K-Nearest Neighbors and Decision Trees

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Introduction

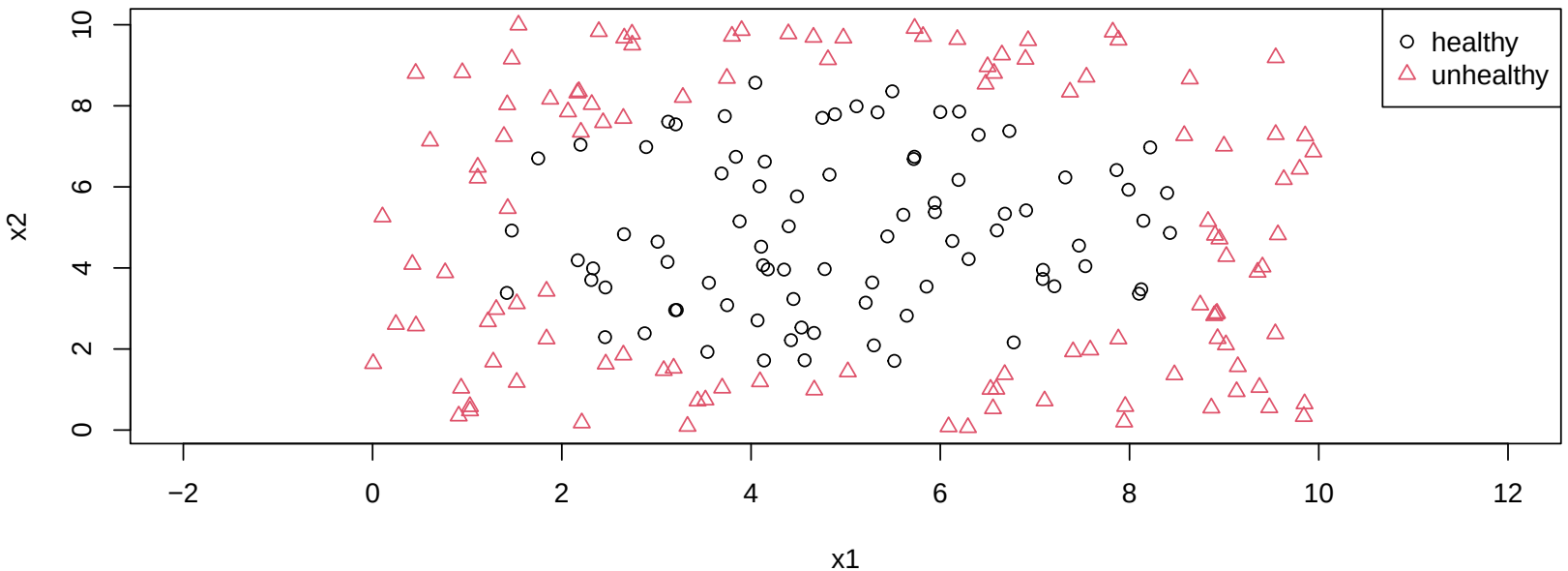
Last time we introduced:

- The general framework for classification and regression tasks: outcome $= f(X) +$ noise
- Reducible vs. irreducible error
- Training vs. testing
- Bias-variance trade off

Today we'll address the question of "how do we actually estimate $f(X)$?" by studying two methods, K-nearest neighbors (KNN) and decision trees, focusing on how each algorithm balances flexibility and generalization

