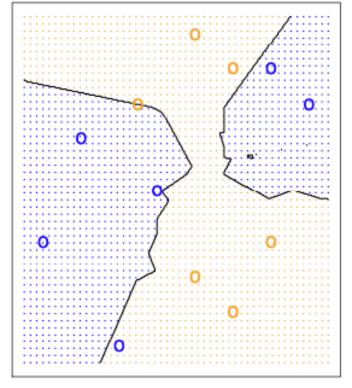


KNN illustration: Classify a test point based on majority vote among 3 nearest neighbors.



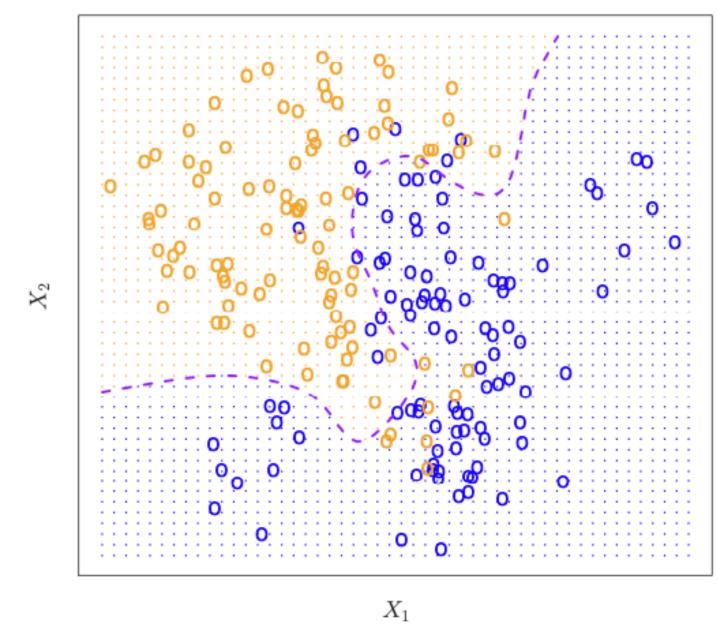
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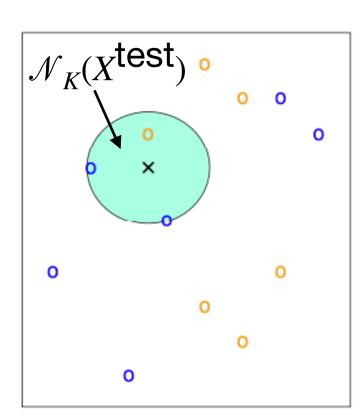


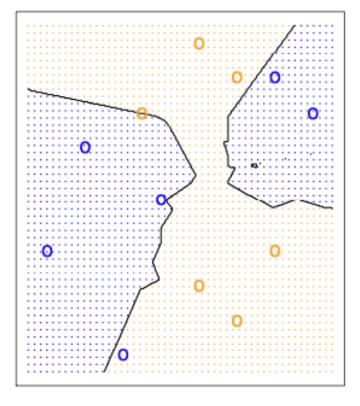
KNN illustration: Classify a test point based on majority vote among 3 nearest neighbors.

$$\widehat{p}(X^{\mathsf{test}}) = \frac{1}{K} \sum_{i \in \mathcal{N}_K} I(Y_i^{\mathsf{train}} = 1).$$



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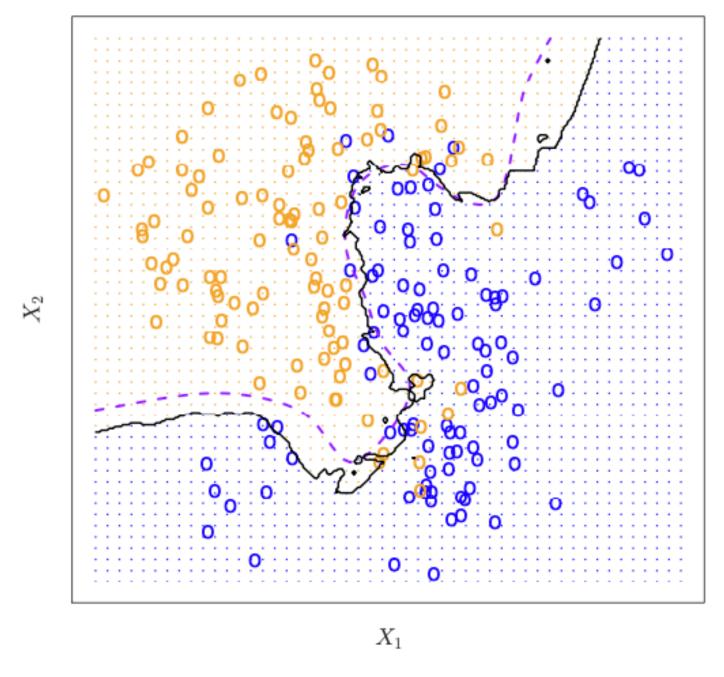




