CSC380: Principles of Data Science

Predictive Modeling and Classification 2

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Outline

- Decision tree variations
- KNN
- Model selections and evaluations

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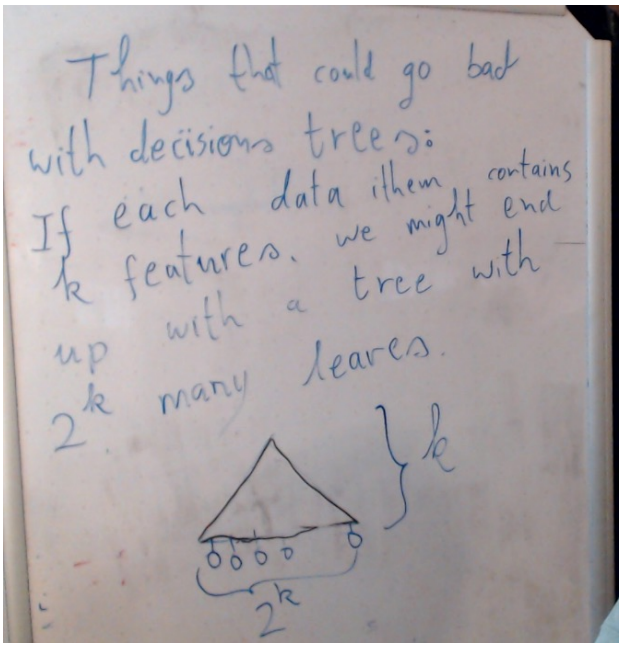
Things that could go bad with decisions trees:
If each data ithem contains k features, we might end up with a tree with 2^k many leaves.
k
2^k

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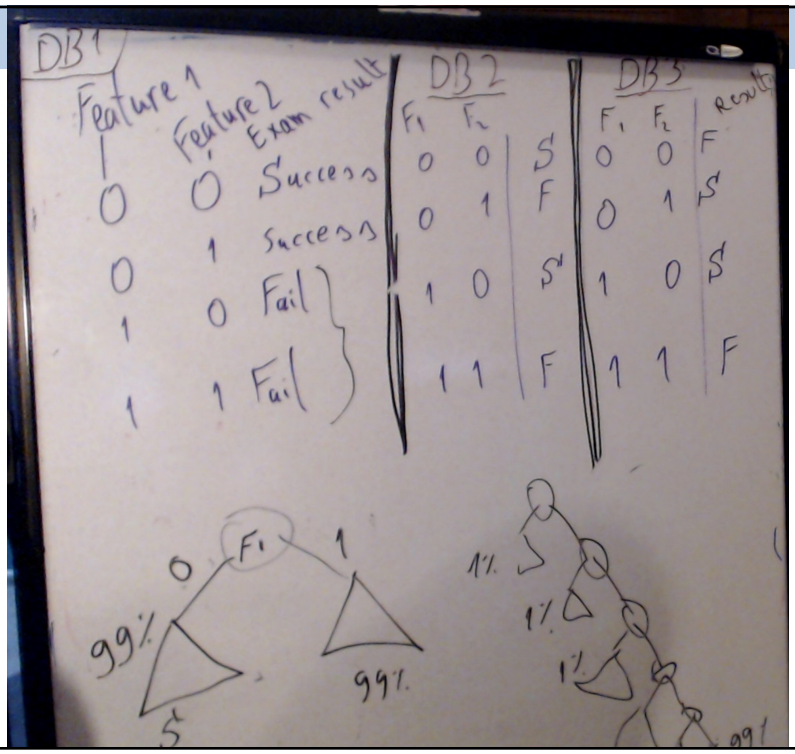
DB1
Feature 1
Feature 2
Exam result
0 0 Success
0 1 Success
1 0 Fail
1 1 Fail
DB2
DB3
Result
F1
99%
99%
1%
1%
1%

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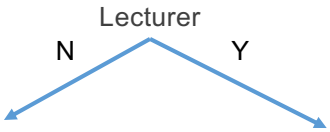
Review: criterion is accuracy



True label: +, +, +, +, +, +, +, +, +, + | +, +, -, -, -, -, -, -, -, -

Predicted label: +, +, +, +, +, +, +, +, +, + | -, -, -, -, -, -, -, -, -, -

Accuracy: $\frac{10}{20} \cdot \frac{10}{10} + \frac{10}{20} \cdot \frac{8}{10} = \frac{18}{20} = 0.9$

- Sum of (fraction of subgroup * fraction of correct answer in subgroup)
- What if we change it to Sum of (fraction of a subgroup * some function on that subgroup)?

