Computer Science

CSC380: Principles of Data Science

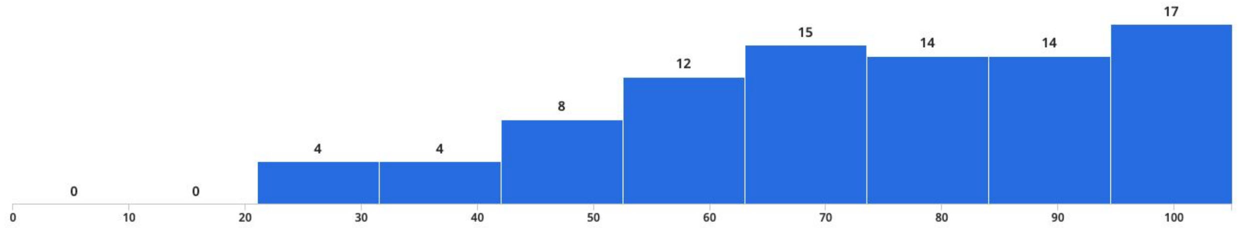
Predictive Modeling and Classification 2

Xinchen Yu

Midterm statistics

Total points 100:

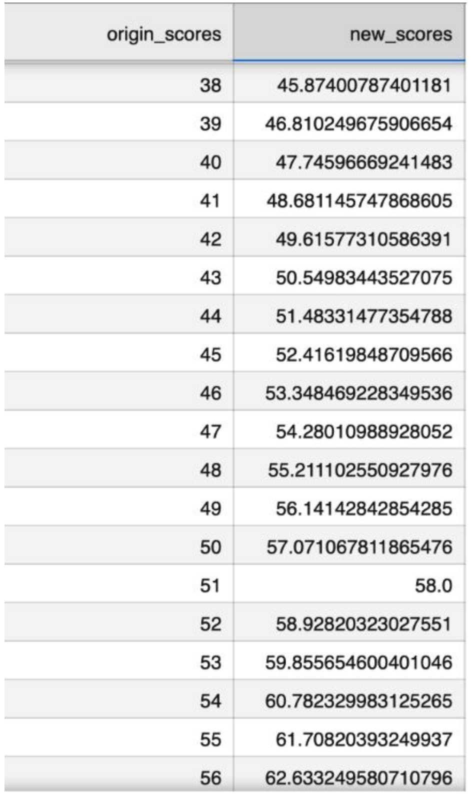
- 8 students = 100
- 24 students >= 90
- 35 students >= 80



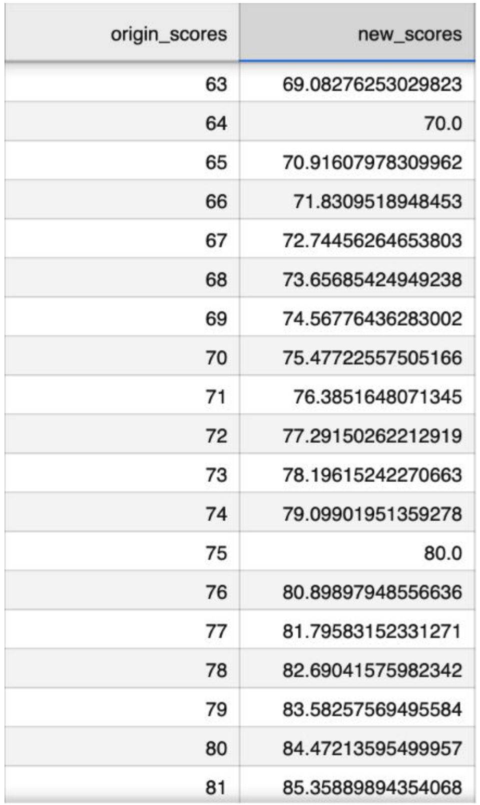
Minimum	Median	Maximum	Mean	Std Dev
27.0	74.25	105.0	72.42	20.94