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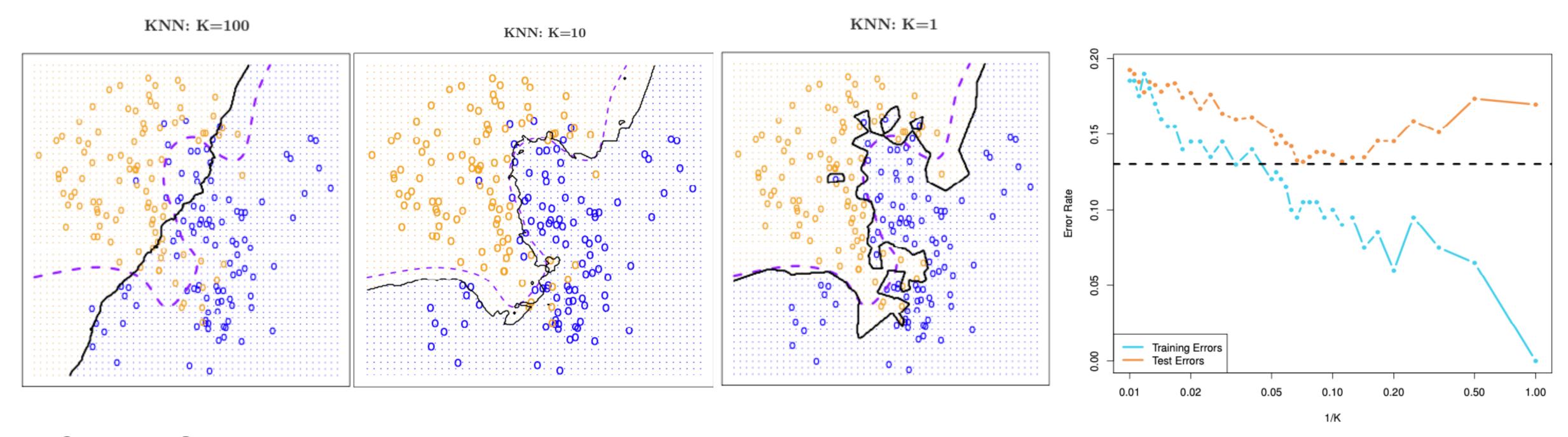
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Applying KNN with K = 10 to simulated data.

## Model complexity and misclassification error



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).

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• Bias:  $\mathbb{E}[\hat{p}(X)] - p(X)$ 

