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

Toby Dylan Hocking

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.
- $x =$image of digit/clothing, $y \in \{0, \ldots, 9\}$ (ten classes).
- $x =$vector of word counts in email, $y \in \{1, 0\}$ (spam or not).
- $x =$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 $\textsc{Learn}$ 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: $\textsc{Learn}(\mathbf{X}, \mathbf{y}) \rightarrow f$.
- 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/cs499-599-fall-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

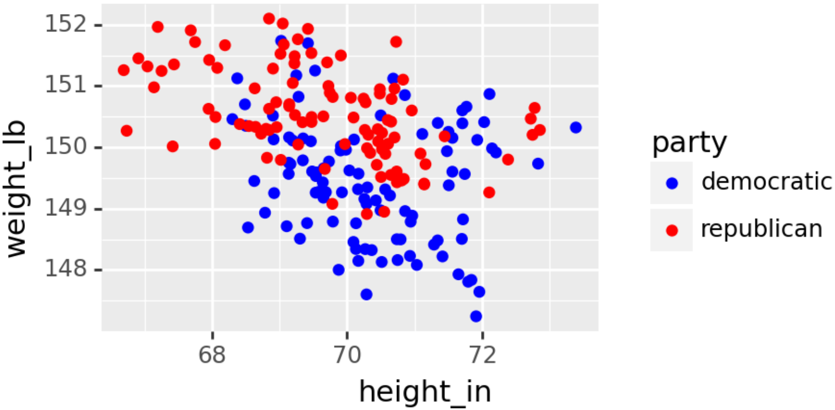
```
##          0     1     2  ...   55    56  57
## 0     0.00  0.64  0.64  ...   61   278   1
## 1     0.21  0.28  0.50  ...  101  1028   1
## 2     0.06  0.00  0.71  ...  485  2259   1
## 3     0.00  0.00  0.00  ...   40   191   1
## 4     0.00  0.00  0.00  ...   40   191   1
## ...    ...   ...   ...  ...  ...   ...  ..
## 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

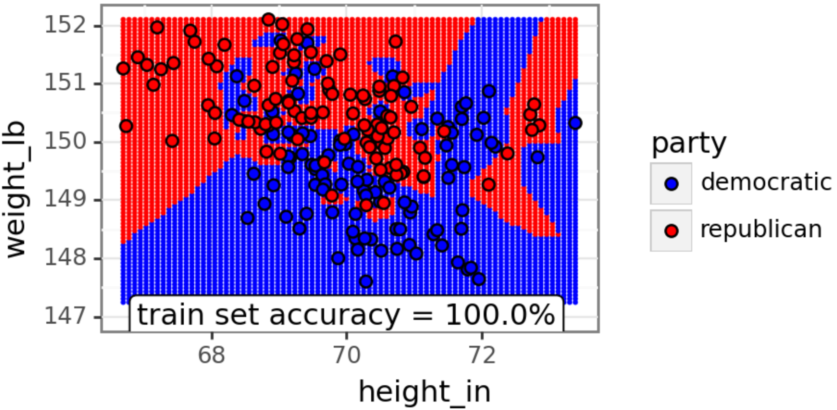
- Each axis represents one column of the **X** matrix.
- Each point represents one row of the **X** matrix.
- Color represents class label **y**.