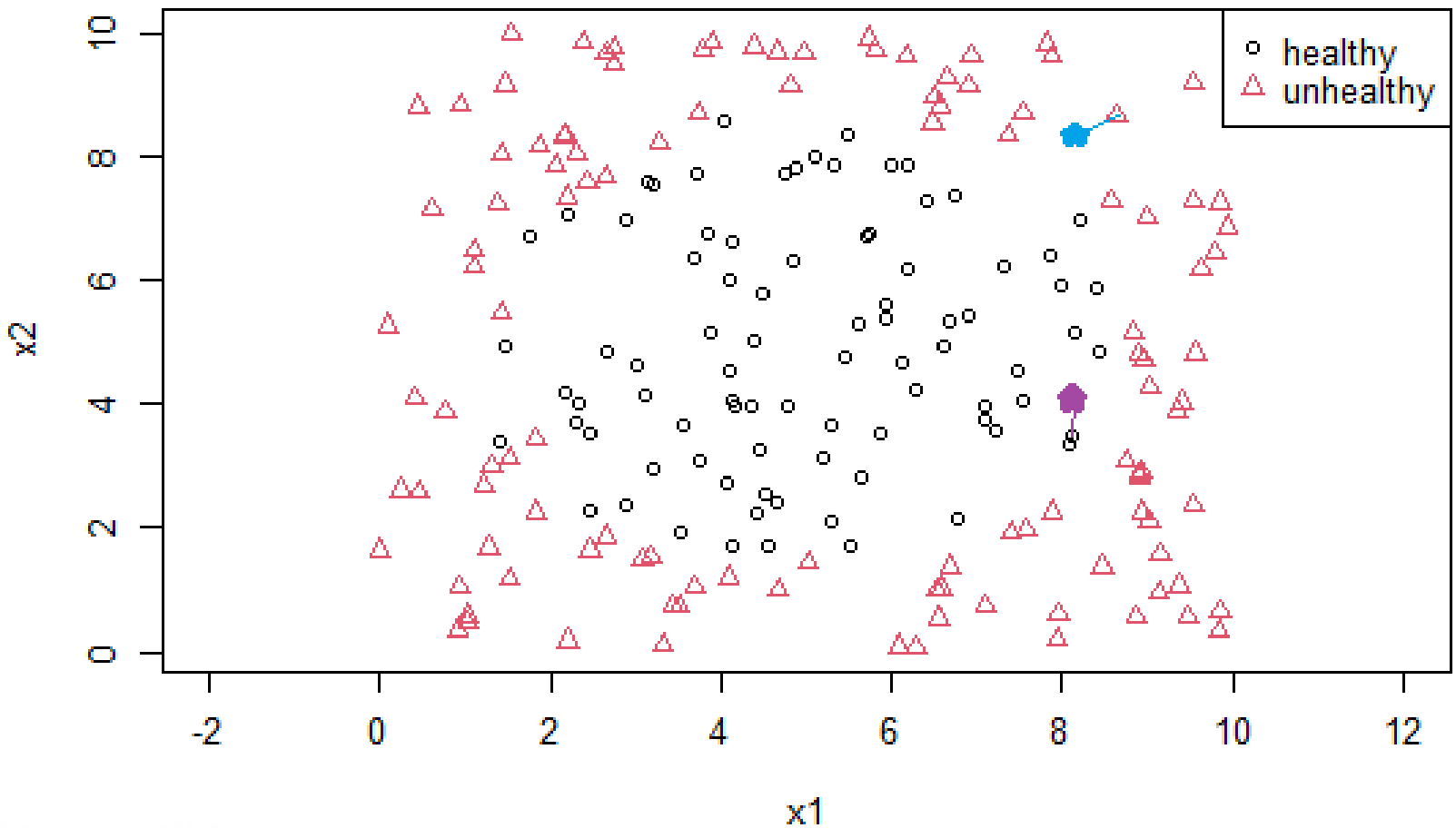
Introduction

We'll begin with the toy data example from last time:



K-Nearest Neighbors

A simple rule is to classify each new data-point using its *nearest neighbor*, or the observation closest to its (x_1, x_2) coordinates:



K-Nearest Neighbors

To implement this approach, we need a method of identifying neighbors.

$$d_{a,b} = \left(\sum_{j=1}^{m} |x_{a,j} - x_{b,j}|^p \right)^{1/p}$$

- Minkowski distance, $d_{a,b}$, measures the distance between data-points a and b
  - The formula sums *pairwise coordinate differences* across m dimensions (features)
  - The power parameter, p, is chosen by the analyst, with $p = 2$ (euclidean distance) being a popular choice

K-Nearest Neighbors

Once neighbors are identified they must be used to make predictions. There are two common ways to do this:

1. **Uniform weighting** - all neighbors contribute equally, so if 4 of 5 neighbors of the new data-point are "healthy" the predicted probability of "healthy" is 80%
2. **Distance weighting** - neighbors are weighted by the inverse of their distance, allowing closer data-points to contribute more to the prediction (ie: a weighted proportion)

Note: when the outcome is numeric *KNN regression* averages the target variable among neighbors (rather than taking proportions)

Hyperparameters

KNN will not achieve state-of-the-art performance in most applications, but it is an interesting algorithm to study because it illustrates two important ideas in machine learning:

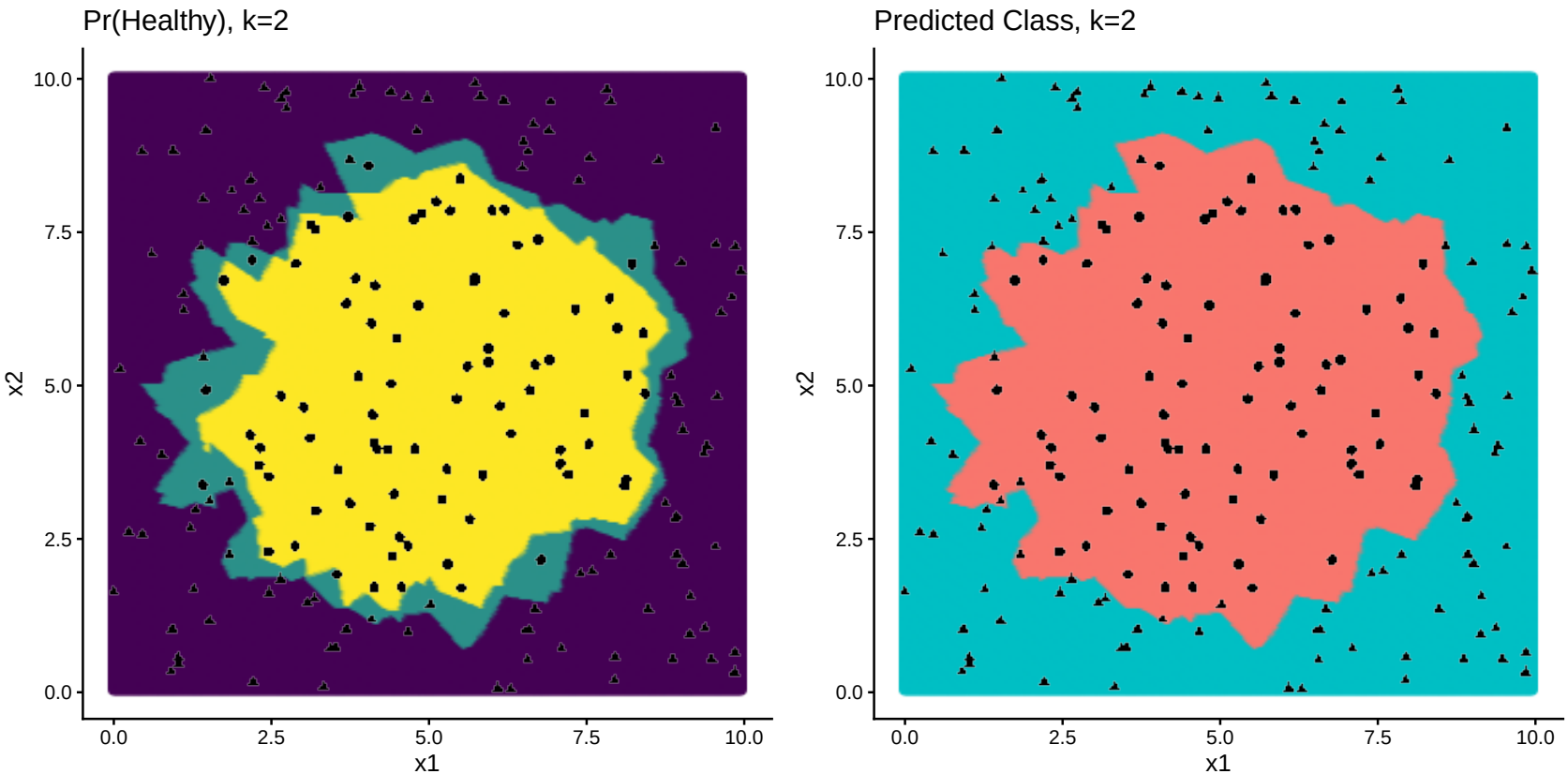
1. **hyperparameters** - configurable values that must be set before the algorithm can be used
2. **pre-processing** - steps that must be applied to the data in order for the algorithm to be effective