Midterm score curving

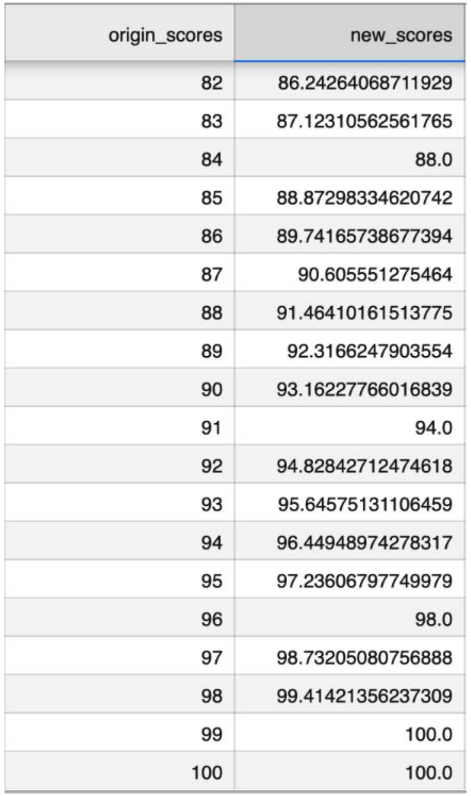
$$new = score + \sqrt{1 - score}$$



origin_scores	new_scores
38	45.87400787401181
39	46.810249675906654
40	47.74596669241483
41	48.681145747868605
42	49.61577310586391
43	50.54983443527075
44	51.48331477354788
45	52.41619848709566
46	53.348469228349536
47	54.28010988928052
48	55.211102550927976
49	56.14142842854285
50	57.071067811865476
51	58.0
52	58.92820323027551
53	59.855654600401046
54	60.782329983125265
55	61.70820393249937
56	62.633249580710796



origin_scores	new_scores
63	69.08276253029823
64	70.0
65	70.91607978309962
66	71.8309518948453
67	72.74456264653803
68	73.65685424949238
69	74.56776436283002
70	75.47722557505166
71	76.3851648071345
72	77.29150262212919
73	78.19615242270663
74	79.09901951359278
75	80.0
76	80.89897948556636
77	81.79583152331271
78	82.69041575982342
79	83.58257569495584
80	84.47213595499957
81	85.35889894354068



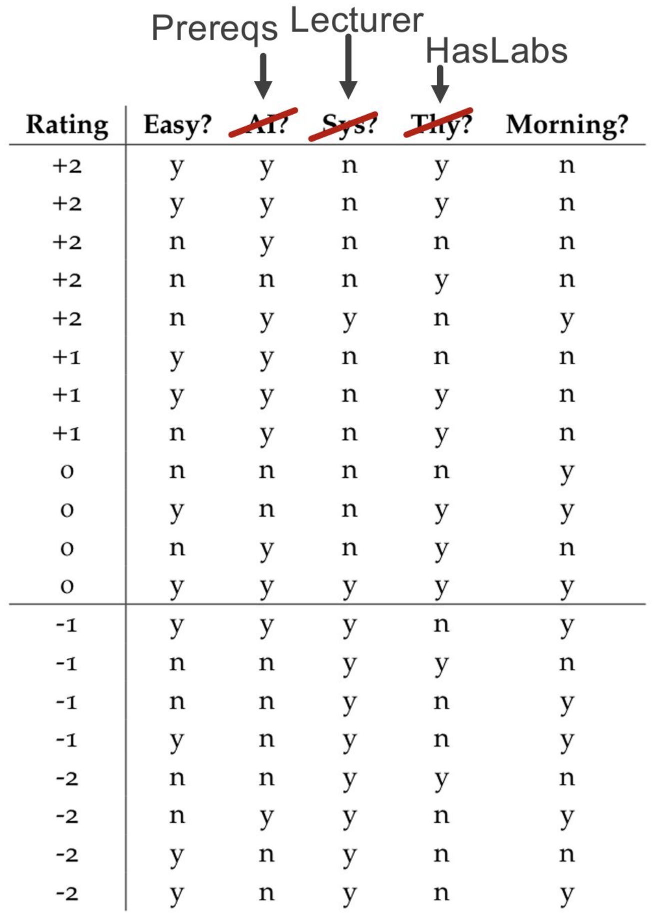
origin_scores	new_scores
82	86.24264068711929
83	87.12310562561765
84	88.0
85	88.87298334620742
86	89.74165738677394
87	90.605551275464
88	91.46410161513775
89	92.3166247903554
90	93.16227766016839
91	94.0
92	94.82842712474618
93	95.64575131106459
94	96.44948974278317
95	97.23606797749979
96	98.0
97	98.73205080756888
98	99.41421356237309
99	100.0
100	100.0

