

# Introduction to supervised machine learning, k-fold cross-validation, nearest neighbors, and linear models

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## Supervised machine learning

- ▶ Goal is to learn a function  $f(\mathbf{x}) = y$  where  $\mathbf{x}$  is an input/feature vector and  $y$  is an output/label.
- ▶  $\mathbf{x} =$ image of digit/clothing,  $y \in \{0, \dots, 9\}$  (ten classes).
- ▶  $\mathbf{x} =$ vector of word counts in email,  $y \in \{1, 0\}$  (spam or not).
- ▶  $\mathbf{x} =$ image of retina,  $y =$ risk score for heart disease.
- ▶ This week we will focus on a specific kind of supervised learning problem called binary classification, which means  $y \in \{1, 0\}$ .

## Learning algorithm

- ▶ We want a learning algorithm  $\text{LEARN}$  which inputs a training data set and outputs a prediction function  $f$ .
- ▶ In math a training data set with  $n$  observations and  $p$  features is a matrix  $\mathbf{X} \in \mathbb{R}^{n \times p}$  with a label vector  $\mathbf{y} \in \{0, 1\}^n$ .
- ▶ On computers it is a CSV file with  $n$  rows and  $p + 1$  columns.
- ▶ Want:  $\text{LEARN}(\mathbf{X}, \mathbf{y}) \rightarrow f$ .
- ▶ We will use three such data sets from Elements of Statistical Learning book by Hastie et al. (mixture slightly modified)

name	observations, $n$	inputs/features, $p$	outputs/labels
zip.test	images, 623	pixel intensities, 256	0/1 digits
spam	emails, 4601	word counts, 57	spam=1/not=0
mixture	people, 200	height/weight, 2	democratic/republican

<https://github.com/tdhock/cs570-spring-2022/tree/master/data>

<https://hastie.su.domains/ElemStatLearn/data.html>

## Mixture data table

```
##                 party height_in weight_lb
## 0    democratic   71.741421 149.565034
## 1    democratic   69.582283 149.275446
## 2    democratic   69.983547 149.961470
## 3    democratic   69.908764 150.021178
## 4    democratic   69.195491 150.111237
## ..
## ...
## 195   republican   69.472078 151.537588
## 196   republican   71.140501 149.409036
## 197   republican   70.517269 150.236183
## 198   republican   69.223459 151.486248
## 199   republican   69.019082 149.795387
##
## [200 rows x 3 columns]
```

## Spam data table

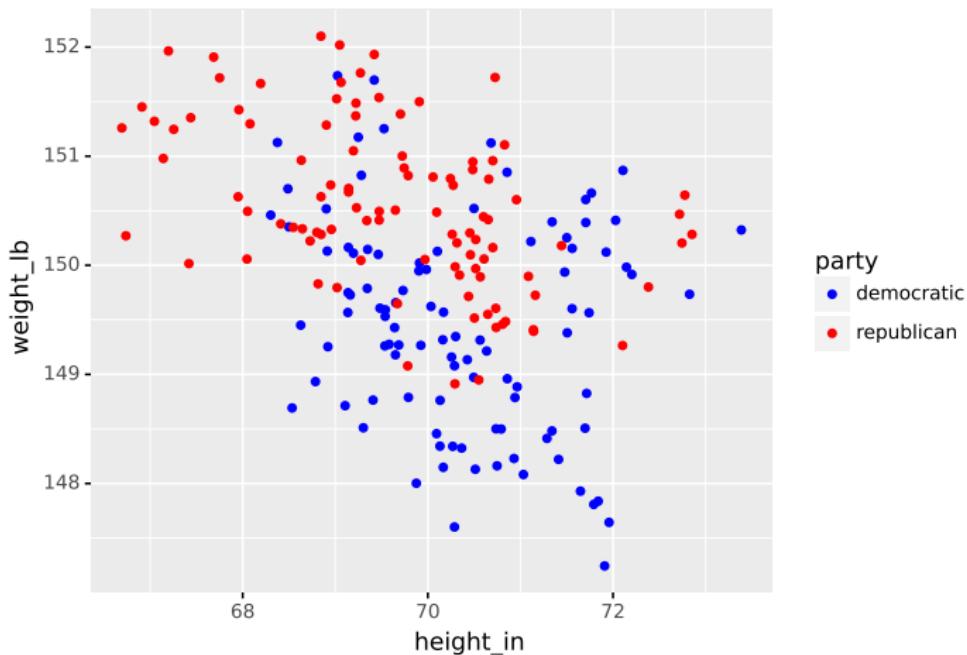
```
##          0      1      2     ...     55     56     57
## 0    0.00  0.64  0.64   ...    61   278     1
## 1    0.21  0.28  0.50   ...   101  1028     1
## 2    0.06  0.00  0.71   ...   485 2259     1
## 3    0.00  0.00  0.00   ...    40   191     1
## 4    0.00  0.00  0.00   ...    40   191     1
## ...
## 4596  0.31  0.00  0.62   ...     3    88     0
## 4597  0.00  0.00  0.00   ...     4    14     0
## 4598  0.30  0.00  0.30   ...     6   118     0
## 4599  0.96  0.00  0.00   ...     5    78     0
## 4600  0.00  0.00  0.65   ...     5    40     0
##
## [4601 rows x 58 columns]
```

## Zip.test data table

```
##          0      1      2      ...     254     255     256
## 0      9 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 1      6 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 2      3 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 3      6 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 4      6 -1.0 -1.0 ... -1.0 -1.0 -1.0
## ...
## 2002    3 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 2003    9 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 2004    4 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 2005    0 -1.0 -1.0 ... -1.0 -1.0 -1.0
## 2006    1 -1.0 -1.0 ... -1.0 -1.0 -1.0
##
## [2007 rows x 257 columns]
```