Hyperparameters

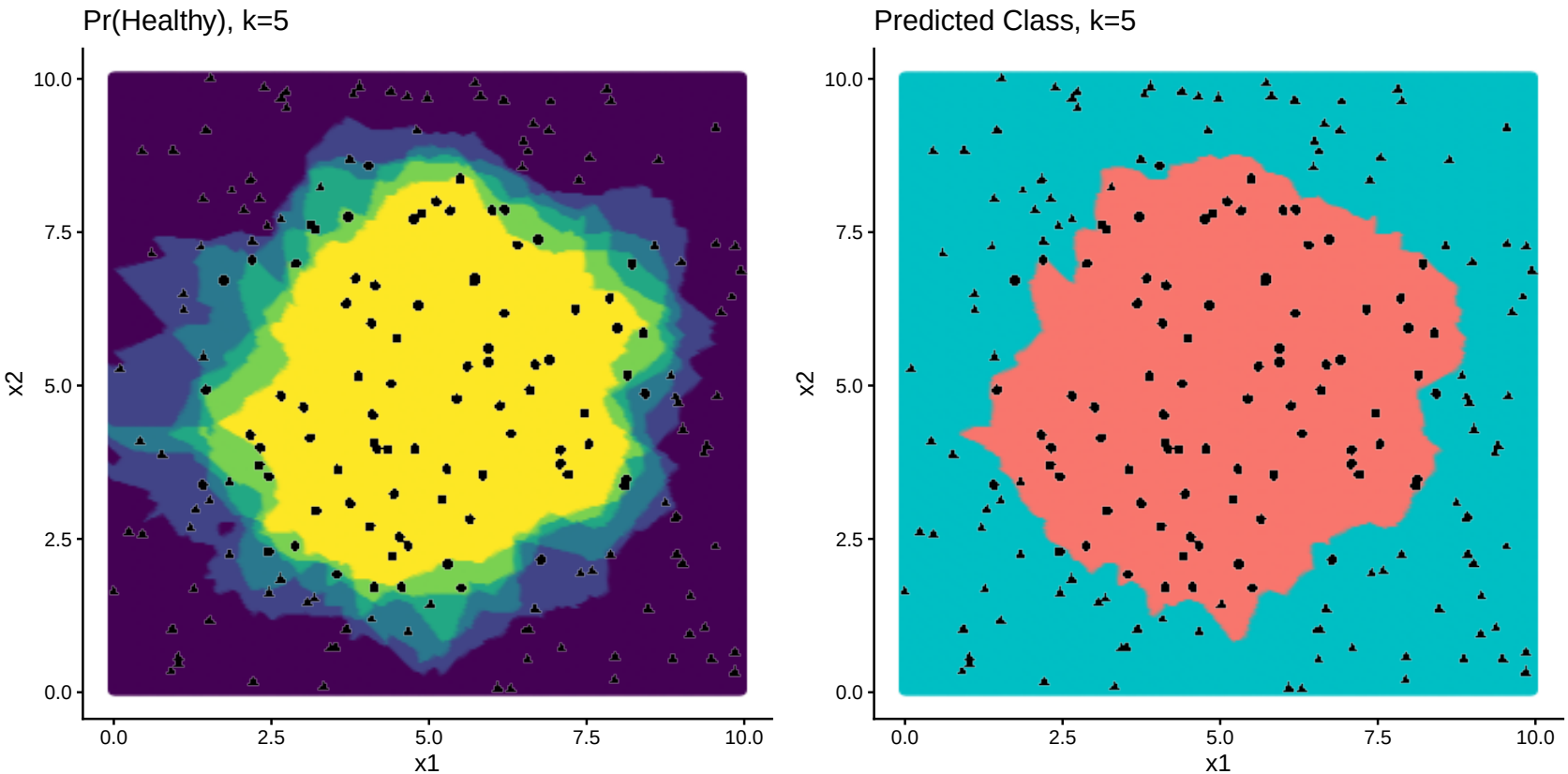
We will discuss pre-processing in our next lecture. For now we'll focus on hyperparameters, which include (for KNN):