Outline

- Decision tree variations
- KNN
- Model selections and evaluations

How to construct a tree

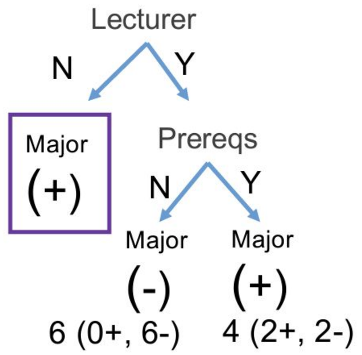
- Assign all training instances to the root of the tree. Set current node to root node.
- For each feature:
  a. Partition all data instances at the node by the value of the feature.
  b. Compute the accuracy from the partitioning.
- Identify feature that results in the highest accuracy. Set this feature to be the splitting criterion at the current node.


Prereqs
Lecturer
HasLabs

Rating	Easy?	~~AI?~~	~~Sys?~~	~~Thy?~~	Morning?
+2	y	y	n	y	n
+2	y	y	n	y	n
+2	n	y	n	n	n
+2	n	n	n	y	n
+2	n	y	y	n	y
+1	y	y	n	n	n
+1	y	y	n	y	n
+1	n	y	n	y	n
0	n	n	n	n	y
0	y	n	n	y	y
0	n	y	n	y	n
0	y	y	y	y	y
-1	y	y	y	n	y
-1	n	n	y	y	n
-1	n	n	y	n	y
-1	y	n	y	n	y
-2	n	n	y	y	n
-2	n	y	y	n	y
-2	y	n	y	n	n
-2	y	n	y	n	y

How to construct a tree

- Partition all instances according to attribute value of the best feature.
- Denote each partition as a child node of the current node.
- For each child node:
  a. If the child node is “pure” (has instances from only one class) tag it as a leaf and return.
  b. If not set the child node as the current node and recurse to step 2.

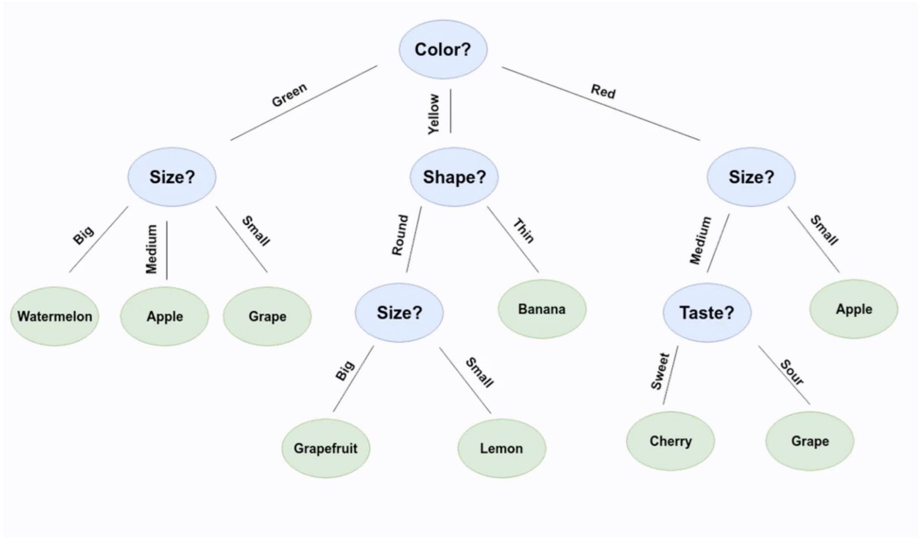


Types of features

- 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 $c \in C$.