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Types of features

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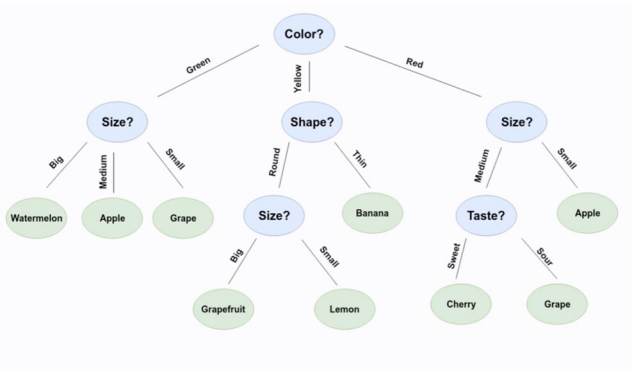
- Binary
- Categorical: values in $\{1, \ldots, C\}$ e.g., occupation, blood type
  - Option 1: Instead of 2 children, have C children.
  - Option 2: Derive C features of the form "feature=c?" for every $c \in C$.

↑ binary features!

Option 1:



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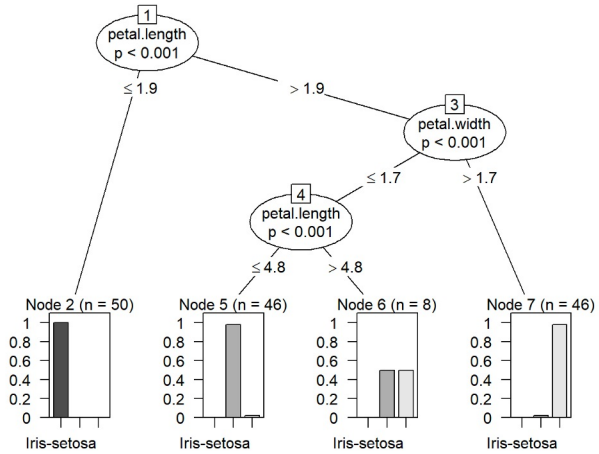
Types of labels

- Binary
- Multiclass: What changes do we need to make?
  - Almost none!
  - Just extend the accuracy to multiclass.



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Different selection criterions

Idea – want to make each subset (after the partition) as homogenous as possible
In the case that labels are Boolean (Success/Fail), this is similar to majority vote.

Notions of uncertainty: general case

Suppose in $S \subseteq \mathcal{X} \times \mathcal{Y}$, a p_k fraction are labeled as k (for each $k \in \mathcal{Y}$).

1. **Classification error**:
$$u(S) := 1 - \max_{k \in \mathcal{Y}} p_k$$
Gini impurity
2. **Gini index**:
$$u(S) := 1 - \sum_{k \in \mathcal{Y}} p_k^2$$
3. **Entropy**:
$$u(S) := \sum_{k \in \mathcal{Y}} p_k \log \frac{1}{p_k}$$

Each is *maximized* when $p_k = 1/|\mathcal{Y}|$ for all $k \in \mathcal{Y}$
(i.e., equal numbers of each label in S)

Each is *minimized* when $p_k = 1$ for a single label $k \in \mathcal{Y}$
(so S is **pure** in label)

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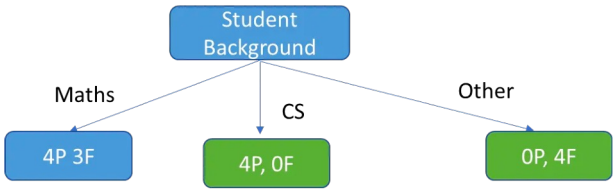
Different selection criterions - Gini index

Gini index:

$$u(S) := 1 - \sum_{k \in \mathcal{Y}} p_k^2$$



$$Gini_{maths} = 1 - \left(\frac{4}{7}\right)^2 - \left(\frac{3}{7}\right)^2 = .4897$$

$$Gini_{CS} = 1 - \left(\frac{4}{4}\right)^2 - \left(\frac{0}{4}\right)^2 = 0$$

$$Gini_{others} = 1 - \left(\frac{0}{4}\right)^2 - \left(\frac{4}{4}\right)^2 = 0$$

$$Gini_{bkgrd} = \frac{7}{15} * .4897 + \frac{4}{15} * 0 + \frac{4}{15} * 0 = .2286$$

Pick the one with lowest Gini index as root

https://towardsdatascience.com/decision-trees-explained-entropy-information-gain-gini-index-ccp-pruning-4d78070db36c

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k-Nearest Neighbors (k-NN)

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Background: Train Error vs Test Error

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Error := 1 – accuracy.

Suppose we have trained a function $\hat{f}$ on $D = \{(x^{(i)}, y^{(i)})\}_{i=1}^{m}$ using a supervised learning algorithm.

- Train error: Evaluate on D.

$$\widehat{err}_D(f) := \frac{1}{|D|} \sum_{(x,y)\in D} \mathbf{I}\{f(x) \neq y\}$$

- Test error: Evaluate on $D' = \{(x^{(i)}, y^{(i)})\}_{i=1}^{m'}$ not used for training.