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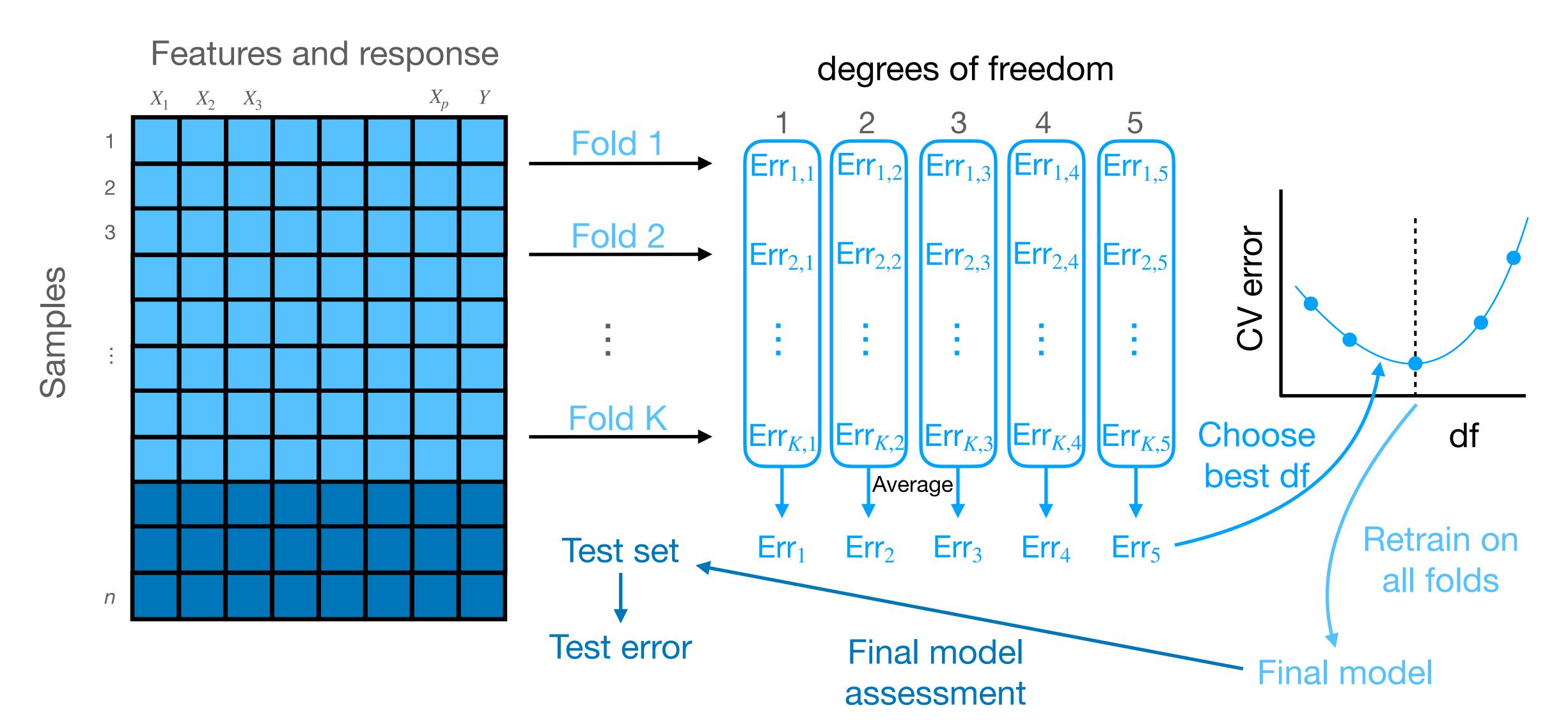
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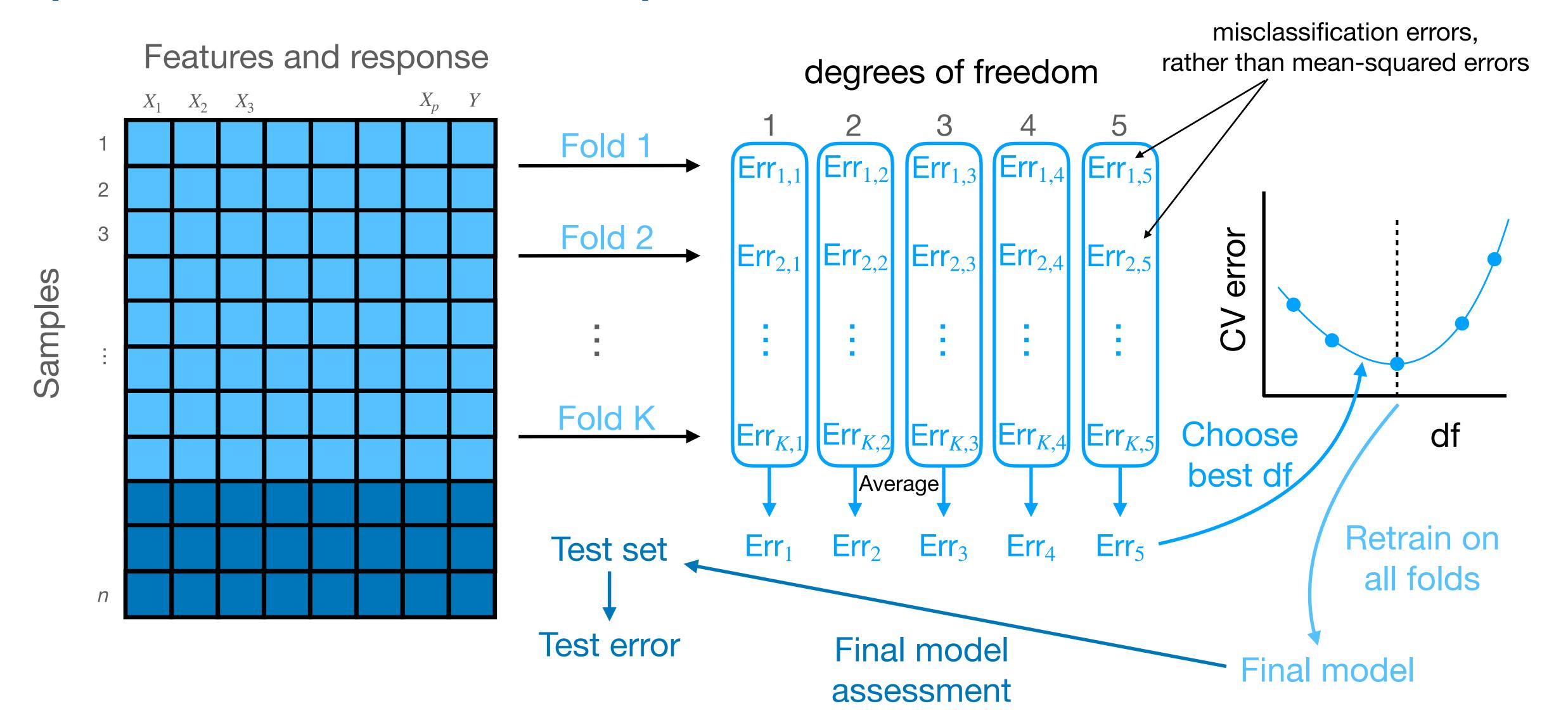
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  - Variance: Prediction varies with training set, to the extent  $\hat{p}$  fluctuates above or below 0.5
    - Irreducible error (AKA Bayes error): Error incurred by Bayes classifier because  $0 < \mathbb{P}[Y = 1 | X] < 1$ .