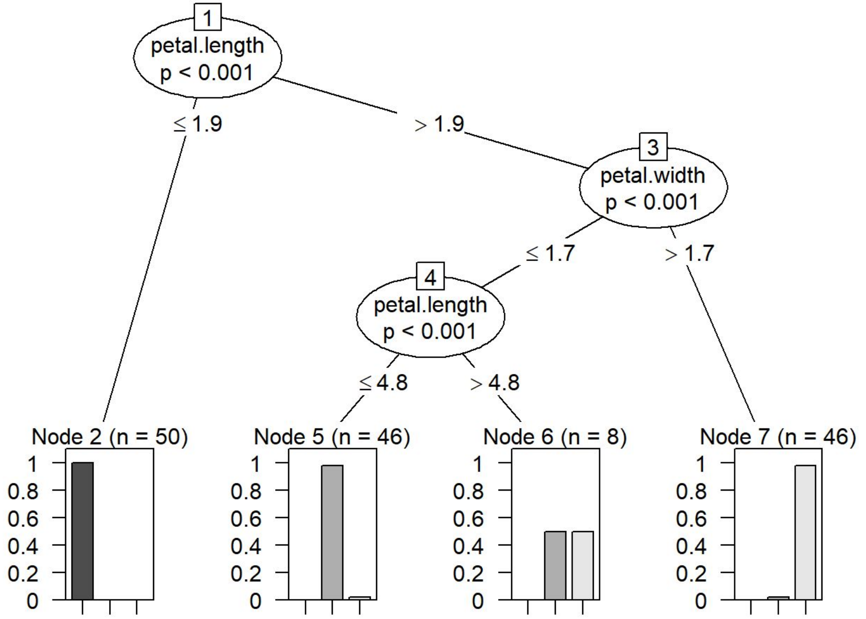
↑ binary features!

Option 1:



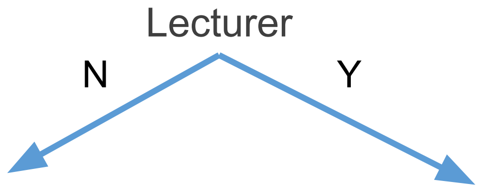
Types of labels

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



Iris Versicolor **Iris Setosa** **Iris Virginica**

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)?

Different selection criterions

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

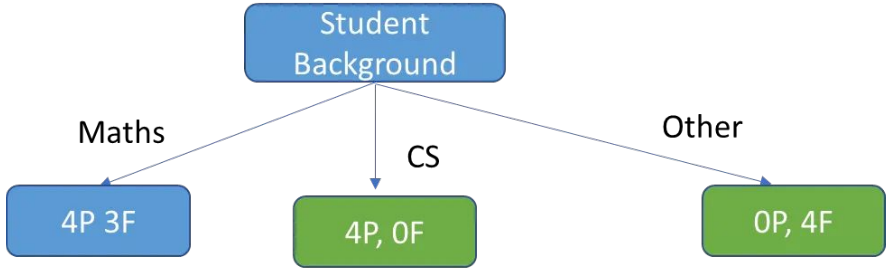
Each is *maximized* when $p_k = 1/|\mathcal{Y}|$ for all $k \in \mathcal{Y}$
(i.e., equal numbers of each label in S)

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

Different selection criterions - Gini index

❷ **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

k-Nearest Neighbors (k-NN)

Background: Train Error vs Test Error

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

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

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

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

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.