## Visualize mixture data set

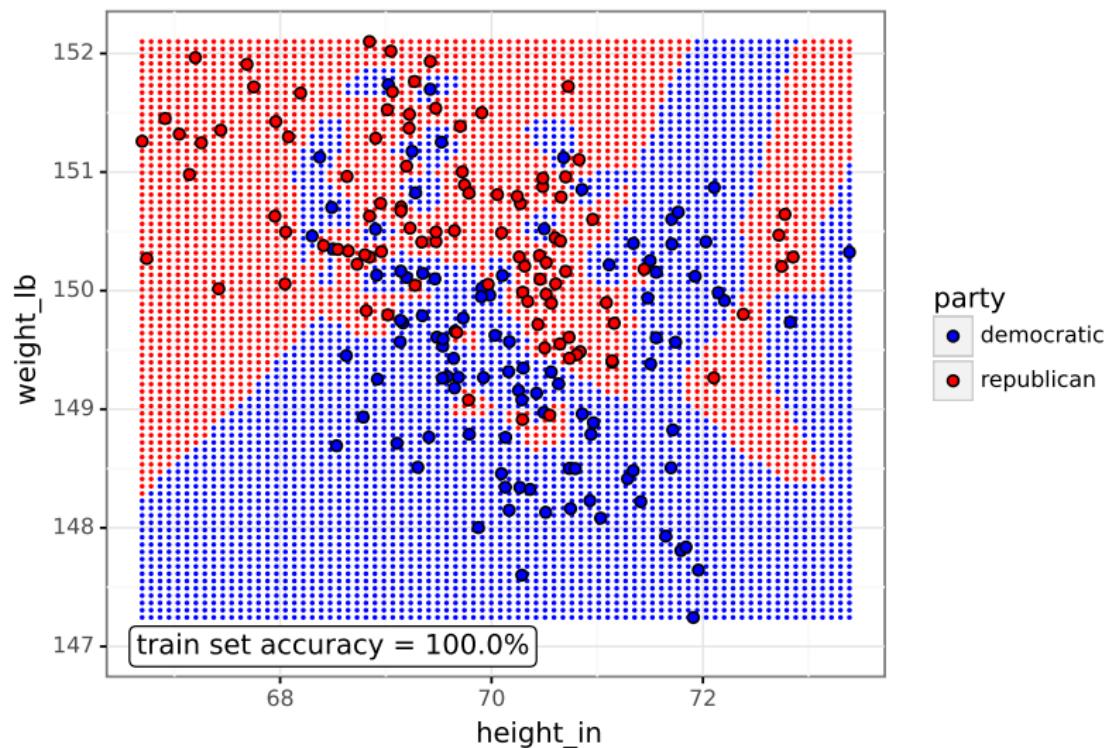
- ▶ Each axis represents one column of the  $\mathbf{X}$  matrix.
- ▶ Each point represents one row of the  $\mathbf{X}$  matrix.
- ▶ Color represents class label  $\mathbf{y}$ .



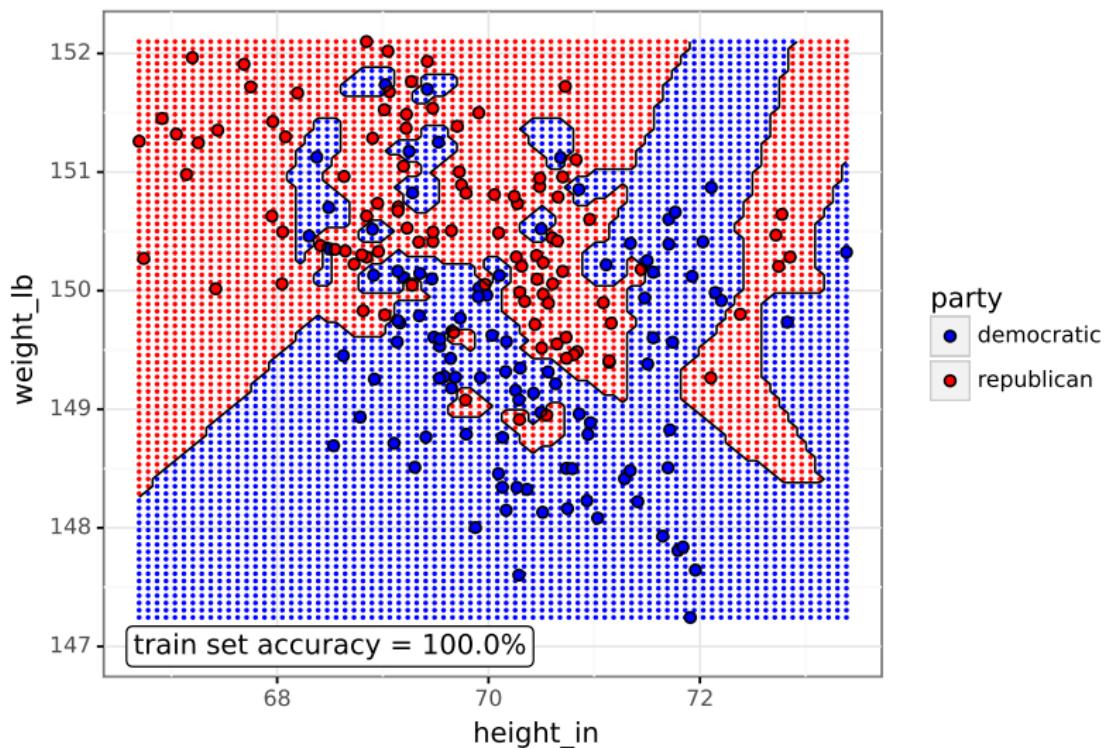
## A basic machine learning algorithm

- ▶ Goal of supervised learning is to learn a function which predicts the label for new inputs  $x \in \mathbb{R}^2$ .
- ▶ K-Nearest neighbors: a simple non-linear algorithm.
- ▶ For any new data point, predict the average label of the K nearest neighbors.