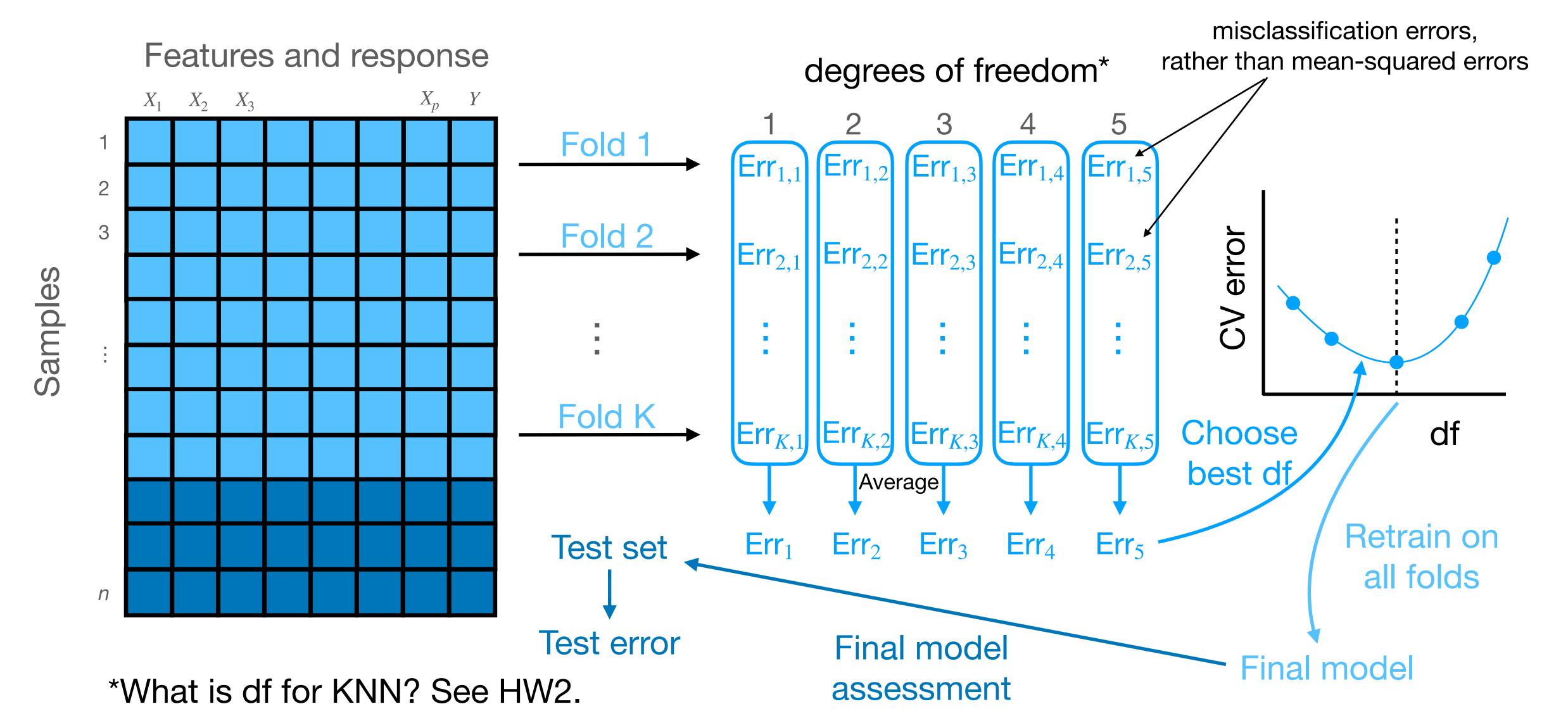
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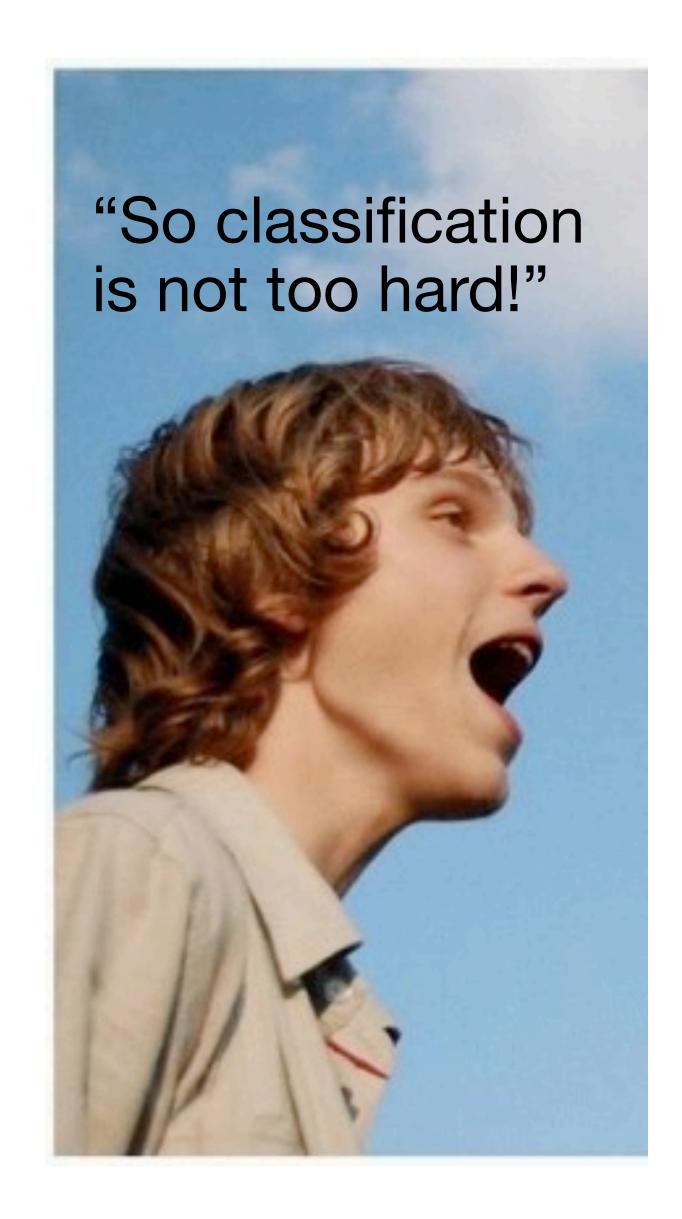