Q: Choose one:
(1) train error ≥ test error (2) train error ≈ test error (3) train error ≤ test error

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Background: Train Error

Suppose our train set:

Index	Ground Truth	Predicted
0	0	1
1	1	1
2	0	0
3	0	1
4	1	0
5	0	0
6	1	1

$$\frac{1}{6} \cdot (1 + 0 + 0 + 1 + 1 + 0) = \frac{1}{2}$$

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Background: Workflow of Training a Classifier

Standard practice:

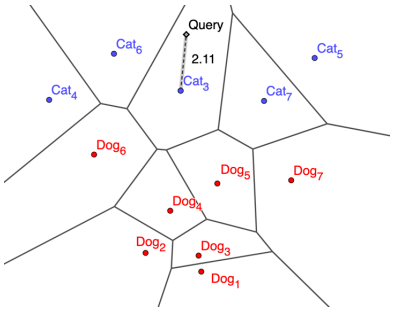
- Given a data set D, split it into train set D_{train} and D_{test}
  - large data: 90-10 ratio
  - medium data: 80-20 ratio
  - small data: 70-30 ratio

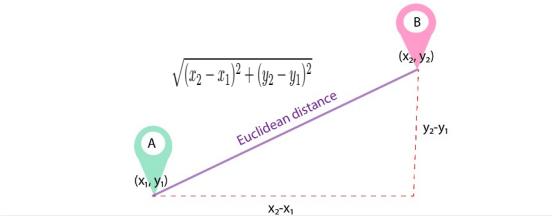
(these are guidelines only)

- Train on D_{train} and evaluate error rate on D_{test}. You trust that D_{test} will be the performance when you deploy the trained classifier.

Classier via Nearest Neighbor. Voronoi Diagram

- Given – set of Dogs, and Set of cats, decide for a query whether a Dog or a Cat
- Assume: Data is labeled. Also given –weight and height of each animal
- Given a query, find a close data point, and return its label (that is, dog/cat)
- Needed: A distance function from Query to each data point. Say x is weight, and y-axis is height.
- Distance function= $(\Delta(Weight)^2 + \Delta(Height)^2)^{1/2}$
- Report type of nearest animal
- Voronoi Diagram-partition of the space into cells, each cell with unique closest data point.





k-nearest neighbor: main concept

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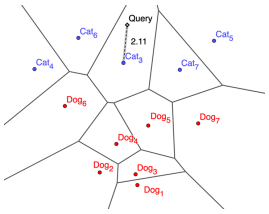
- Train set: $S = \{ (x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)}) \}$
- **Idea**: given a new, unseen data point x, its label should resemble the labels of **nearby points**
- What function?
  - Input: $x \in \mathbb{R}^d$

E.g., Euclidean distance



  - From S, find the k nearest points to x from S; call it $N(x)$
  - Output: the majority vote of $\{y_i : i \in N(x)\}$
    - For regression, take the average label.

Finding say 3-Nearest Nbrs gives better resilience to noise (but more expensive)

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k-NN example

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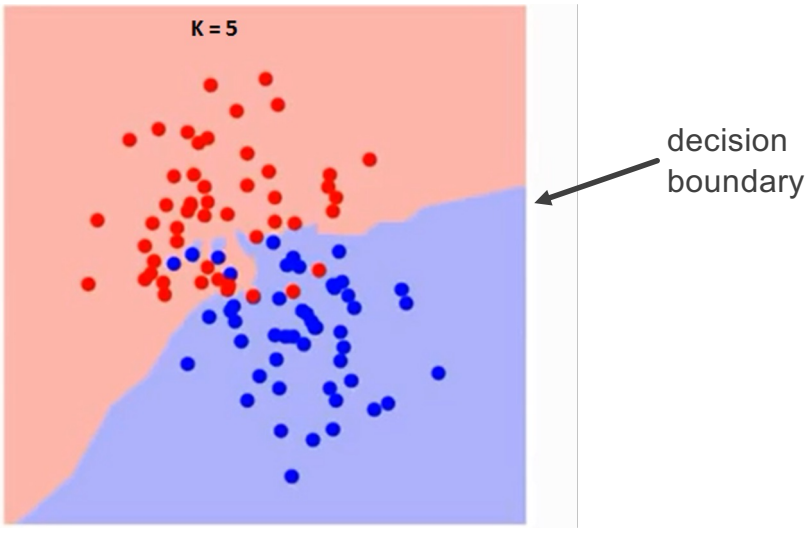

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Finding k nearest neighbours

- For a query point q, and a data set D in d-dimensions, we can find the 1-NN in linear time – could be very expensive if data is large, multiple queries and d is large
- For mid-size d (at most 30) Multiple data structures exists that could expedite the search (for example kD-trees). They usually don't give the exact nearest neibors by a good approximation.
- For higher dimension, it is common to project the data (via dimensionality-reduction techniques) and perform the search on the projeccted data.
- Larger k is not always better (example on board). It is possibe to ask for the 4-NN, if there a need, ask for the 8-NN, 16 if needed and so on.