# Visualize predictions of 1-nearest neighbor algorithm



Also plot decision boundary in black

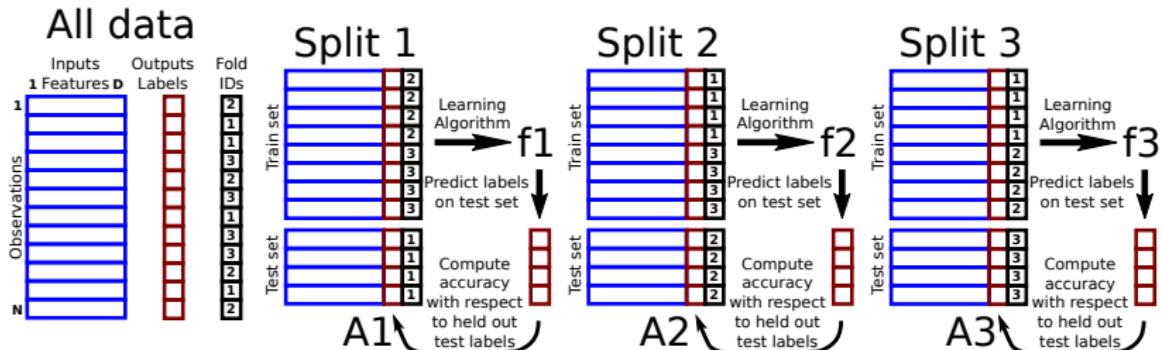


## Is it good to have 100% accuracy on train data?

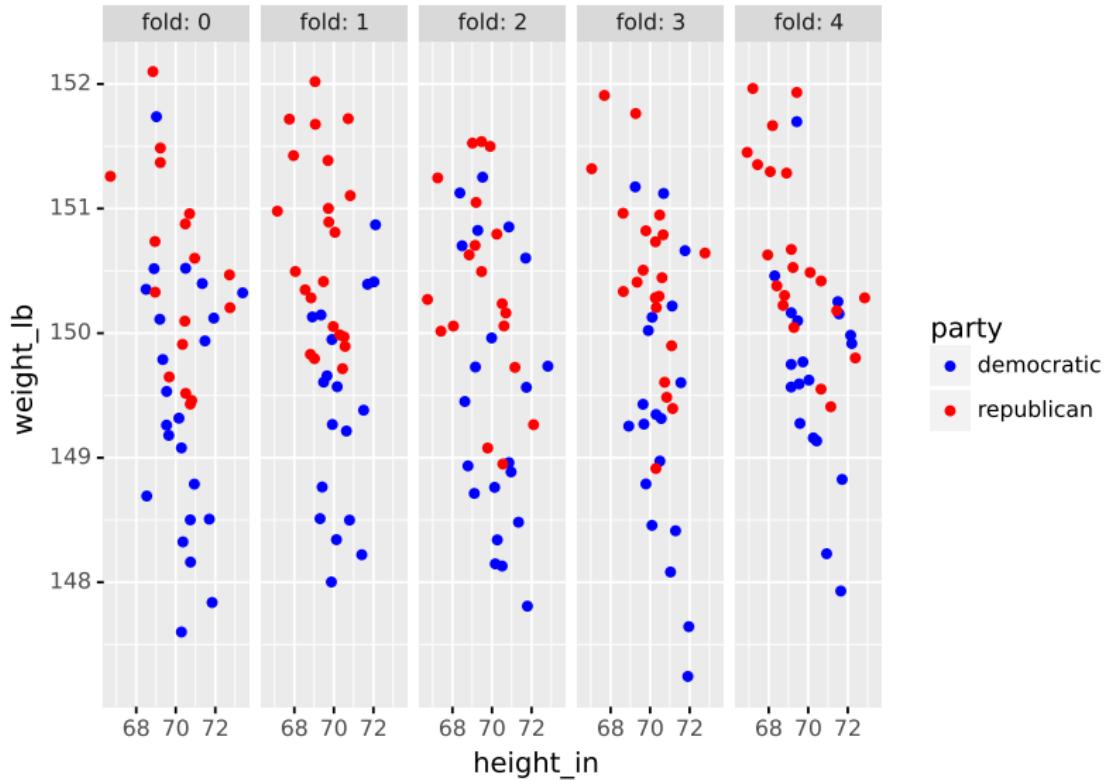
- ▶ Remember: goal is function  $f$  with accurate predictions on new inputs.
- ▶ What is a new input?
- ▶ We must assume that new/test inputs are similar to old/train inputs.
- ▶ In the statistical literature this is the iid (independent and identically distributed) assumption.
- ▶ We can therefore split the full data set into train/test sets.
- ▶ Train set is used to learn the prediction function  $f$ .
- ▶ Test set (simulated new inputs) is used to evaluate the accuracy of the function  $f$  (but can not be used to learn function  $f$ ).

# K-fold cross-validation for splitting data

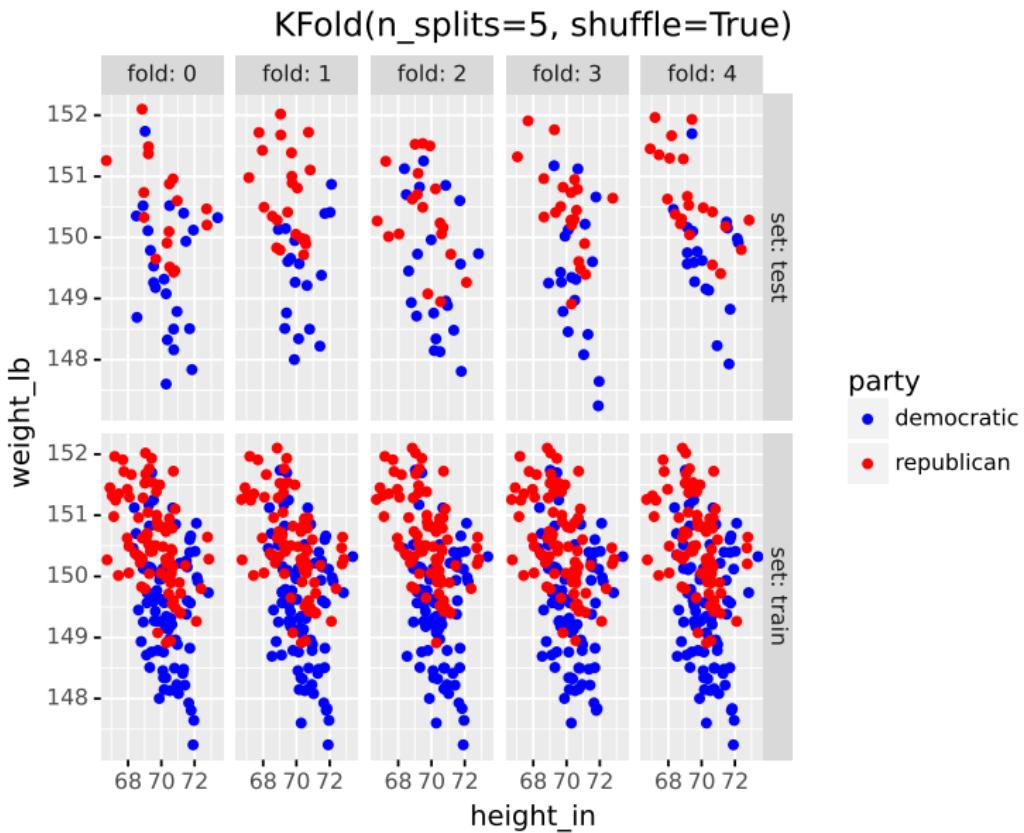
- ▶ One way to split is via K-fold cross-validation.
- ▶ Each row is assigned a fold ID number from 1 to K.
- ▶ For each fold ID, those data are held out, and other data are kept.
- ▶ Popular relative to other splitting methods because of simplicity and fairness (each row is held out one time).