k-nearest neighbor: main concept

- Train set: $S = \{ (x^{(1)}, y^{(1)}), \ldots , (x^{(m)}, y^{(m)})\}$

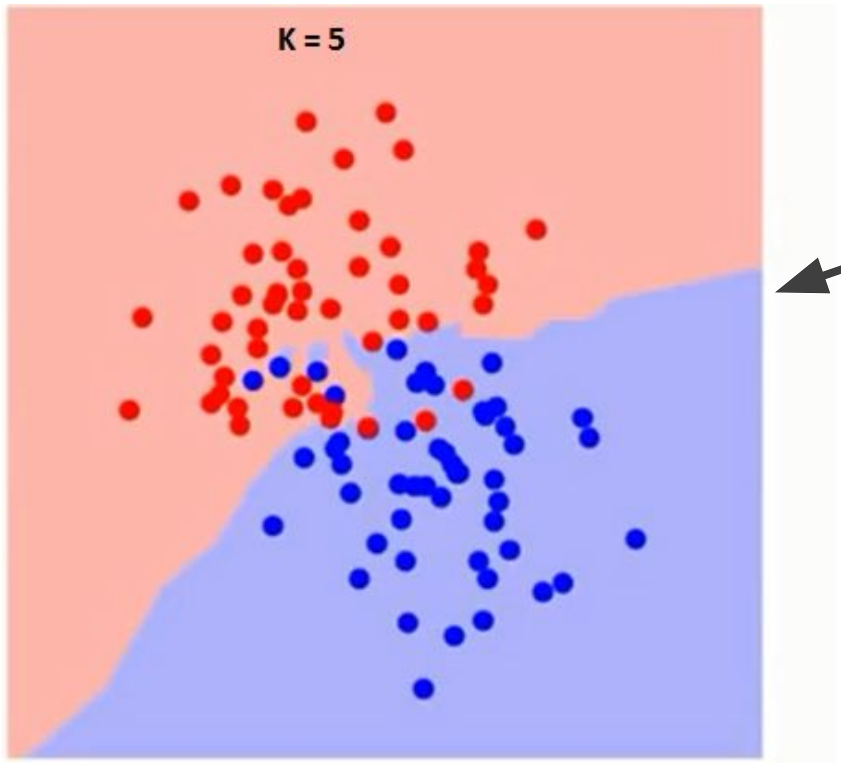
- **<u>Idea</u>**: given a new, unseen data point x, its label should resemble the labels of **nearby points**

- 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.