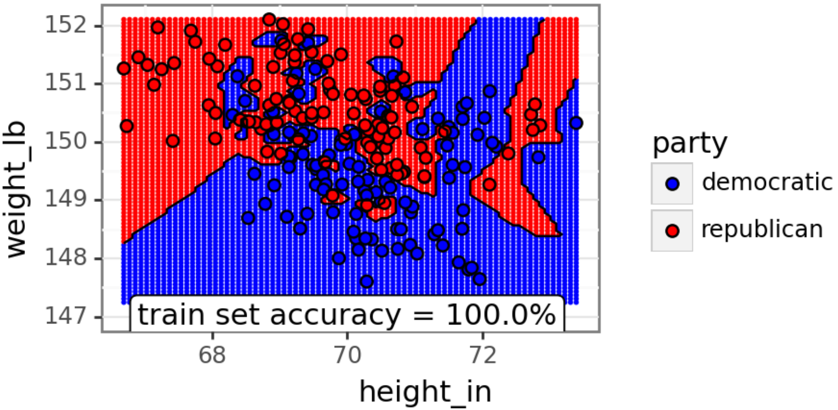
A basic machine learning algorithm

- 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

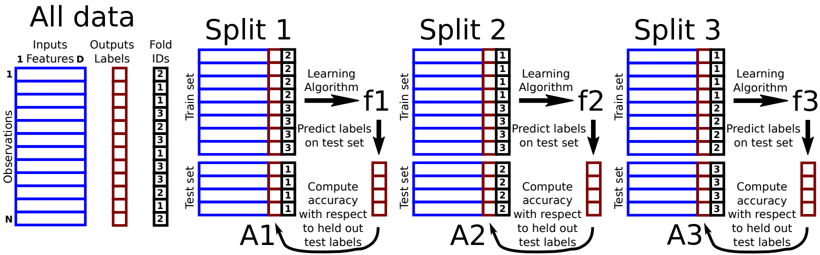


Is it good to have 100% accuracy on train data?

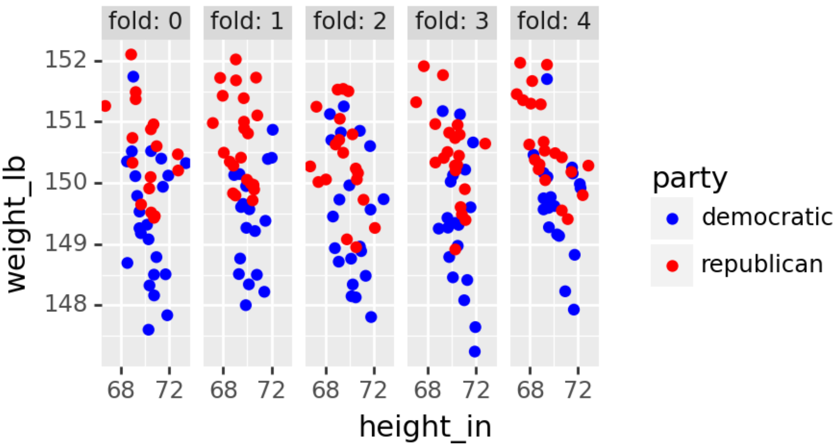
- Remember: goal is function f with accurate predictions on new inputs.
- What is a new input?
- We must assume that new/test inputs are similar to old/train inputs.
- In the statistical literature this is the iid (independent and identically distributed) assumption.
- We can therefore split the full 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

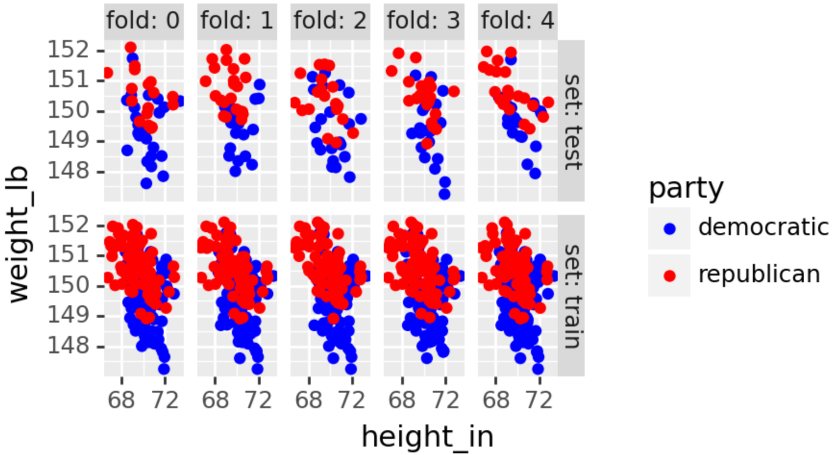
- One way to split is via K-fold cross-validation.
- Each row is assigned a fold ID number from 1 to K.
- For each for ID, those data are held out, and other data are kept.
- Popular relative to other splitting methods because of simplicity and fairness (each row is held out one time).



