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.
- $x =$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/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

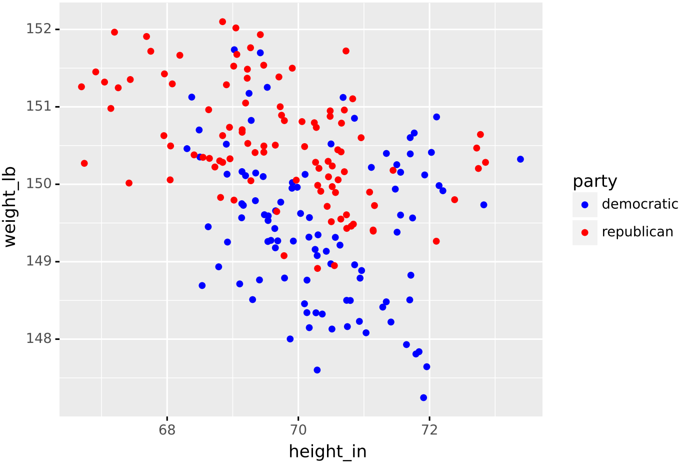
```
##         0     1     2   ...   55    56  57
## 0     0.00  0.64  0.64  ...   61   278   1
## 1     0.21  0.28  0.50  ...  101  1028   1
## 2     0.06  0.00  0.71  ...  485  2259   1
## 3     0.00  0.00  0.00  ...   40   191   1
## 4     0.00  0.00  0.00  ...   40   191   1
## ...    ...   ... 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

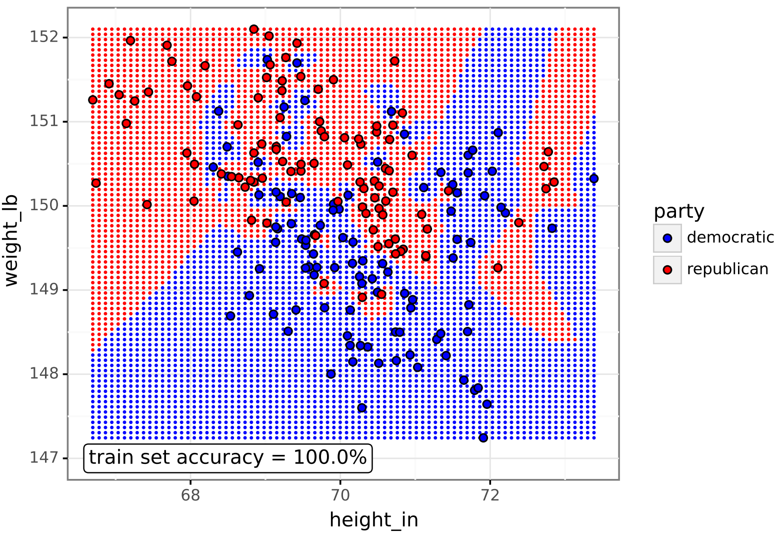
- Each axis represents one column of the **X** matrix.
- Each point represents one row of the **X** matrix.
- Color represents class label **y**.



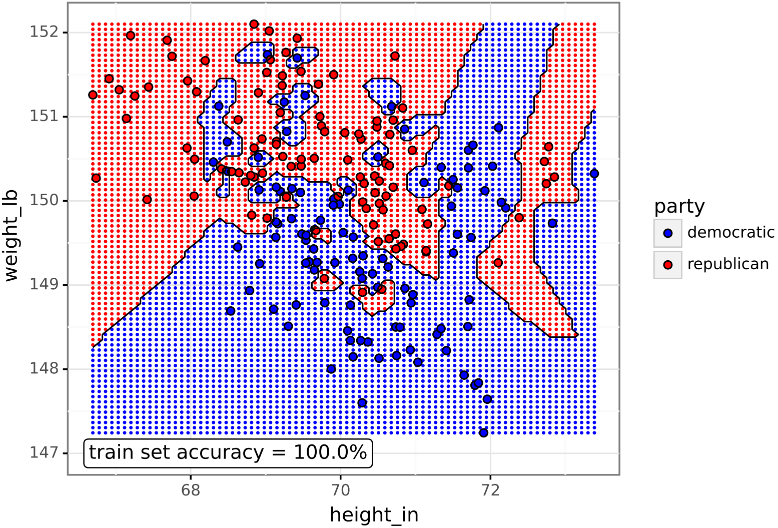
A basic machine learning algorithm

- 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

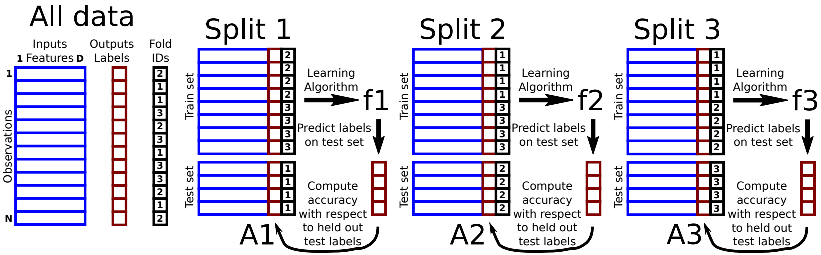


Is it good to have 100% accuracy on train data?

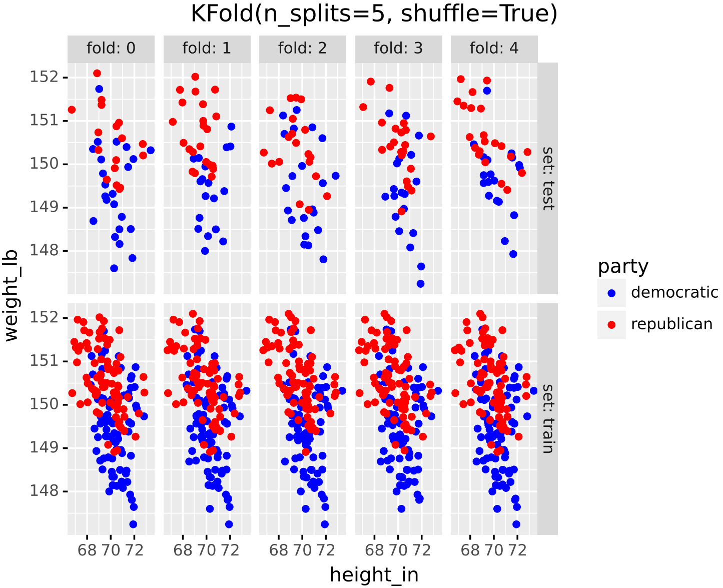
- Remember: goal is function f with accurate predictions on new inputs.
- What is a new input?
- We must assume that new/test inputs are similar to old/train inputs.
- In the statistical literature this is the iid (independent and identically distributed) assumption.
- We can therefore split the full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



Visualization of splits/sets in input/feature space



Two kinds of splits

- Full data into train/test.
- Train into subtrain/validation.

Basic idea of linear model

Visualize iris data without labels

- Let $X \in \mathbb{R}^{150 \times 2}$ be the data matrix (input for clustering).