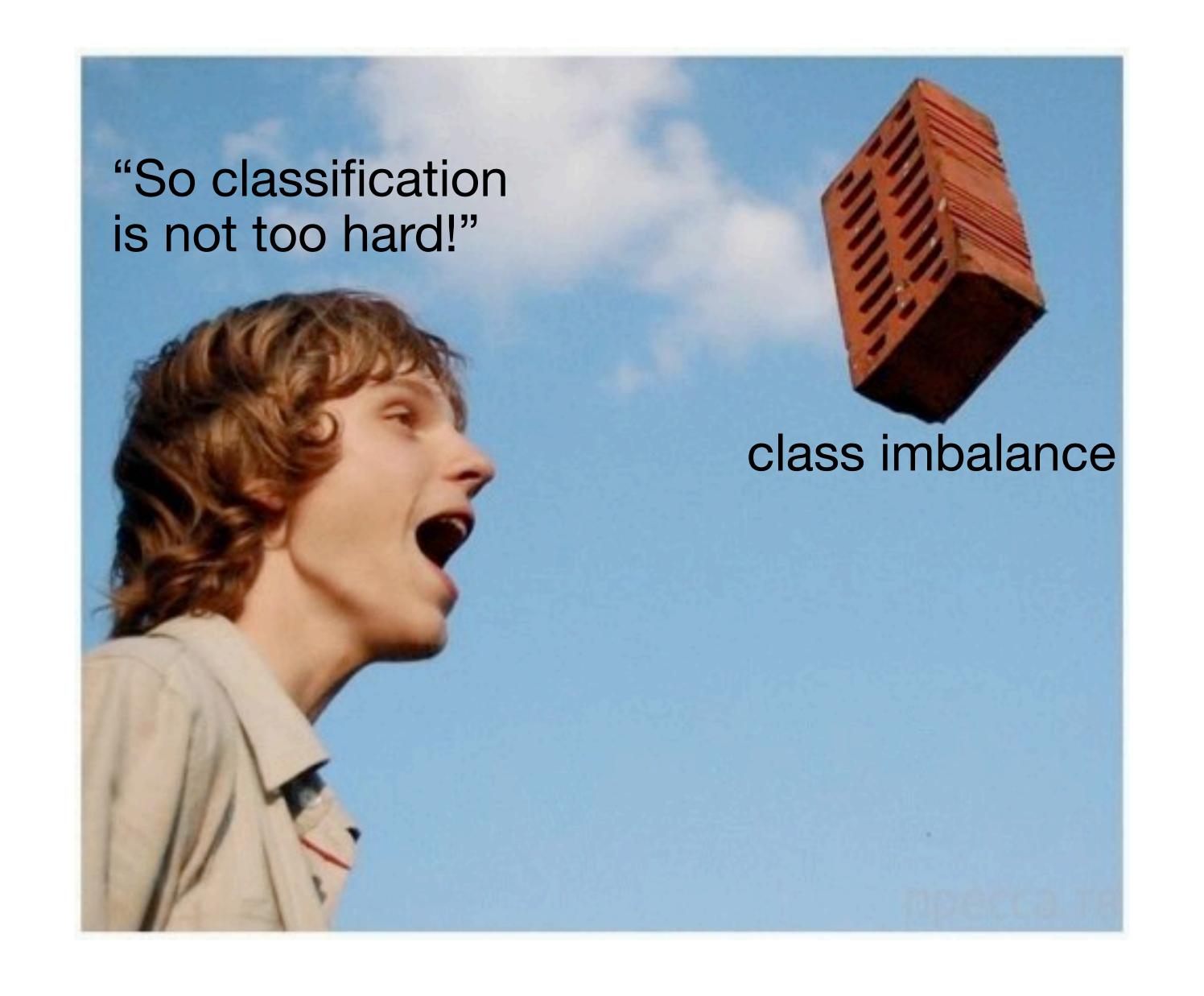
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Cross-validation based on misclassification error leads to overly simple models that ignore the minority class.