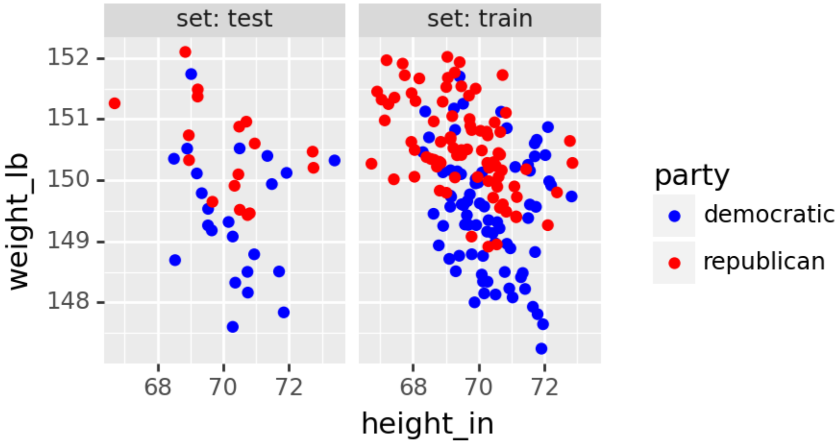
Visualization of fold IDs in input/feature space



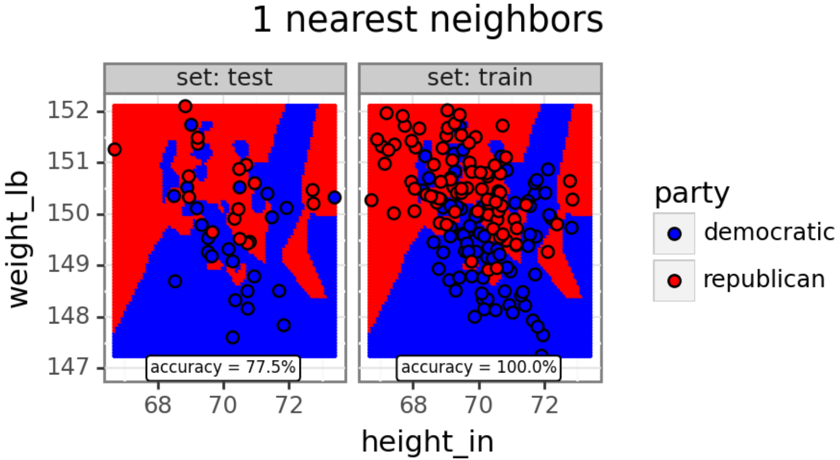
Visualization of splits/sets in input/feature space



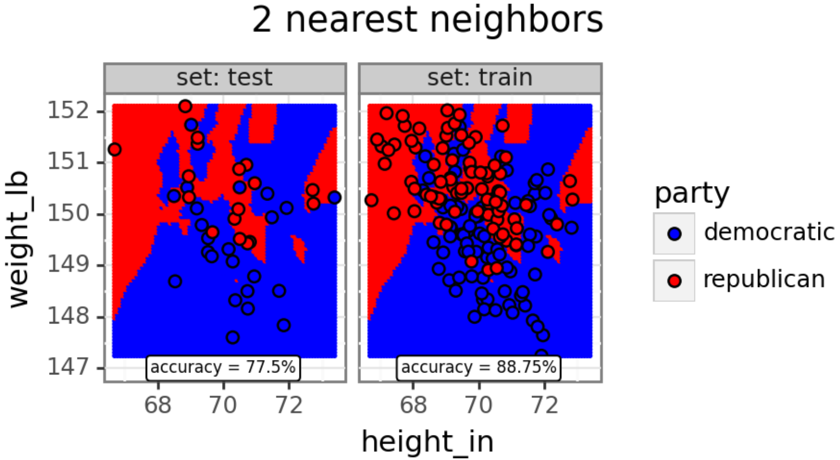
One split


set: test
set: train
weight_lb
152
151
150
149
148
68
70
72
height_in
party
democratic
republican

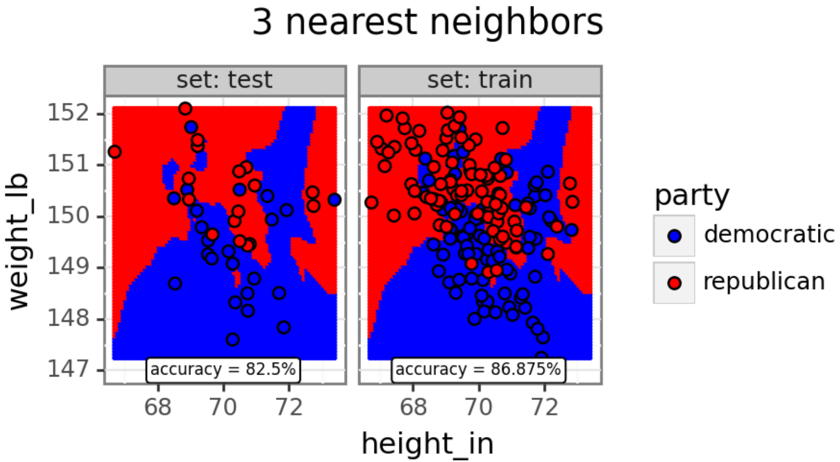
Nearest neighbor predictions



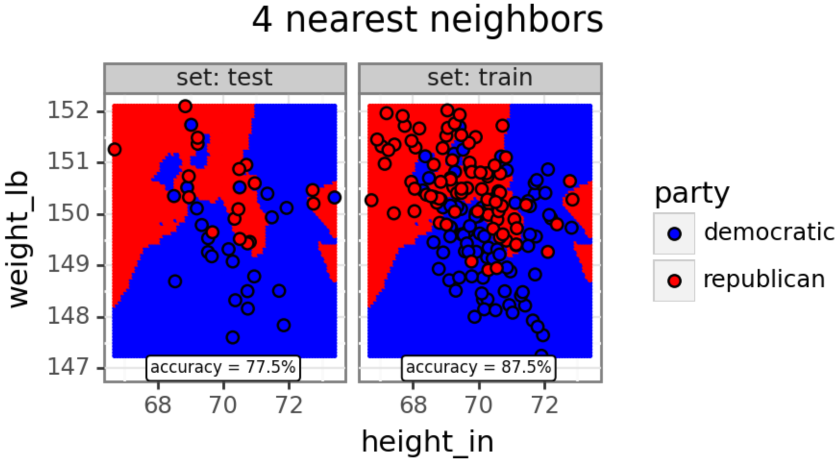
Nearest neighbor predictions



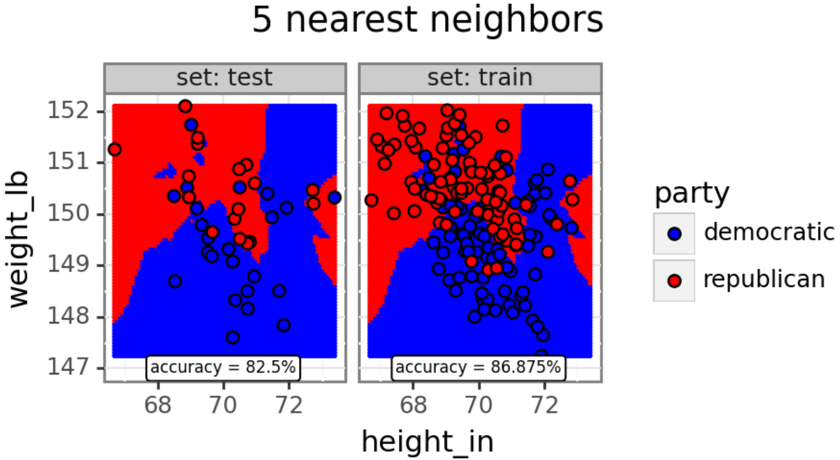
Nearest neighbor predictions



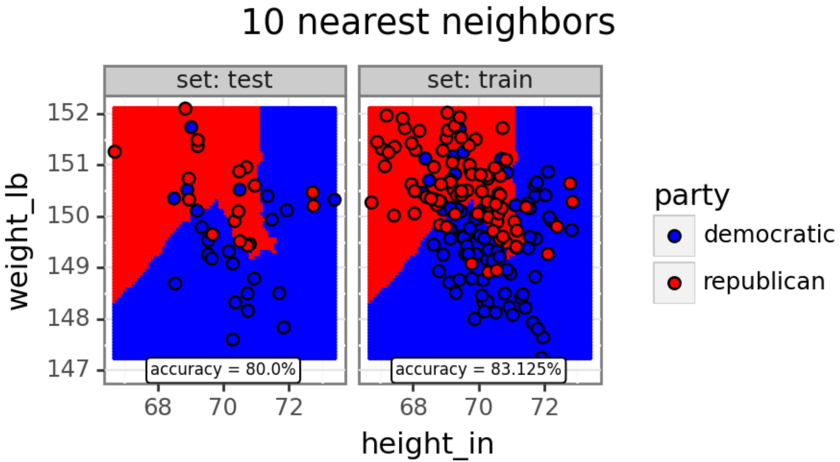