- k or `n_neighbors` - the number of neighbors that contribute to predictions
- p - the power parameter used in Minkowski distance calculations
- `weights` - whether *uniform* or *distance* weighting is used

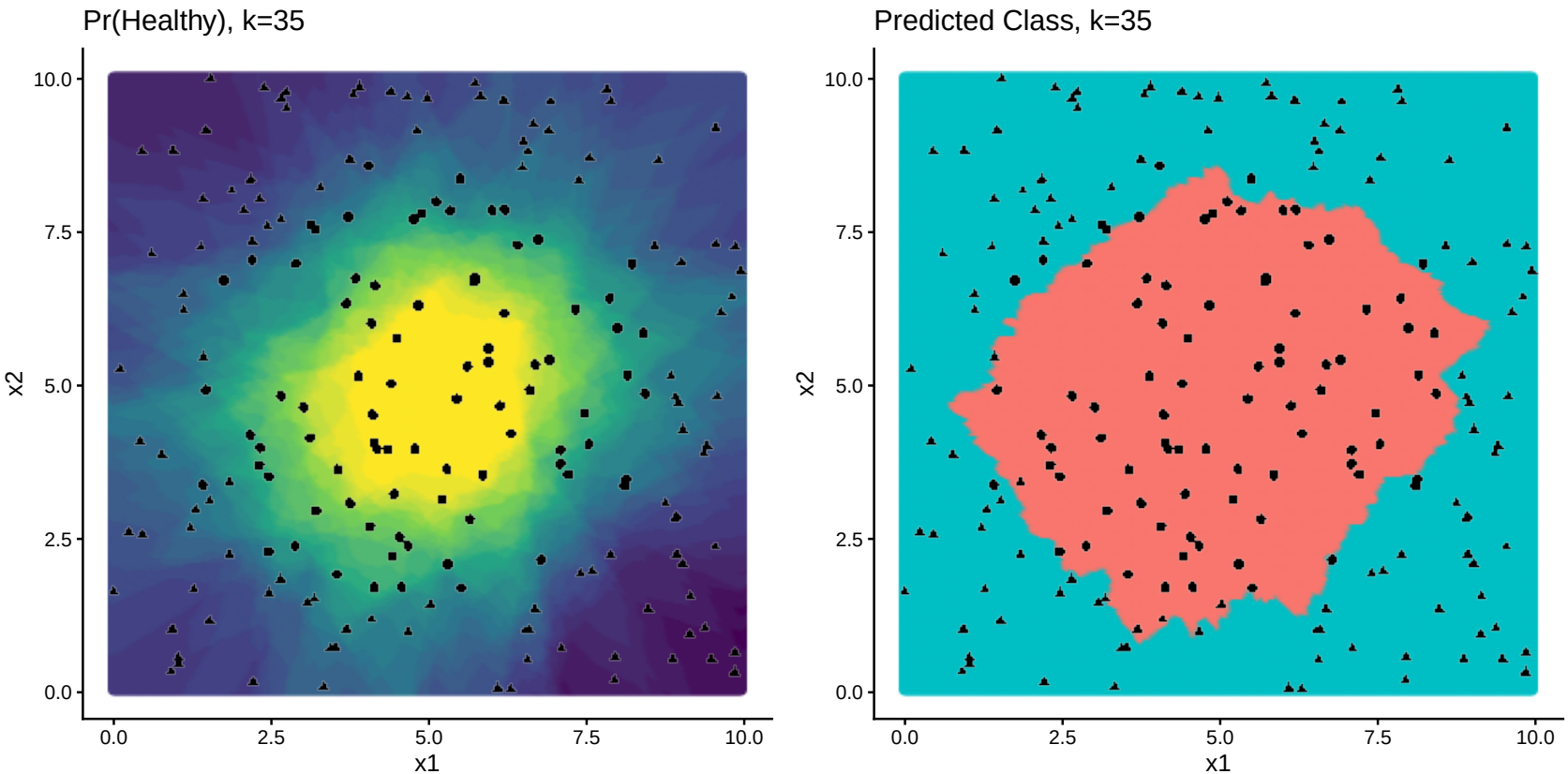
K-Nearest Neighbors Prediction Surface (k=2)



K-Nearest Neighbors Prediction Surface (k=5)



K-Nearest Neighbors Prediction Surface (k=35)