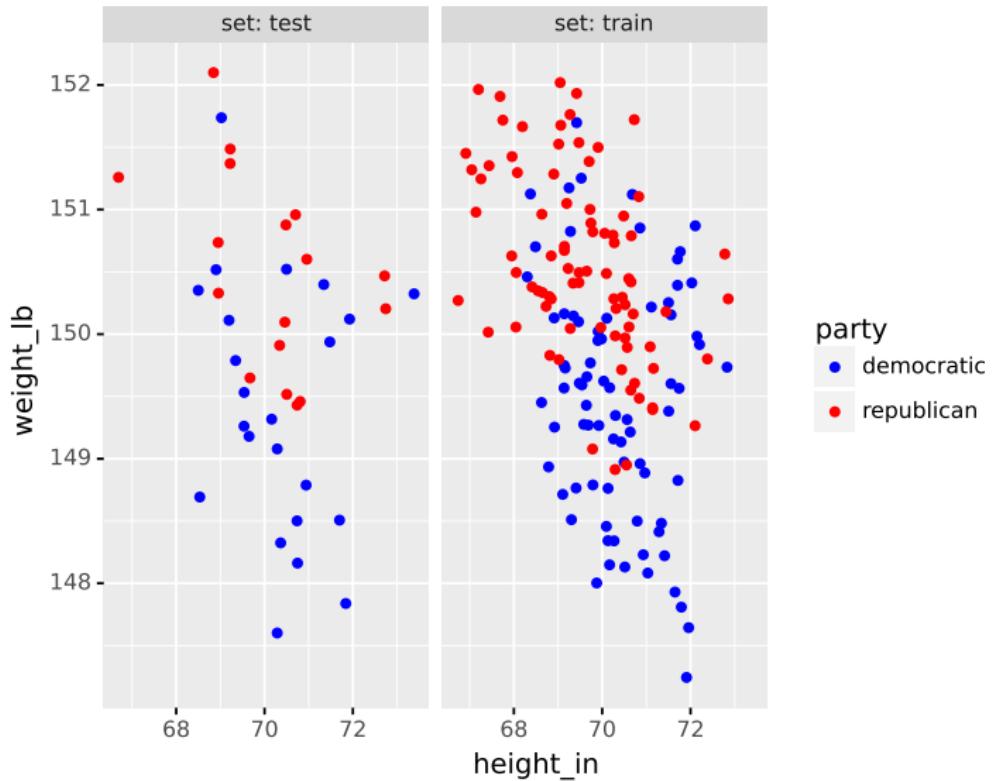
# Visualization of fold IDs in input/feature space