Nearest neighbor predictions



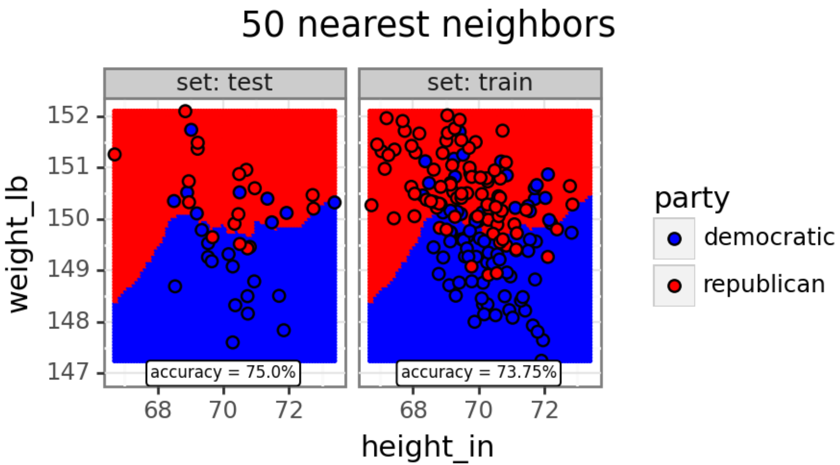
Nearest neighbor predictions



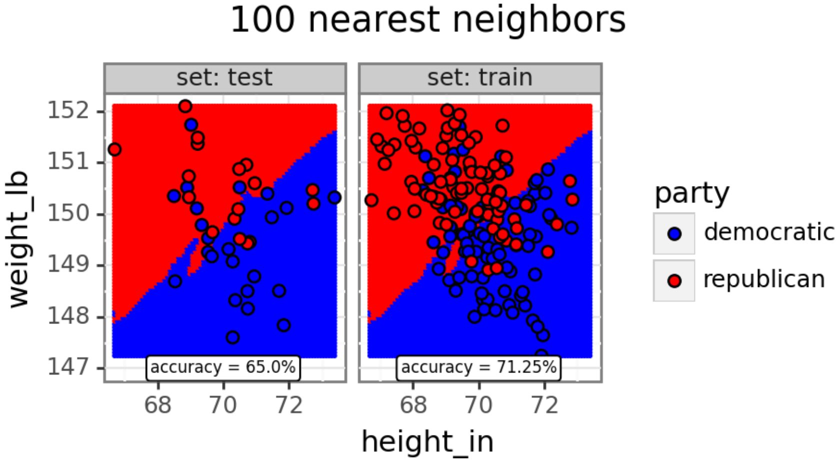
Nearest neighbor predictions



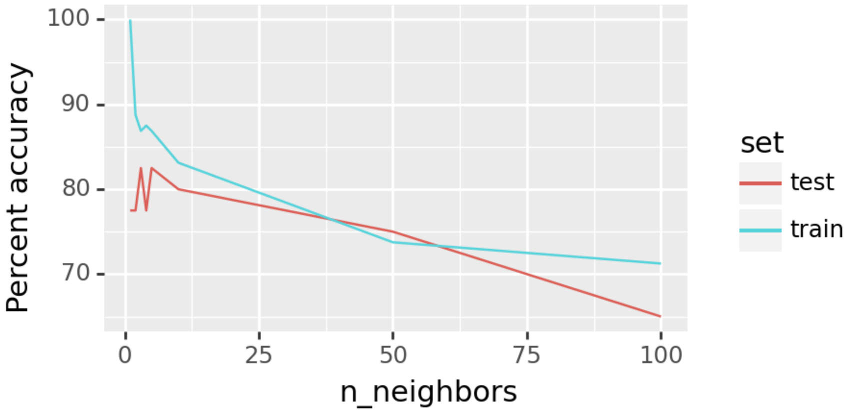
Nearest neighbor predictions



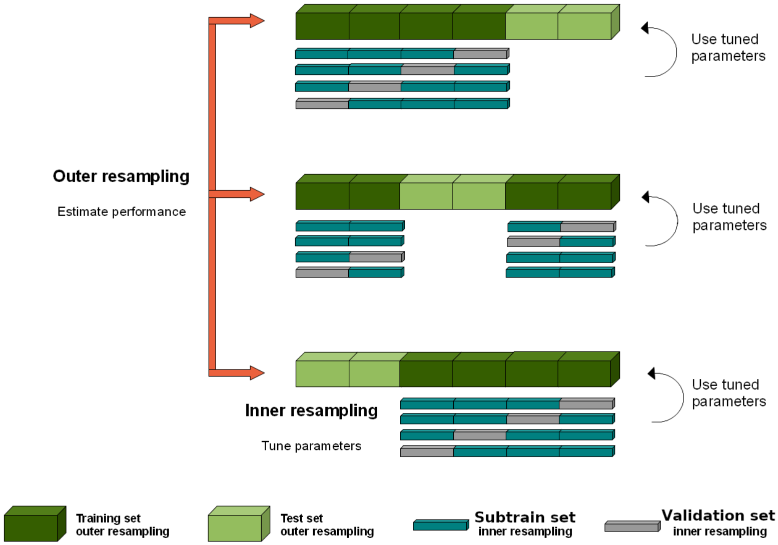
Nearest neighbor predictions



Accuracy for each model size



Two kinds of splits

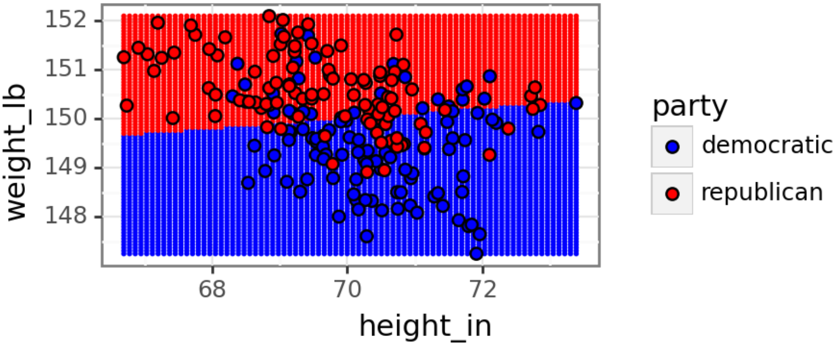


Implementing splits in python

- 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

- Learn a function $f(\mathbf{x}) = \hat{y} = \mathbf{w}^T\mathbf{x} + \beta \in \mathbb{R}$, larger values for more likely to be positive class.
- Predict positive class when $f(\mathbf{x}) > 0$.
- Optimize weights $\mathbf{w}$ and intercept β to minimize logistic loss.
- If labels are recoded as $y \in \{-1, 1\}$ then logistic loss is $\ell(\hat{y}, y) = \log[1 + \exp(-\hat{y}y)]$.



How to fairly compare linear model with nearest neighbors?

- Use cross validation!
- For each train/test split, use the train set as input to each learning algorithm.
- Train set may be further split into subtrain/validation sets for learning hyper-parameters.
  - Nearests neighbors: number of neighbors, done automatically if you use `KNeighborsClassifier` with `GridSearchCV`.
  - Linear model: amount of L2 or early stopping regularization, done automatically by `sklearn.linear_model.LogisticRegressionCV`.
- Compute predictions of learned models on test set.
- Also compute a featureless baseline: predict, for every item in test set, the most frequent class in train labels.
  - if there is any learnable relationship at all between inputs/features and outputs/labels, then algorithm should be more accurate than featureless baseline.
- Average over several train/test splits (K folds of CV).