KNN and the Bias-Variance Trade-off

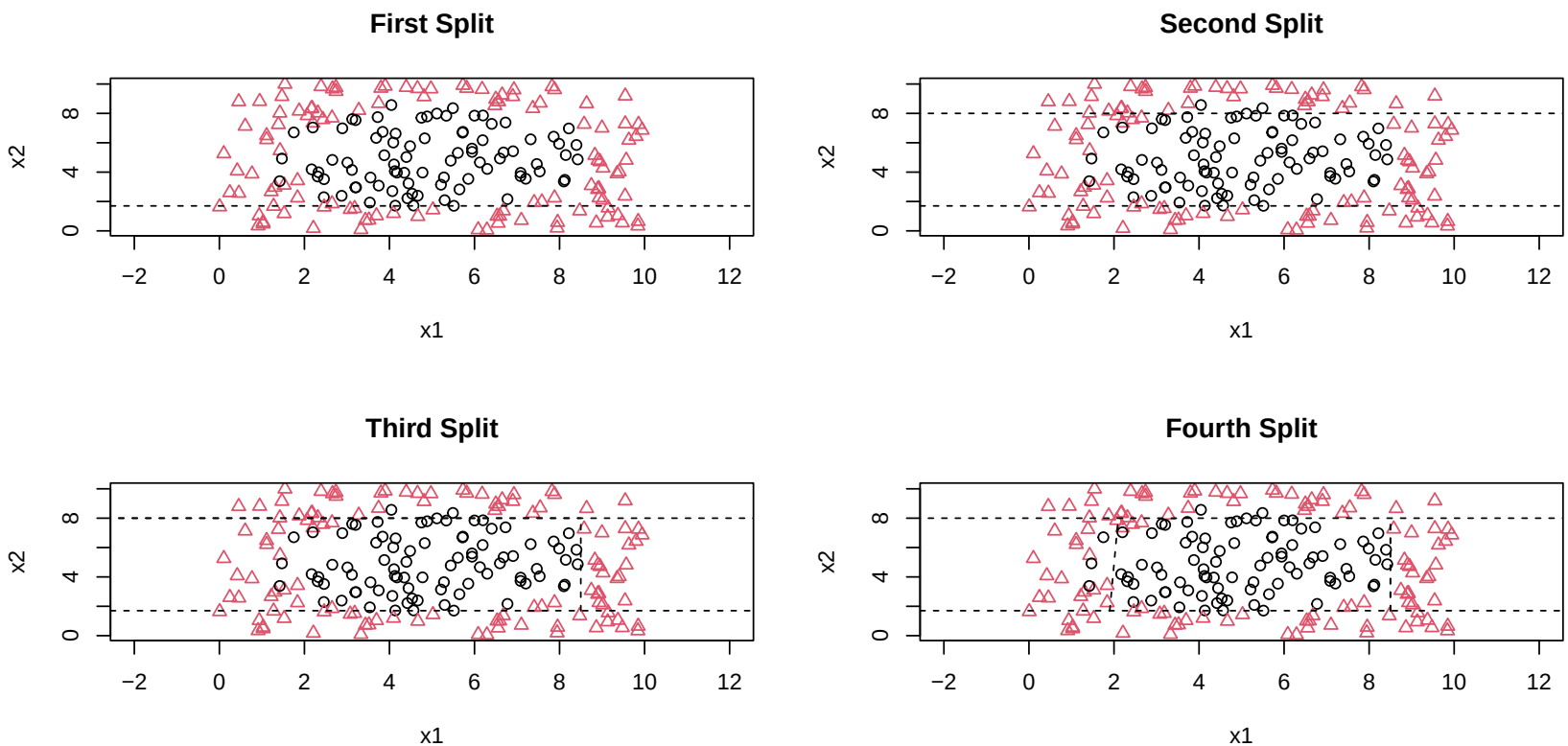
- Smaller values of k lead to more flexible models with *low bias* but *high variance*
- Conversely, larger values of k lead to less flexible models with smoother decision boundaries that are *higher in bias* but *lower in variance*
- Distance weighting gives greater influence to nearby observations. How might this affect the bias-variance trade-off?

Decision Trees

Decision trees are trained by *recursively partitioning* the p-dimensional feature space (defined by the explanatory variables) until an acceptable level of homogeneity or "purity" is achieved within each partition:

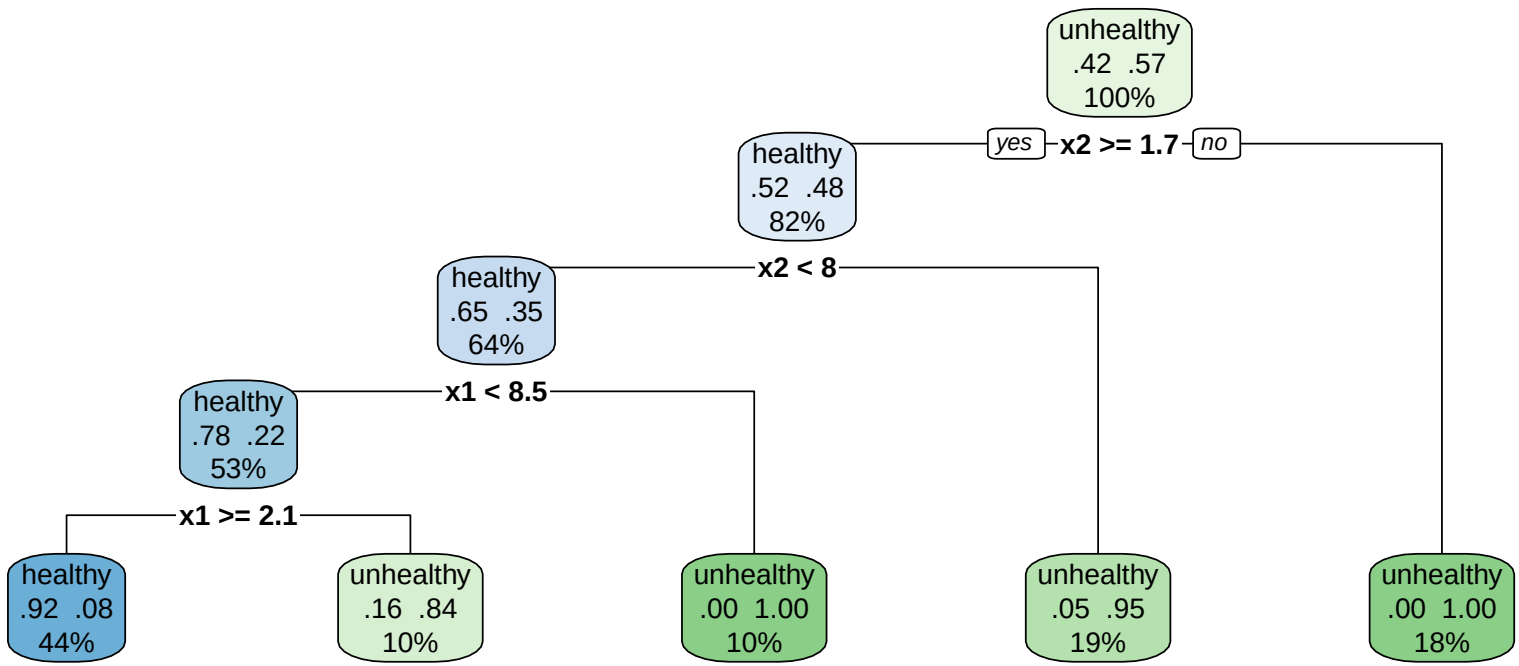
1) Starting with a "parent" node, search for a splitting rule that maximizes the *homogeneity* or *purity* of the "child" nodes
2) Next, considering each node that hasn't yet been split, find another splitting rule that maximizes *purity*
3) Repeat until a stopping criterion has been reached

Decision Trees



Decision Trees

We can express these recursive splits using a tree structure:



Determining the Splits

- The decision tree algorithm considers all possible splits for every feature
  - Only split-points that coincide with observed values are checked, as anything in between won't change purity
- Classification trees most often use **Gini impurity**:

$$Gini = \sum_{j=1}^{k} p_j(1-p_j) = 1 - \sum_{j=1}^{k} p_j^2$$

- For binary classification, Gini impurity reduces to $p_1(1-p_1) + p_2(1-p_2)$
  - The split that yields the greatest improvement in Gini impurity is selected
- Regression trees assess purity using *squared error*, or $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$

Determining the Splits

In our example the initial node's purity was:

$$(0.42 \cdot (1 - 0.42) + 0.58 \cdot (1 - 0.58)) = 0.487$$

Determining the Splits

In our example the initial node's purity was:

$$(0.42 \cdot (1 - 0.42) + 0.58 \cdot (1 - 0.58)) = 0.487$$

The first split created child nodes yielding the following purity:

$$0.82 \cdot (0.52 \cdot (1-0.52) + 0.48 \cdot (1-0.48)) + 0.18 \cdot (0 \cdot (1-0) + 1 \cdot (1-1)) = 0.409$$