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Basics

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How to extract features as **real values**?

- Binary features: Take 0/1
- Categorical {1,…,C} (e.g., movie genres)
  - Binary vector of length C. Set c-th coordinate 1 and 0 otherwise. one-hot encoding

Distance:

- (popular) Euclidean distance: $d(x, x') = \sqrt{\sum_{i=1}^{d} (x_i - x_i')^2}$
- Manhattan distance : $d(x, x') = \sum_{i=1}^{d} |x_i - x_i'|$

L_∞ Distance: $d_\infty(x, x') = \max |x_i - x'|$

A total of d dimensions/features: i from 1 to d

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Issue: features in different scales

Suppose our train set:

Index	Weight (lbs)	Shoe size
0	130	9
1	180	10.5
2	100	6
3	210	12
4	155	7.5
5	170	9.5
6	90	7

Features in different scales can be problematic: "weight" is the dominance in the distance.

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Make sure features are scaled fairly

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- Features having different scale can be problematic. (e.g., weights in lbs vs shoe size)
- [Definition] **Standardization**

$$\text{Features: } (f_1 \dots f_d) = (' weight', ' height' \dots)$$

  - For each feature f, compute $\mu_f = \frac{1}{m}\sum_{i=1}^{m} x_f^{(i)}$, $\sigma_f = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(x_f^{(i)} - \mu_f\right)^2}$
  - Then, transform the data by $\forall f \in \{1, \dots, d\}, \forall i \in \{1, \dots, m\}, \; x_f^{(i)} \leftarrow \frac{x_f^{(i)} - \mu_f}{\sigma_f}$

after transformation, each feature has mean 0 and variance 1

- Be sure to keep the "standardize" function and apply it to the test points.
  - Save $\{(\mu_f, \sigma_f)\}_{f=1}^{d}$
  - For test point x^*, apply $x_f^* \leftarrow \frac{x_f^* - \mu_f}{\sigma_f}, \forall f$

midterm candidate: Assume Norm distribution. Percentage wise, how much of the transformed data is between -1 and 1 ?

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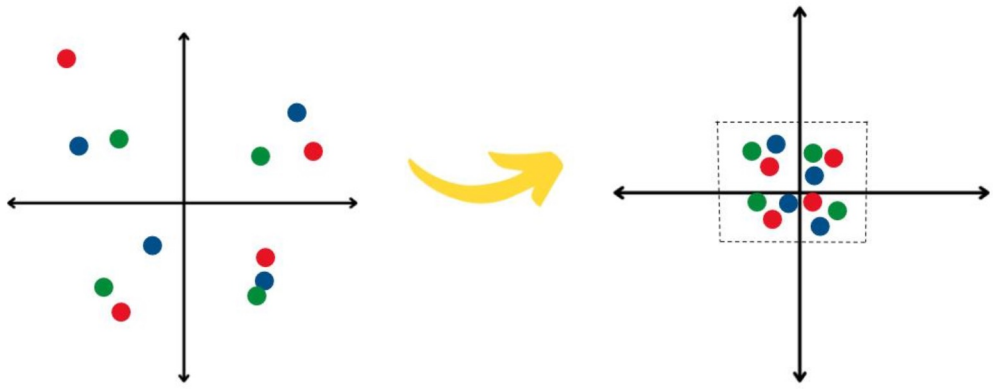
Standardization



After transformation, each feature has mean 0 and variance 1.

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k-NN Summary

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- Given: labeled data D
- Training
  - Compute and save $\{(\mu_f, \sigma_f)\}_{f=1}^{d}$
  - Compute and save standardization of D
- Test
  - Given x^*, apply standardization $x_f^* \leftarrow \frac{x_f^* - \mu_f}{\sigma_f}, \forall f$
  - Compute k nearest neighbors $N(x^*)$
  - Predict by majority vote label in $N(x^*)$ (average label for regression tasks)

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Issues 1: irrelevant features

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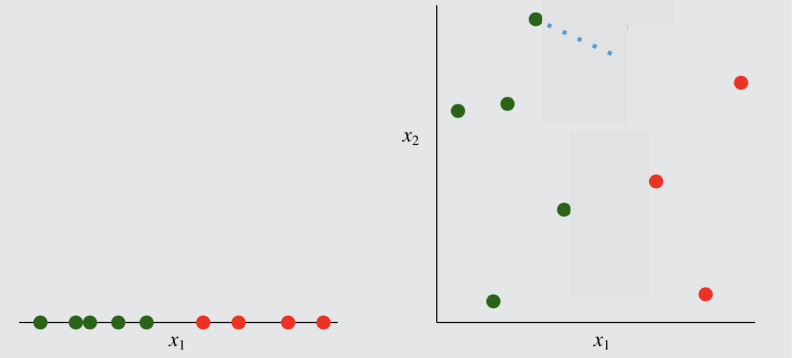
here's a case in which there is one relevant feature x_1 and a 1-NN rule classifies each instance correctly

consider the effect of an irrelevant feature x_2 on distances and nearest neighbors