## Binary classification terminology

```
Positive: Y = 1 (e.g. COVID positive)
```

Negative: Y = 0 (e.g. COVID negative)

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Actually Positive Actually Negative

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(F.g. Sick person

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False Positive (FP)

(E.g. Healthy person testing positive)

False negative (FN)

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True Negative (TN)

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Negative: Y = 0 (e.g. COVID negative)

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#### Weighted misclassification error:

$$\frac{1}{N} \sum_{i=1}^{N} w_i \cdot I(\hat{Y}_i^{\text{test}} \neq Y_i^{\text{test}}), \quad \text{where} \quad w_i = \begin{cases} C_{\text{FP}} & \text{if } Y_i^{\text{test}} = 0 \\ C_{\text{FN}} & \text{if } Y_i^{\text{test}} = 1 \end{cases}.$$

## Thinking about misclassification costs

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 $w_i$  are called observation weights; integer weights like replicating observations.

Many machine learning algorithms accommodate observation weights, i.e. seek to optimize the weighted misclassification error.

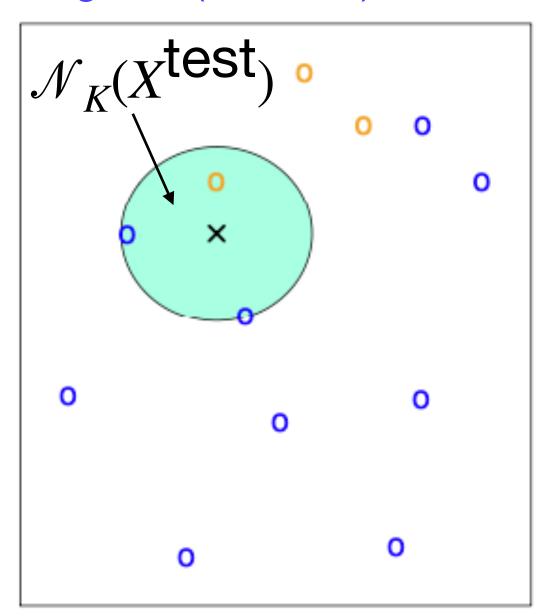
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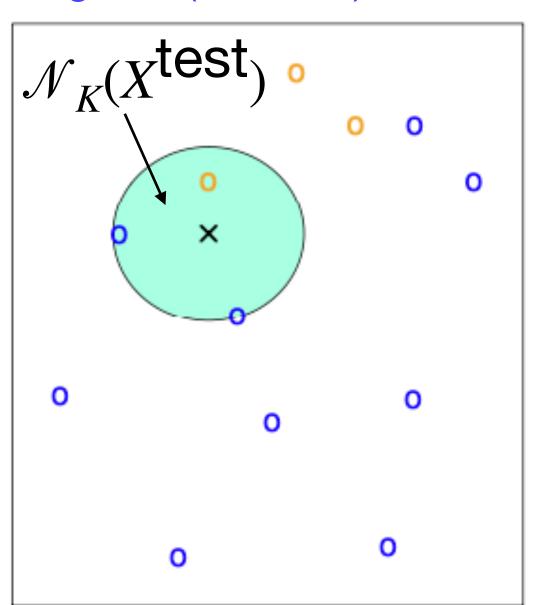
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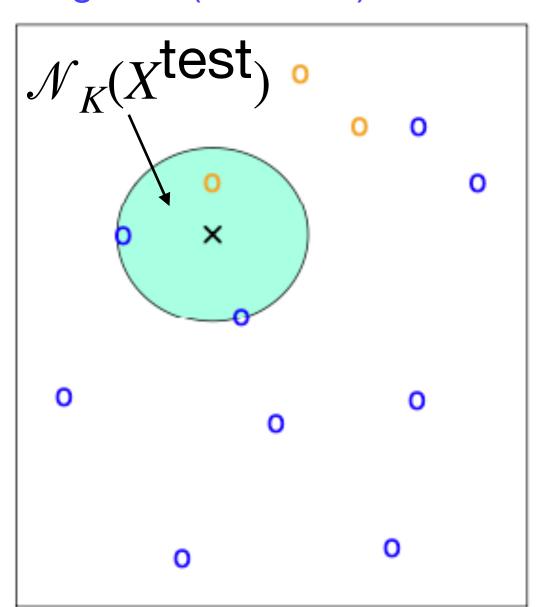
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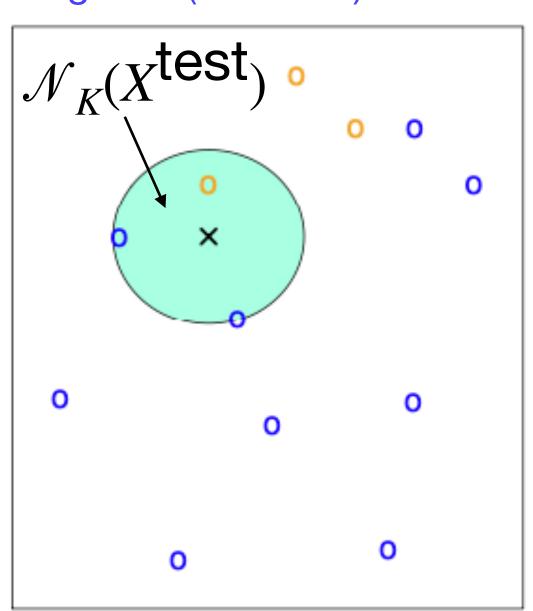