Thus, the *Gini gain* from this split is 0.078

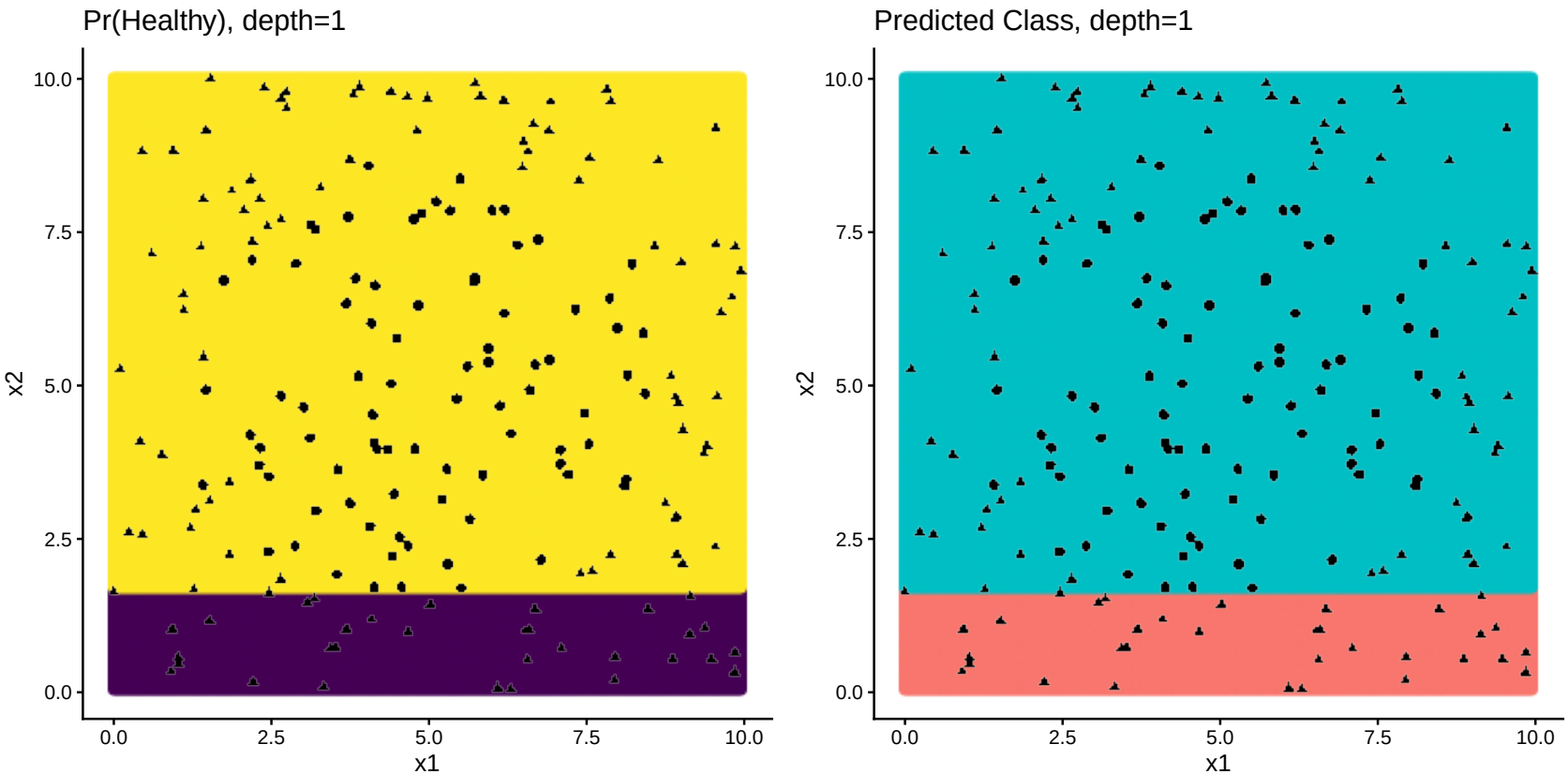
Stopping the Algorithm

Decision trees can be grown until every terminal node is perfectly pure; however, such trees will be very overfit to the training data. We can exploit the bias-variance trade-off in a fitted tree in the following ways:

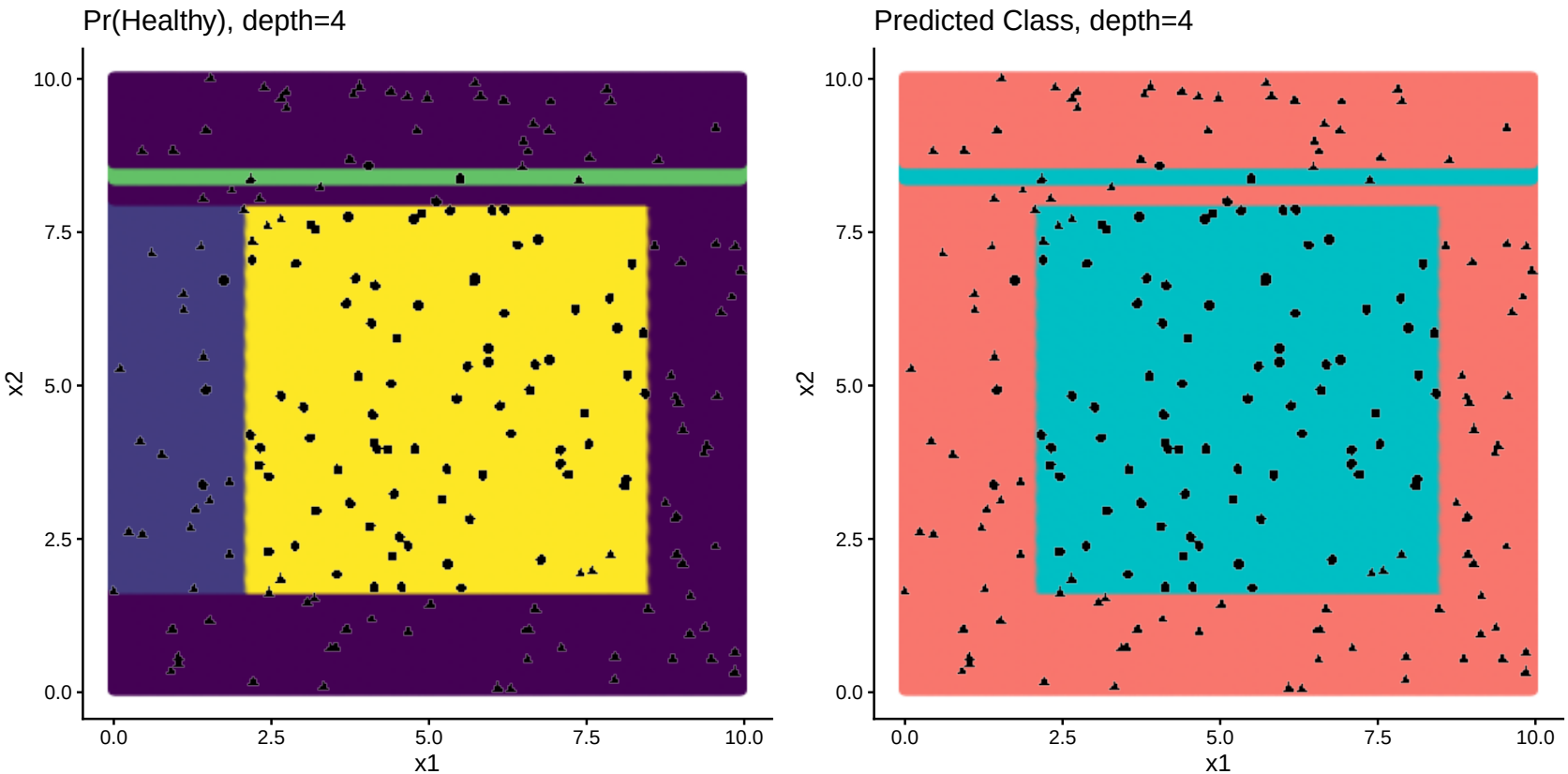
1. Restricting the maximum depth of the tree (ie: the number of sequential rules)
2. Allowing only nodes of sufficient size to be eligible for splitting
3. Requiring a certain improvement in purity for a split to occur

Because all of these are related, it is generally sufficient to focus on maximum depth when tuning hyperparameters.