Q: how did we deal with irrelevant features in decision trees?

not all features are used because (a) we stop adding features when having 0 local accuracy, (b) prune the tree

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Issue 2: choosing k

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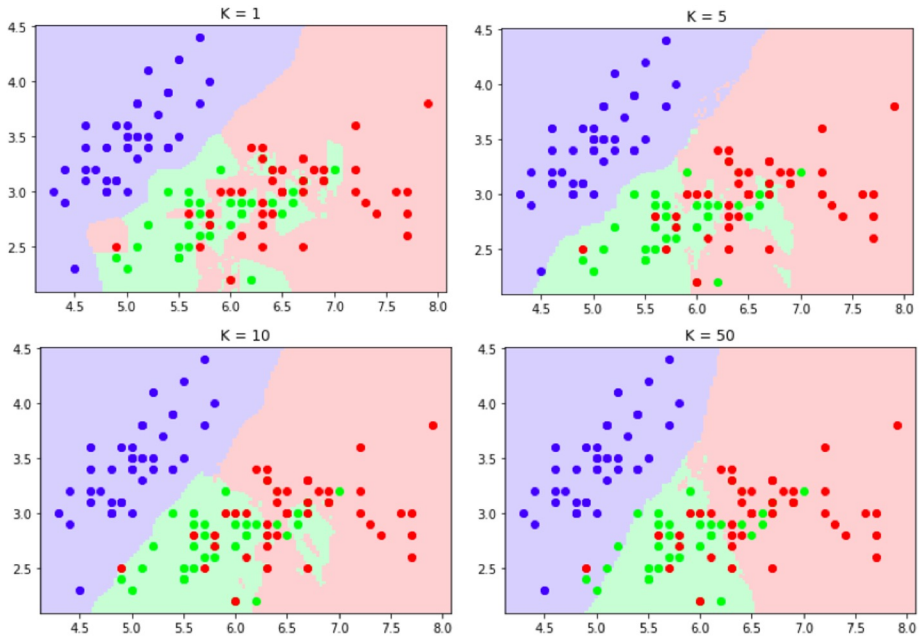

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Model Selection and Evaluation

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Model Selection / Assessment

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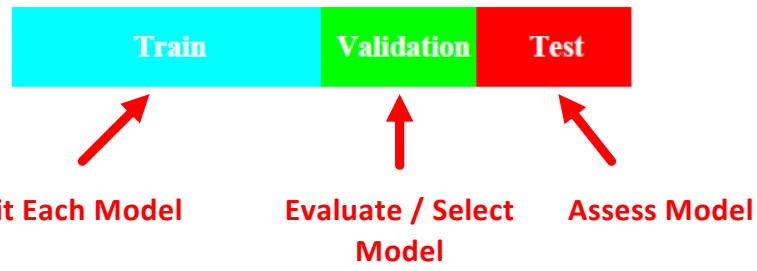
Partition your data into Train-Validation-Test sets



- Ideally, Test set is kept in a "vault" and **only peek at it once model is selected**
- Small dataset: 50% Training, 25% Validation, 25% Test (very loose rule set by statisticians)
- For large data (say a few thousands), 80-10-10 is usually fine.

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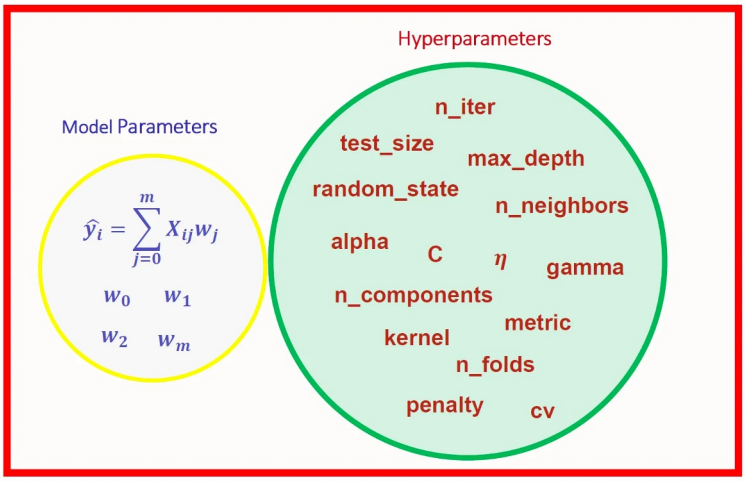
Hyperparameters vs Parameters



hyperparameter: parameters of the model that are not trained automatically by ML algorithms (e.g., k in KNN).

parameters: those that are trained automatically (e.g., tree structures in decision tree)

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Tuning hyperparameters

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Validation set method:

- For each hyperparamter $h \in H$
  - Train $\hat{f}$ on train set with h
  - Compute the error rate of $\hat{f}$ on validation set
- Choose the best performing hyperparameter h^*
- Use h^* to retrain the final model $\hat{f}^*$ with both train and validation set.
- Finally, evaluate $\hat{f}^*$ on test set to estimate its future performance.