k-NN example



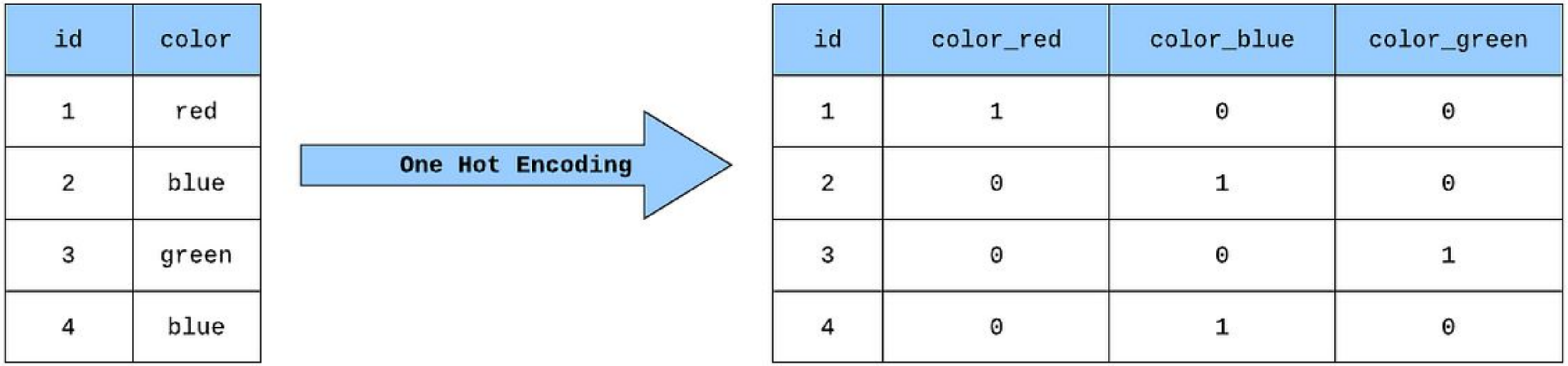
decision boundary

Basics

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



id	color
1	red
2	blue
3	green
4	blue

One Hot Encoding

id	color_red	color_blue	color_green
1	1	0	0
2	0	1	0
3	0	0	1
4	0	1	0

Basics

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

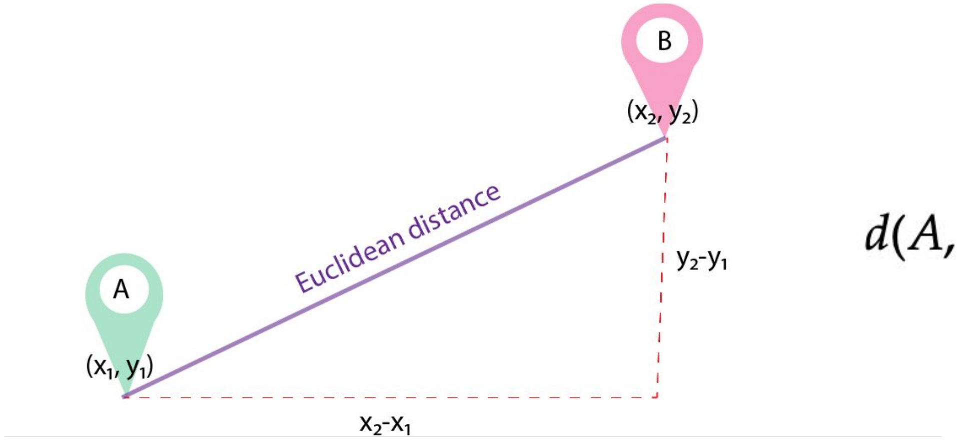
Distance:

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

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

Euclidean distance

Suppose there are only 2 features,
and we have 2 data points A and B:



$$d(A,B) = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}$$

Q: If we shift a feature, would the distance change? no

Q: What about scaling a feature? yes

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.

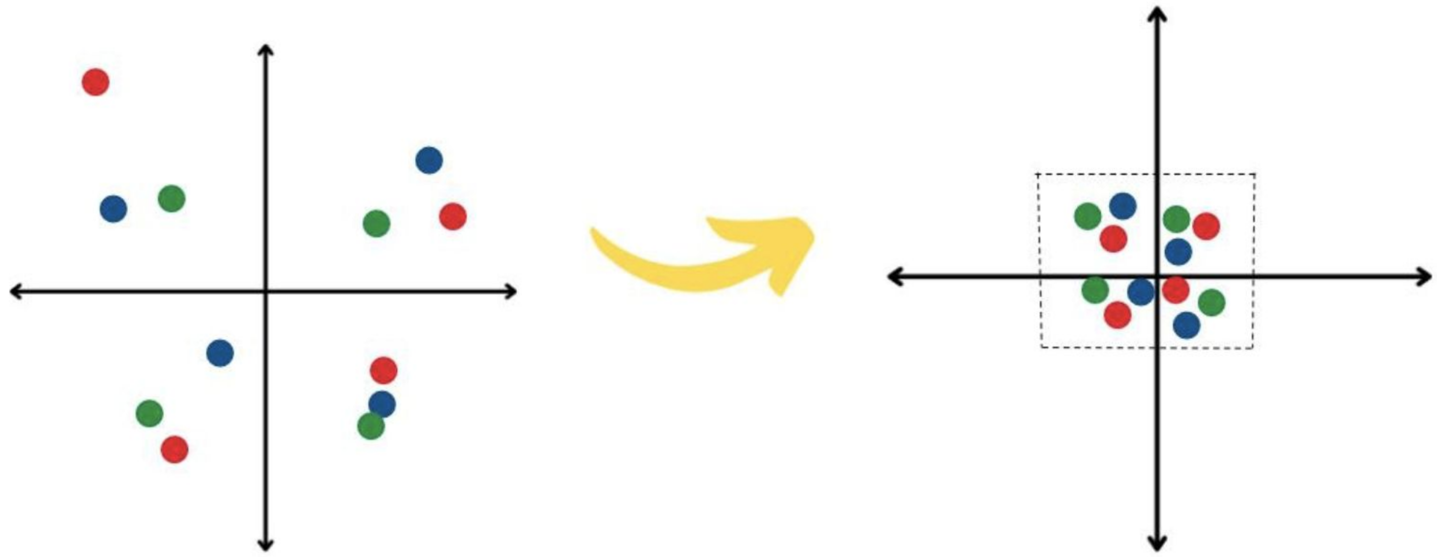
Make sure features are scaled fairly

- Features having different scale can be problematic. (e.g., weights in lbs vs shoe size)
- [Definition] **Standardization**
  - 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 $x_f^* \leftarrow \frac{x_f^* - \mu_f}{\sigma_f}, \forall f$