# Visualization of splits/sets in input/feature space

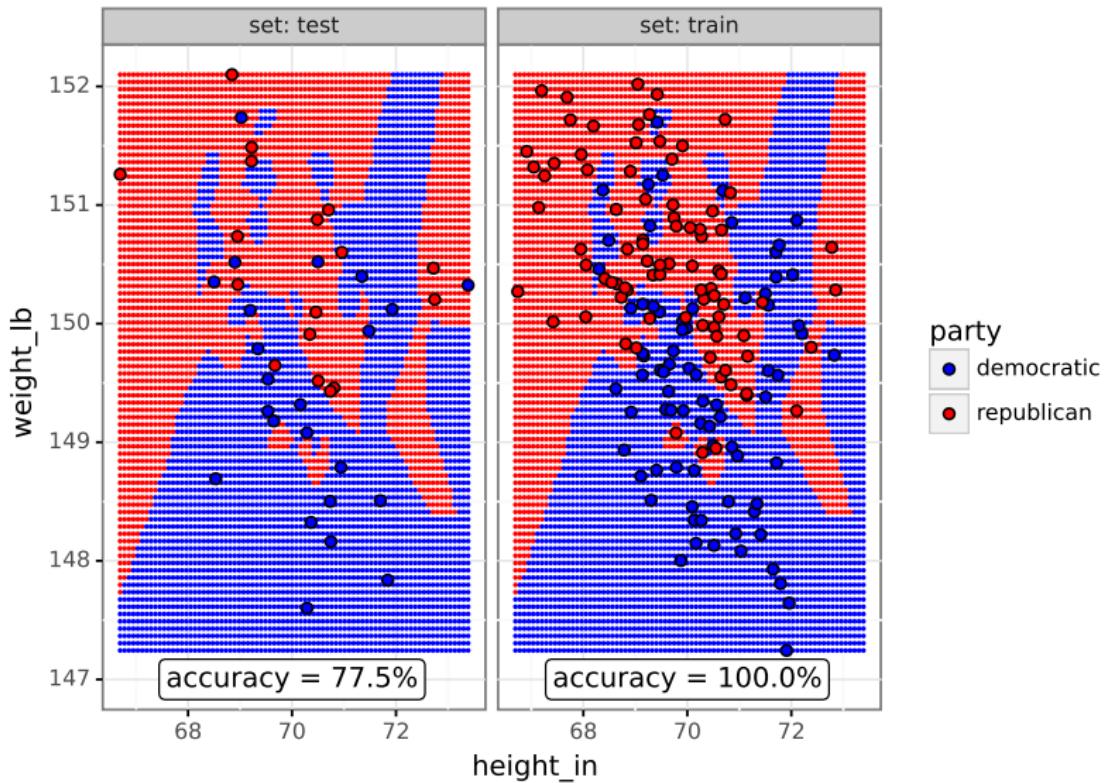


# One split



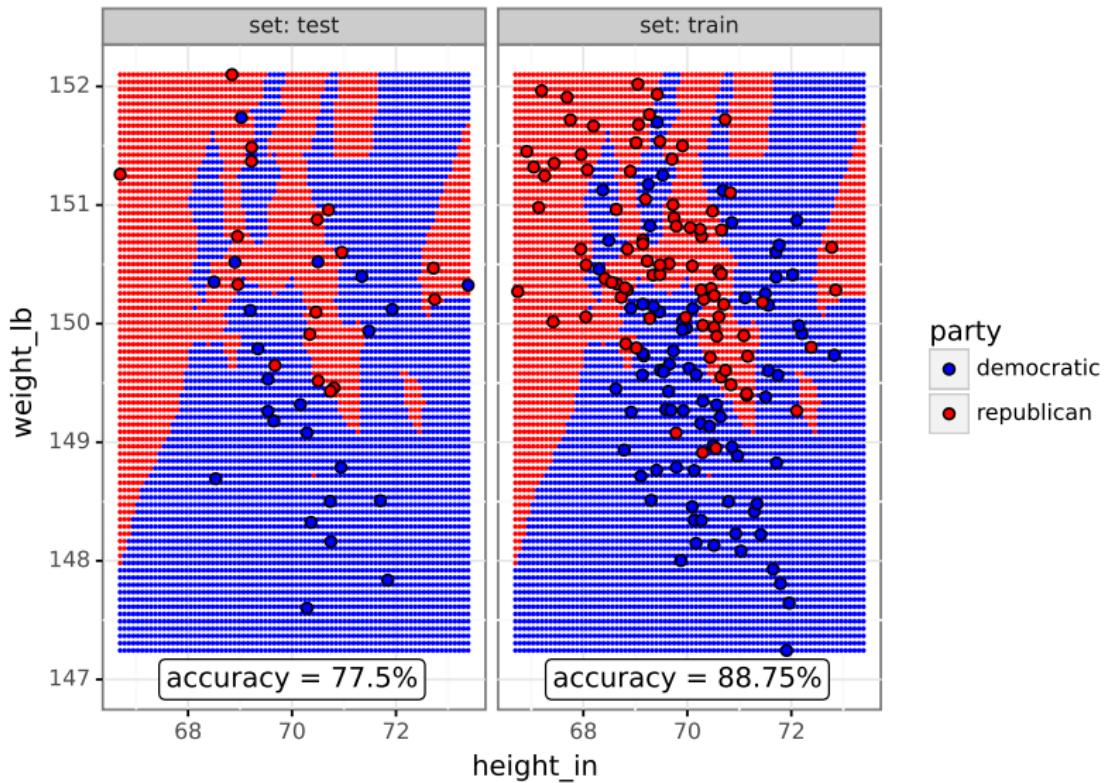
# Nearest neighbor predictions

1 nearest neighbors



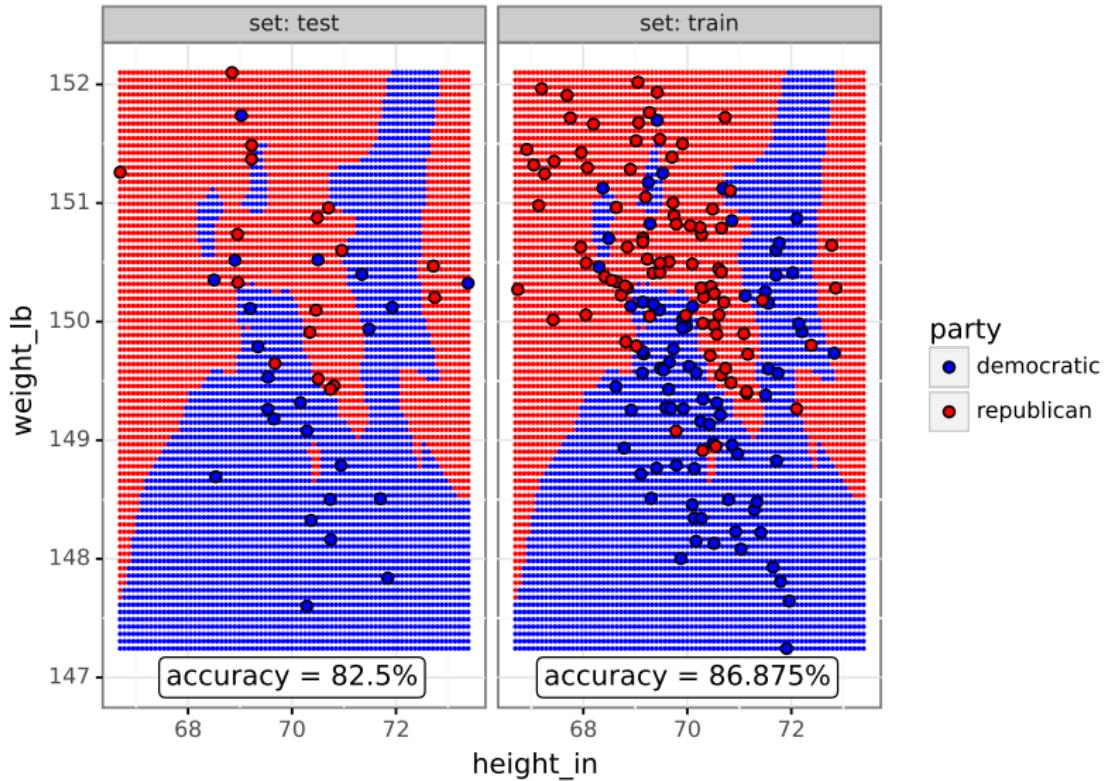
# Nearest neighbor predictions

2 nearest neighbors



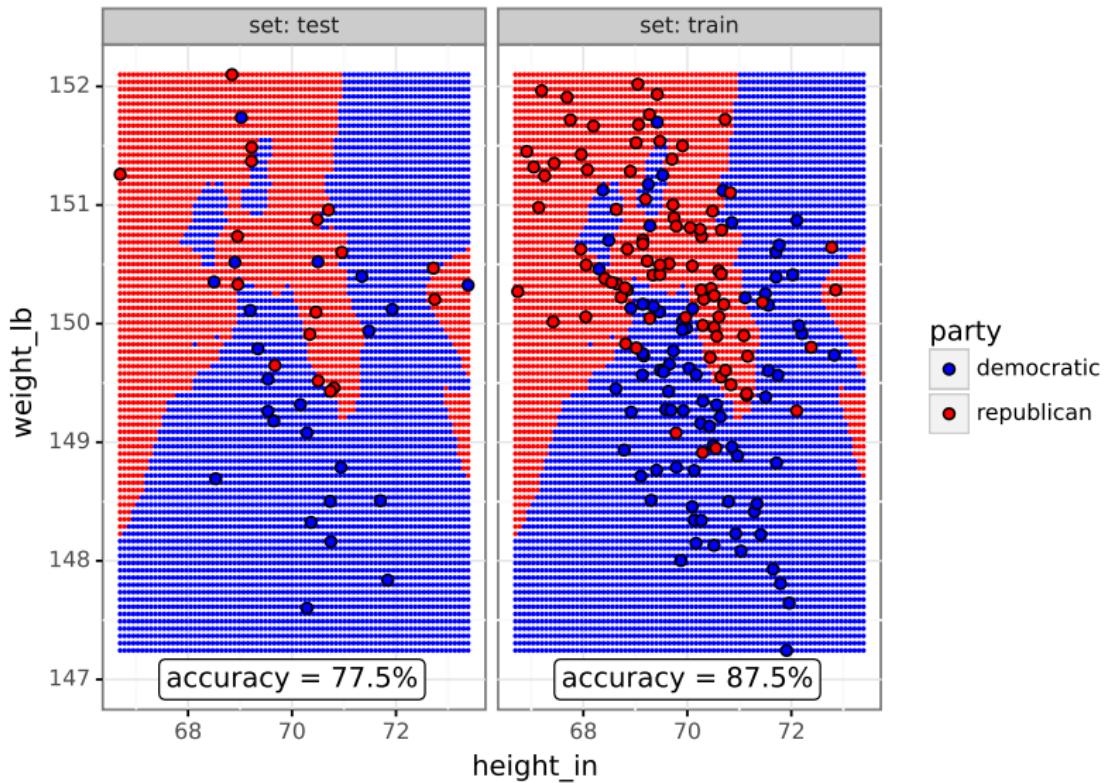