Why not train on the whole set?

Pro tip

- Do not use arithmetic grids; use geometric grids.

Don't k = 1, 3, 5, 7, 9, …
Do k = 1, 2, 4, 8, 16, …

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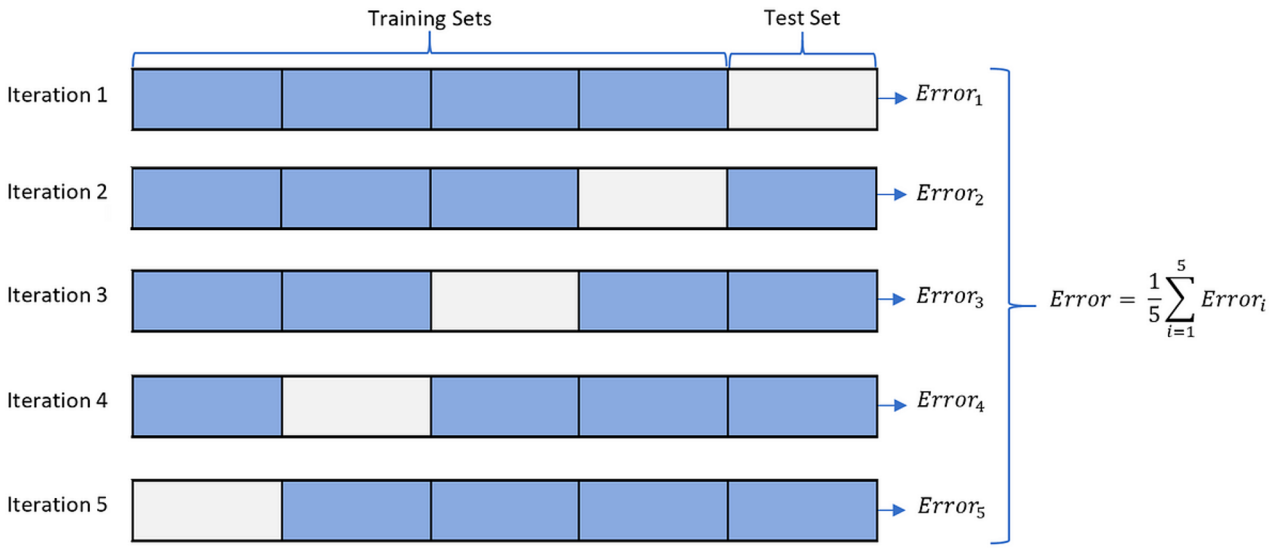
5-fold cross validation



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Tuning hyperparameters

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K-fold cross validation

- Randomly partition train set S into K disjoint sets; call them $\text{fold}_1, \ldots, \text{fold}_K$
- For each hyperparameter $h \in \{1, \ldots, H\}$
  - For each $k \in \{1, \ldots, K\}$
    - train $\hat{f}_k^h$ with $S \setminus \text{fold}_k$
    - measure error rate $e_{h,k}$ of $\hat{f}_k^h$ on fold_k
  - Compute the average error of the above: $\widehat{err}^h = \frac{1}{K}\sum_{k=1}^{K} e_{h,k}$
- Choose $\hat{h} = \arg\min_h \widehat{err}^h$
- Train $\hat{f}^*$ using S (all the training points) with hyperparameter h
- Finally, evaluate $\hat{f}^*$ on test set to estimate its future performance.

K=10 is standard, but K=5 is okay, too

Use when (1) the dataset is small (2) ML algorithm's retraining time complexity is low (e.g., kNN)