Standardization



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

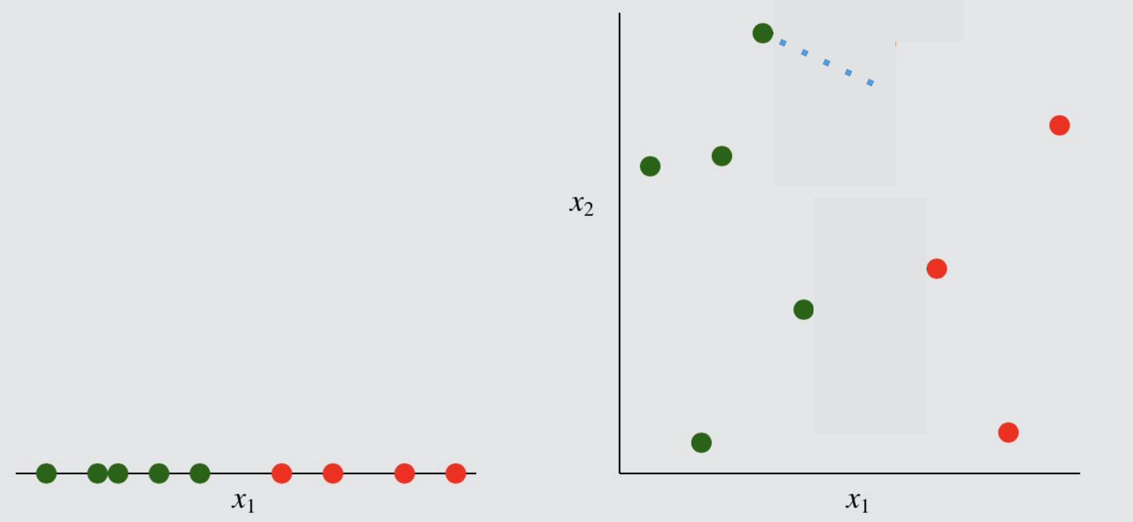
k-NN Summary

- 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)