# Nearest neighbor predictions

3 nearest neighbors



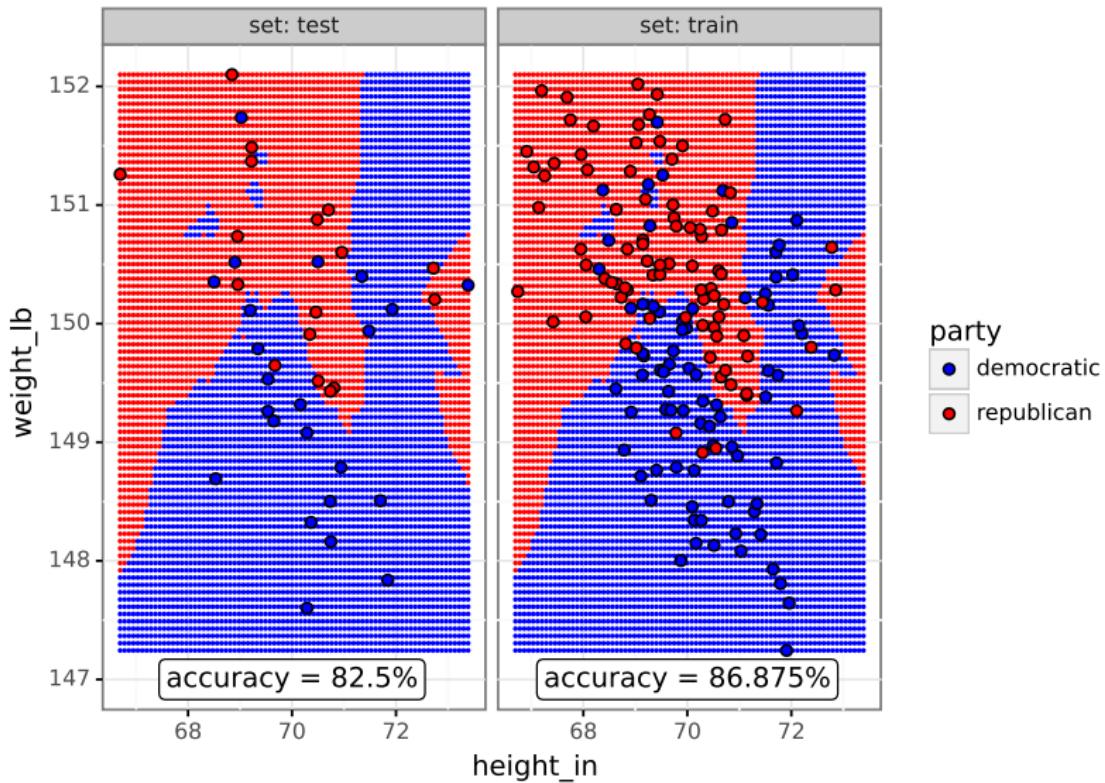
# Nearest neighbor predictions

4 nearest neighbors



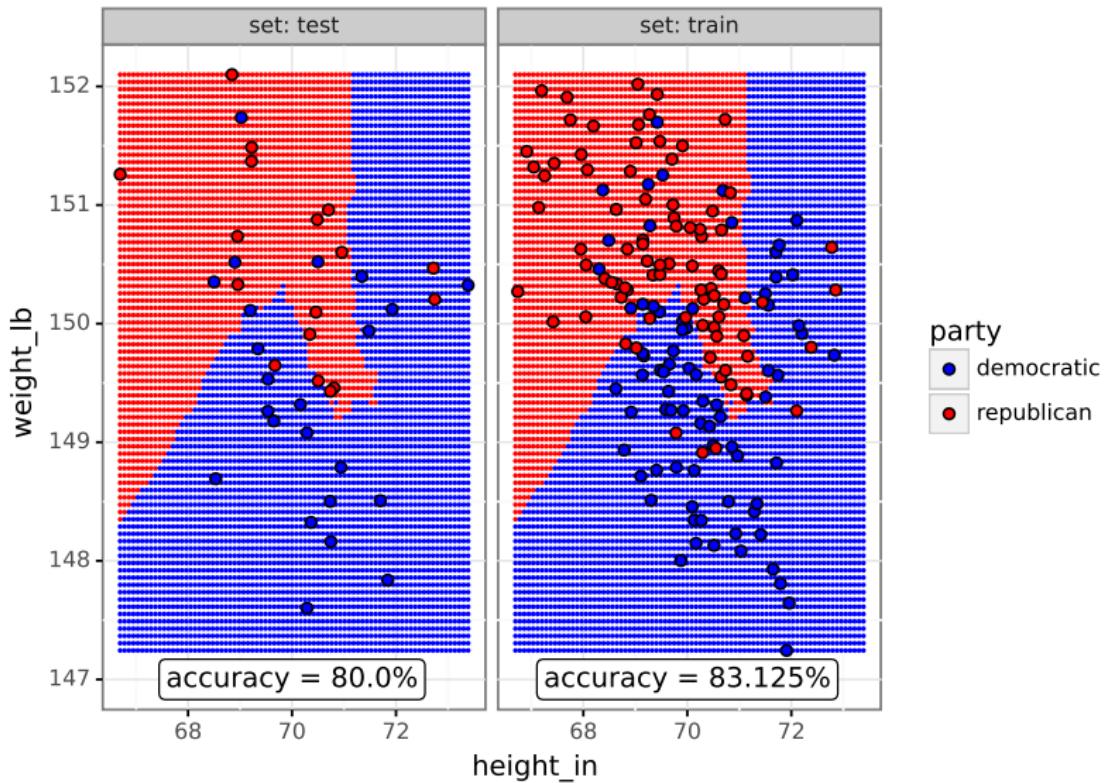
# Nearest neighbor predictions

5 nearest neighbors



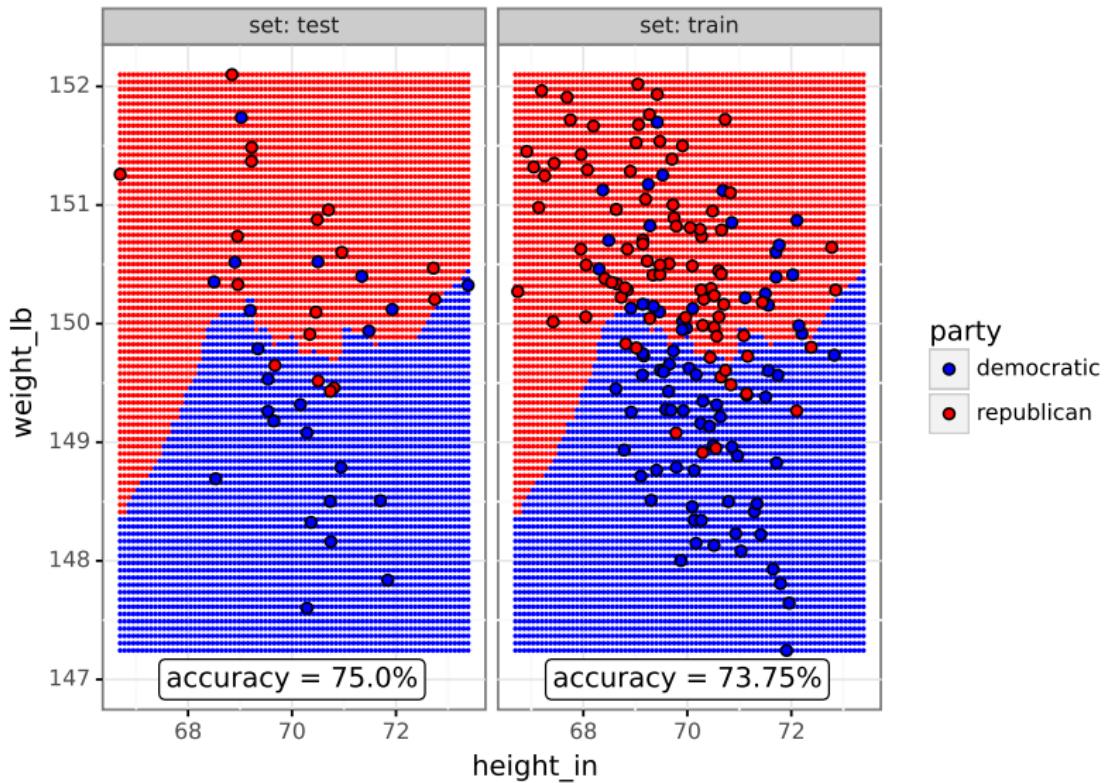
# Nearest neighbor predictions

10 nearest neighbors



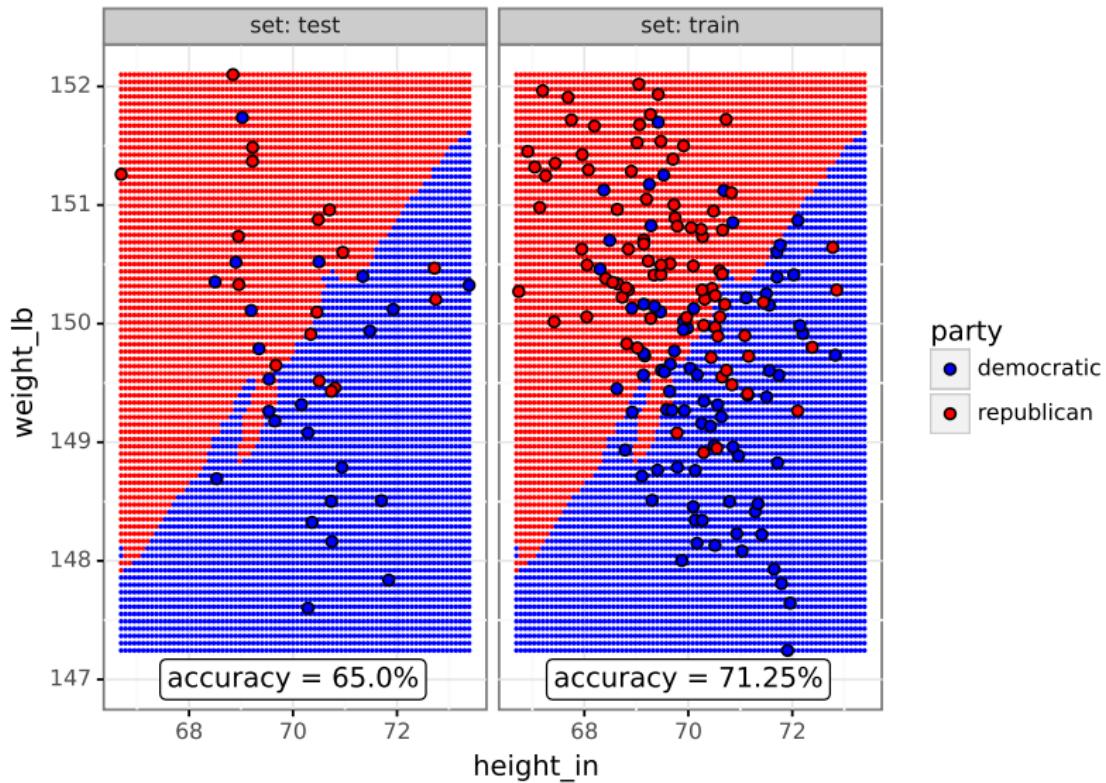