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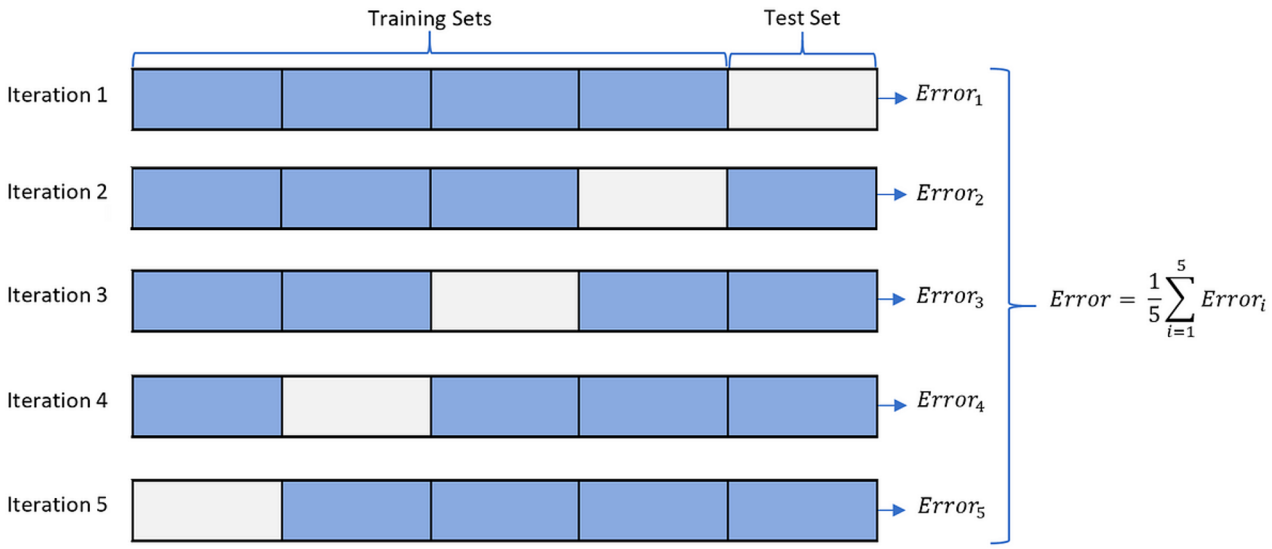
5-fold cross validation



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Scikit-Learn

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Python library for machine learning. Install using Anaconda:

```
$ conda install -c conda-forge scikit-learn
```

Or using PyPi:

```
$ pip install -U scikit-learn
```

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Preprocessing : Encoding Labels

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Oftentimes, categorical labels come as strings, which aren't easily modeled (e.g., with Naïve Bayes),

```
>>> le = preprocessing.LabelEncoder()
>>> le.fit(["paris", "paris", "tokyo", "amsterdam"])
LabelEncoder()
>>> list(le.classes_)
['amsterdam', 'paris', 'tokyo']
>>> le.transform(["tokyo", "tokyo", "paris"])
array([2, 2, 1]...)
>>> list(le.inverse_transform([2, 2, 1]))
['tokyo', 'tokyo', 'paris']
```

`LabelEncoder` transforms these into integer values, e.g. for categorical distributions

fit() is doing the heavy work: create the mapping from string to integers

Can *undo* using `inverse_transform` so we don't have to store two copies of the data

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Preprocessing : Z-Score

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Typical ML workflow starts with *pre-processing* or *transforming* data into some useful form, which Scikit-Learn calls *transformers*:

```
>>> from sklearn.preprocessing import StandardScaler
>>> data = [[0, 0], [0, 0], [1, 1], [1, 1]]
>>> scaler = StandardScaler()
>>> print(scaler.fit(data))
StandardScaler()
>>> print(scaler.mean_)
[0.5 0.5]
>>> print(scaler.transform(data))
[[-1. -1.]
 [-1. -1.]
 [ 1.  1.]
 [ 1.  1.]]
```

Standardization:

$$z = \frac{x-\mu}{\sigma}$$

with mean:

$$\mu = \frac{1}{N}\sum_{i=1}^{N}(x_i)$$

and standard deviation:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2}$$

- Features are standardized independently (columns of X)

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Cross-Validation

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Easily do cross validation for model selection / evaluation…

```
>>> from sklearn import datasets, linear_model
>>> from sklearn.model_selection import cross_val_score
>>> diabetes = datasets.load_diabetes()
>>> X = diabetes.data[:150]
>>> y = diabetes.target[:150]
>>> lasso = linear_model.Lasso()
>>> print(cross_val_score(lasso, X, y, cv=3))
[0.3315057  0.08022103 0.03531816]
```

Linear Model trained with Lasso prior as regularizer

Lasso = Least Absolute Shrinkage and Selection Operator

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Scikit-Learn

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Models can be fit using the `fit()` function.
E.g., Random Forest Classifier,


```
>>> from sklearn.ensemble import RandomForestClassifier
>>> clf = RandomForestClassifier(random_state=0)
>>> X = [[ 1,  2,  3],  # 2 samples, 3 features
...      [11, 12, 13]]
>>> y = [0, 1]  # classes of each sample
>>> clf.fit(X, y)
RandomForestClassifier(random_state=0)
```

`fit()` Generally accepts 2 inputs

- Sample matrix X—typically 2d array (n_samples, n_features)
- Target values Y—real numbers for regression, integer for classification