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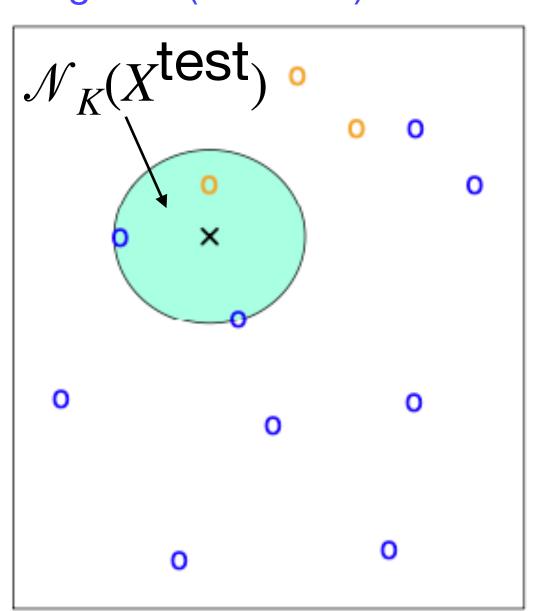
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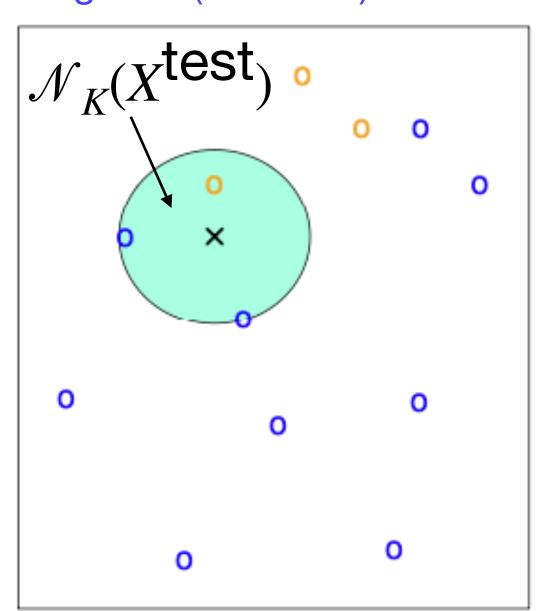
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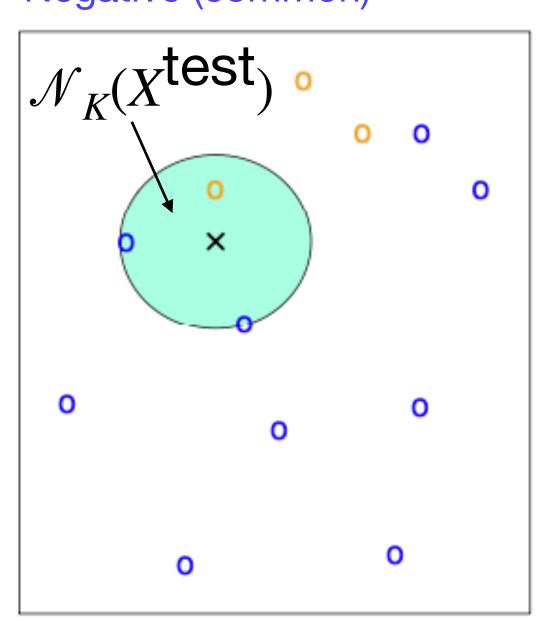
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Note: Only relative values of weights matter, e.g. only  $w_{\rm yellow}/w_{\rm blue}$  matters.

#### Cross-validation with imbalanced classes

- Split the data into folds after stratifying by the response class.
- Use weighted misclassification error when assessing models on in-fold data.

# Evaluating classification errors on a test set

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Another way of assessing classification performance—without quantifying costs—is the confusion matrix and associated metrics (e.g. false positive rate).

#### Confusion matrix

	<b>Actually Positive</b>	<b>Actually Negative</b>
Predicted Positive	10 True Positives (TP) (E.g. Sick people testing positive)	20 False Positives (FP) (E.g. Healthy people testing positive)
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Metrics based on confusion matrix

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True positive rate (TPR) 
$$=\frac{TP}{P}=\frac{10}{50}$$

F-score = 
$$\left(\frac{1}{2}\left(\frac{1}{\text{TPR}} + \frac{1}{\text{TNR}}\right)\right)^{-1} = 0.3$$

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- Performance metrics for classifiers include the weighted misclassification error and confusion matrix based metrics like false positive and false negative rates.