# Nearest neighbor predictions

50 nearest neighbors

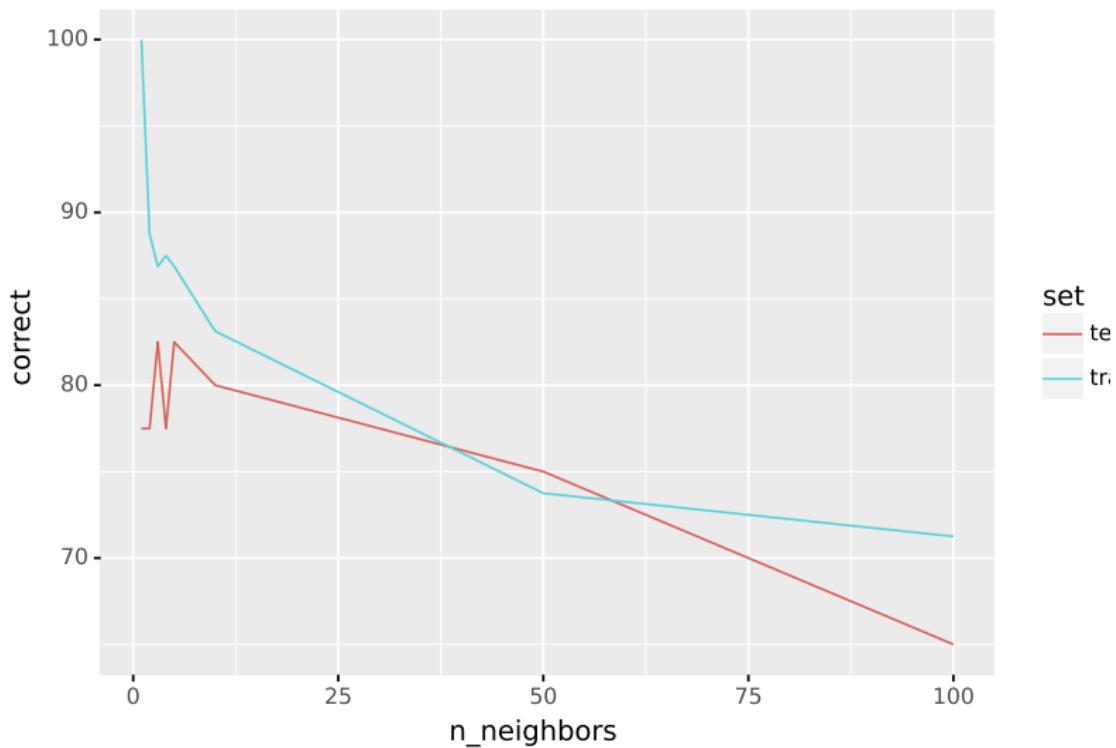


# Nearest neighbor predictions

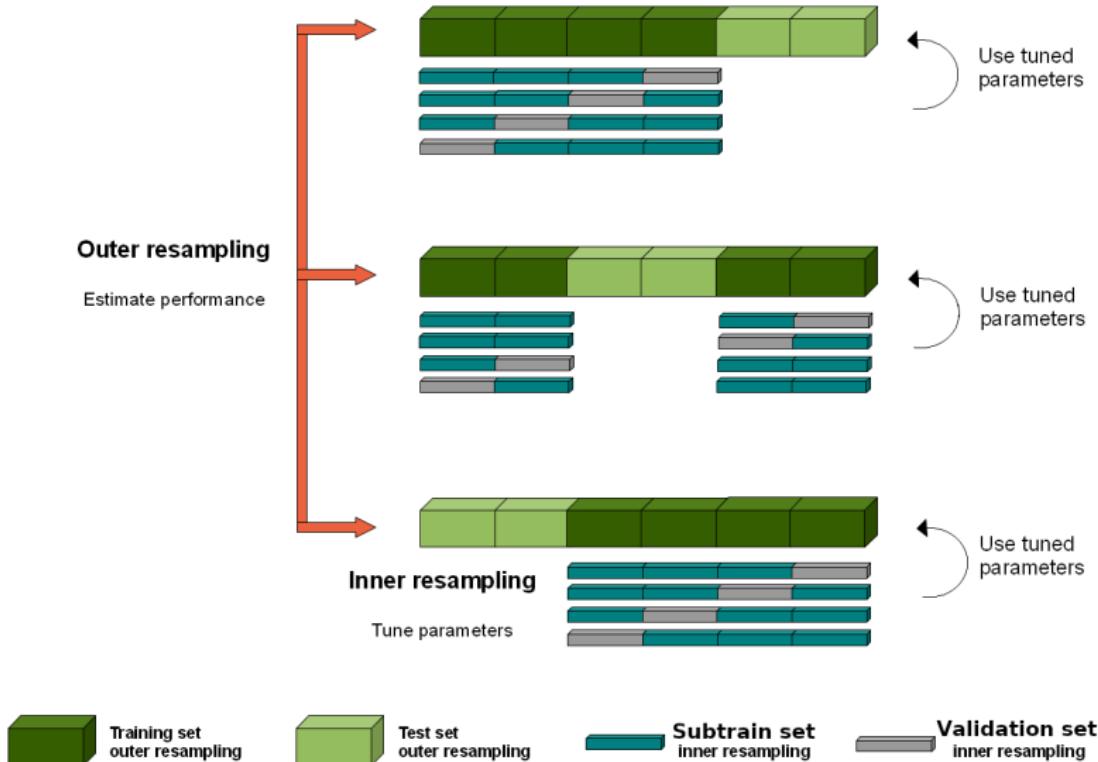
100 nearest neighbors



## Accuracy for each model size



# Two kinds of splits



## Implementing splits in python

- ▶ Full data into train/test ->  
`sklearn.model_selection.KFold`. For evaluating prediction accuracy and comparing different algorithms.
- ▶ Train into subtrain/validation ->  
`sklearn.model_selection.GridSearchCV`. For learning hyper-parameters such as `n_neighbors` which must be fixed before running the learning algorithm / computing predictions.

## Basic idea of linear model

How to fairly compare linear model with nearest neighbors?