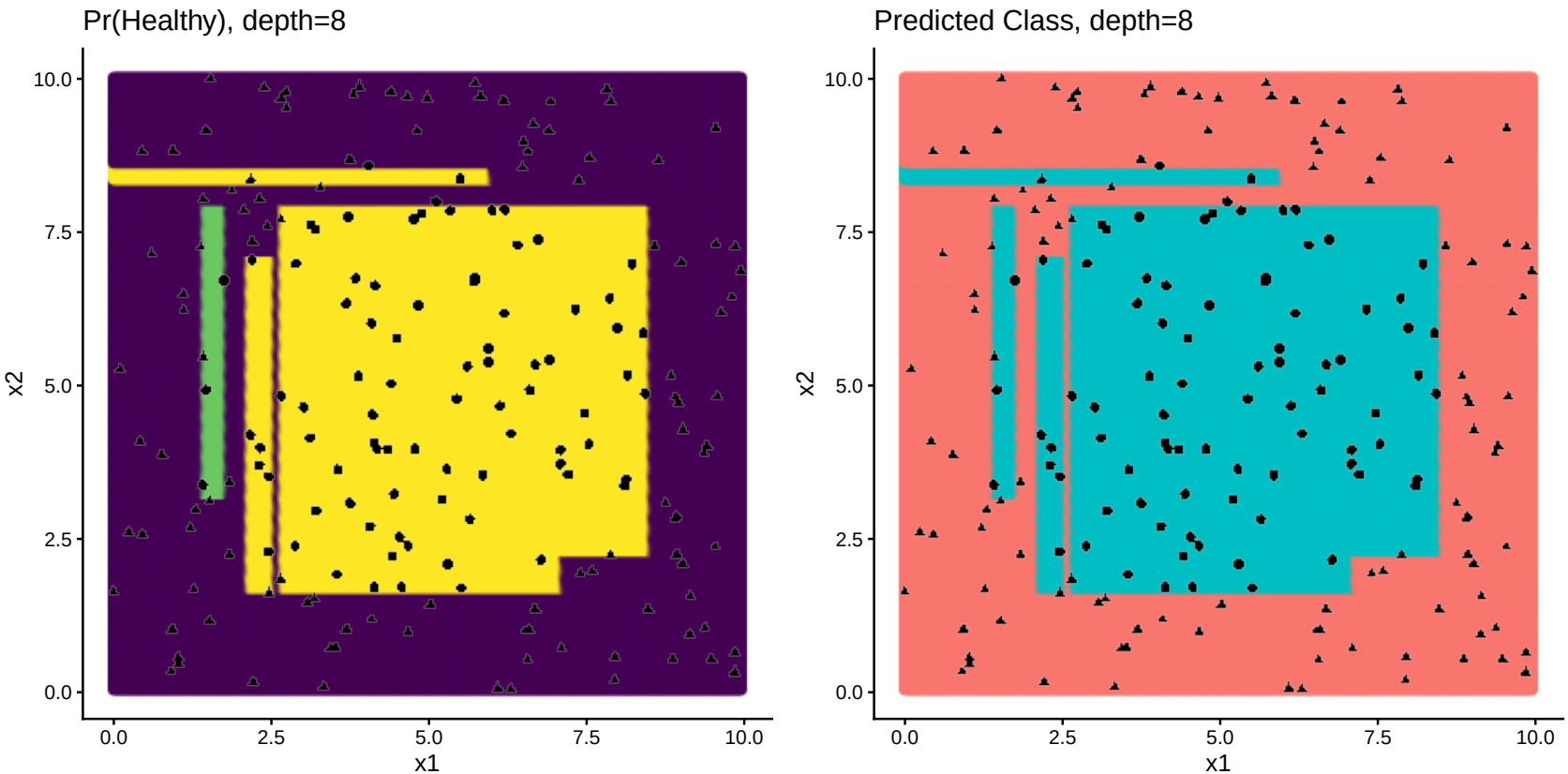
Decision Tree Prediction Surface (`max_depth = 1`)



Decision Tree Prediction Surface (`max_depth = 4`)



Decision Tree Prediction Surface (`max_depth = 8`)



A Few Comments

- KNN produces irregularly shaped decision boundaries that tend to be overly sensitive to the training data for small values of k
- Decision trees produce rectangular decision boundaries and can easily overfit the training data if their maximum depth isn't controlled
- Decision trees are robust to the measurement scale of the predictive features, while KNN is not
  - We will discuss re-scaling (and other data pre-processing steps) next time

Preparing for Quiz #1

The following topics from these slides might appear on our first quiz:

1. Basic steps and properties of the KNN algorithm
2. Basic steps and properties of the decision tree algorithm
3. How various hyperparameter choices in KNN and decision trees relate to the bias-variance trade off