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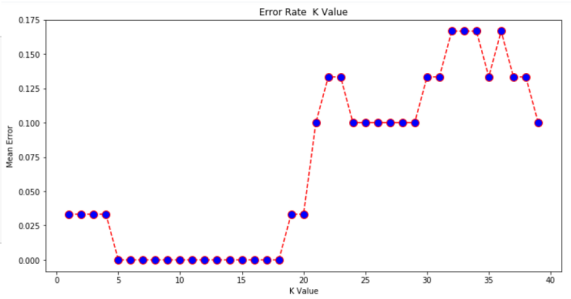
k-Nearest Neighbors

Train / evaluate the KNN classifier for each value K,

```
from sklearn.neighbors import KNeighborsClassifier
error = []

# Calculating error for K values between 1 and 40
for i in range(1, 40):
    knn = KNeighborsClassifier(n_neighbors=i)
    knn.fit(X_train, y_train)
    pred_i = knn.predict(X_val)
    error.append(np.mean(pred_i != y_val))
```

↑ vector operation!



in practice: use geometric grid like 1,2,4,8,…

Print error:

```
plt.figure(figsize=(12, 6))
plt.plot(range(1, 40), error, color='red', linestyle='dashed', marker='o',
         markerfacecolor='blue', markersize=10)
plt.title('Error Rate K Value')
plt.xlabel('K Value')
plt.ylabel('Mean Error')
```

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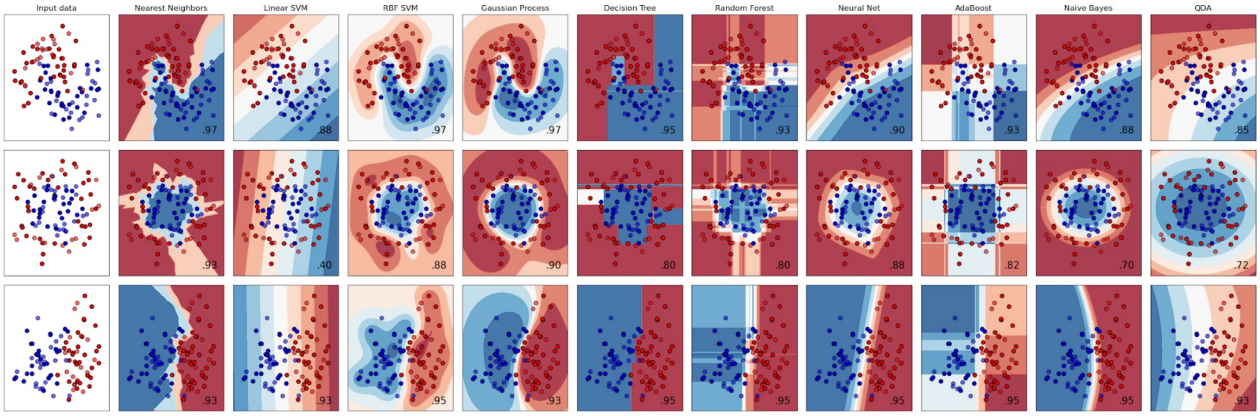
Scikit-Learn

Easily try out *all* the classifiers…



See full code.

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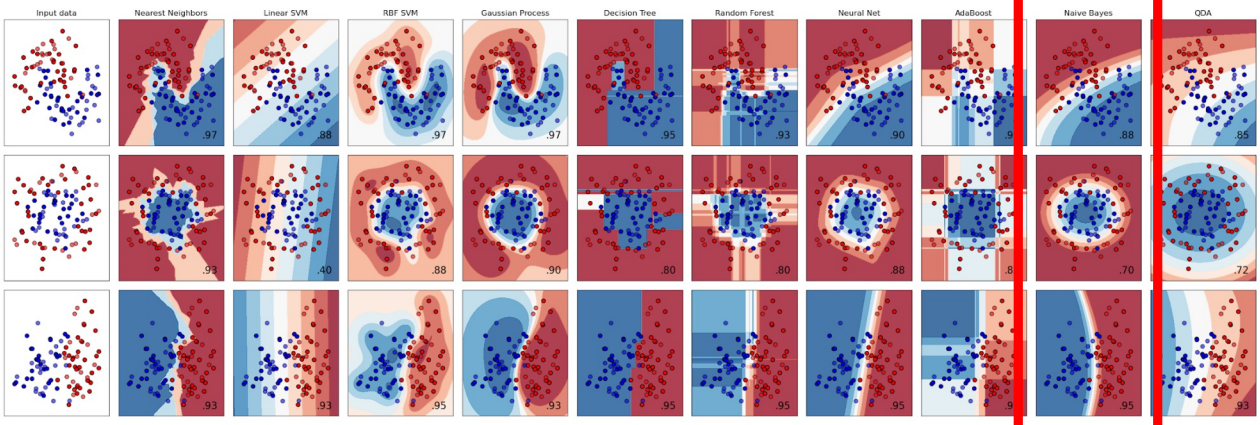
Scikit-Learn

Easily try out *all* the classifiers…

Naïve Bayes



See full code.