Issues 1: irrelevant features

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

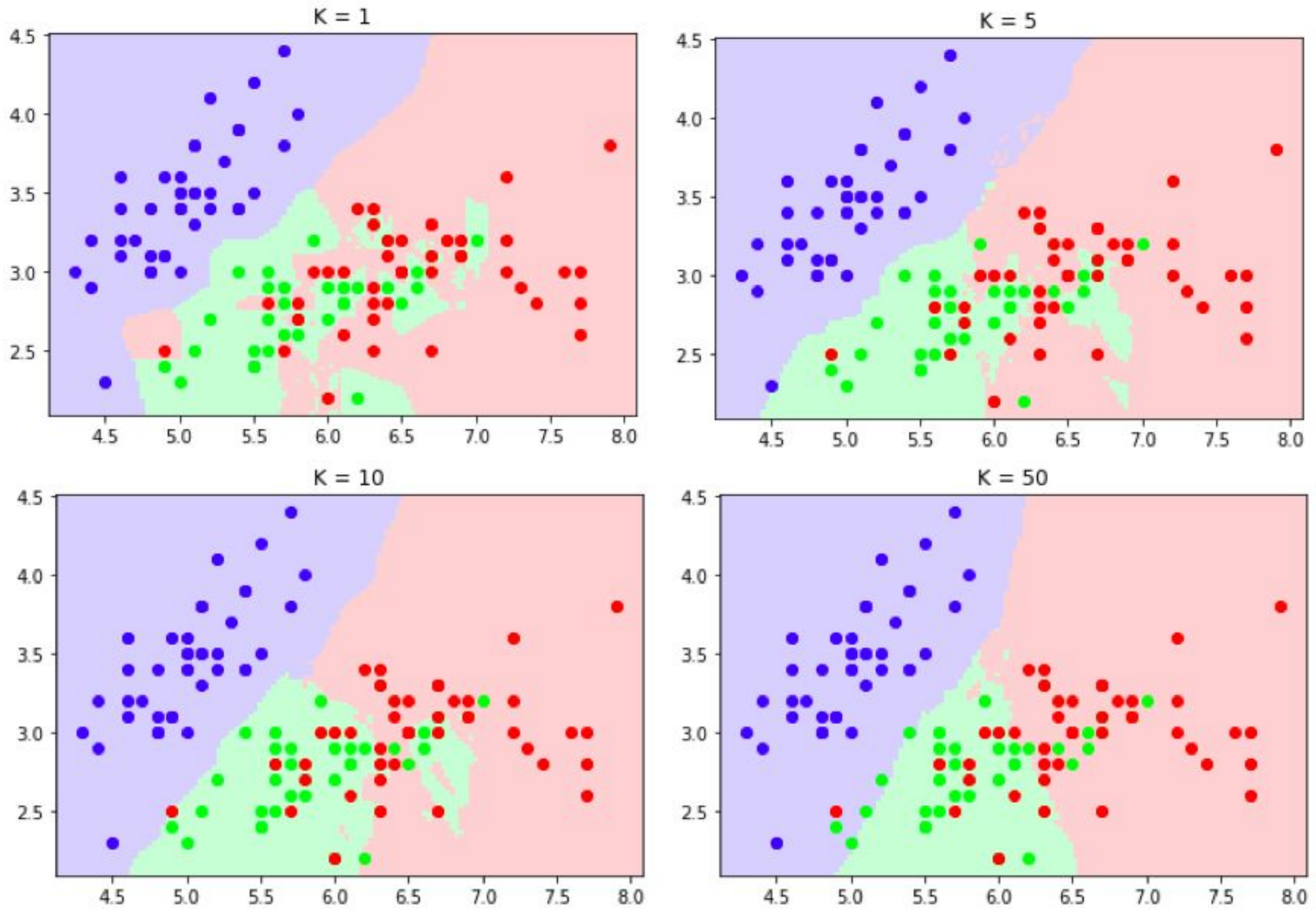
consider the effect of an irrelevant feature x_2 on distances and nearest neighbors



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

Issue 2: choosing k



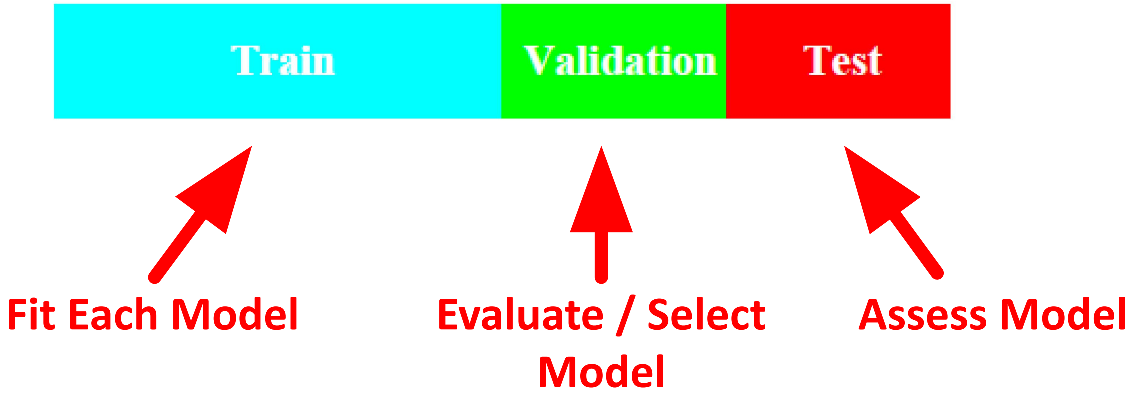
Comparison

	Decision Tree	k-NN
• Interpretability	good	bad
• Sensitivity to irrelevant features	low	high
• train time	$O(dm^2 + dm\log m)$	$O(dm)$
• test time	depth of the tree worst: $O(\min\{d, m\})$ best: $\log(m)$	$O(m(d + \log(m)))$ bad
• test time space complexity	worst: $O(m)$ in general: much smaller	$\Theta(dm)$

Model Selection and Evaluation

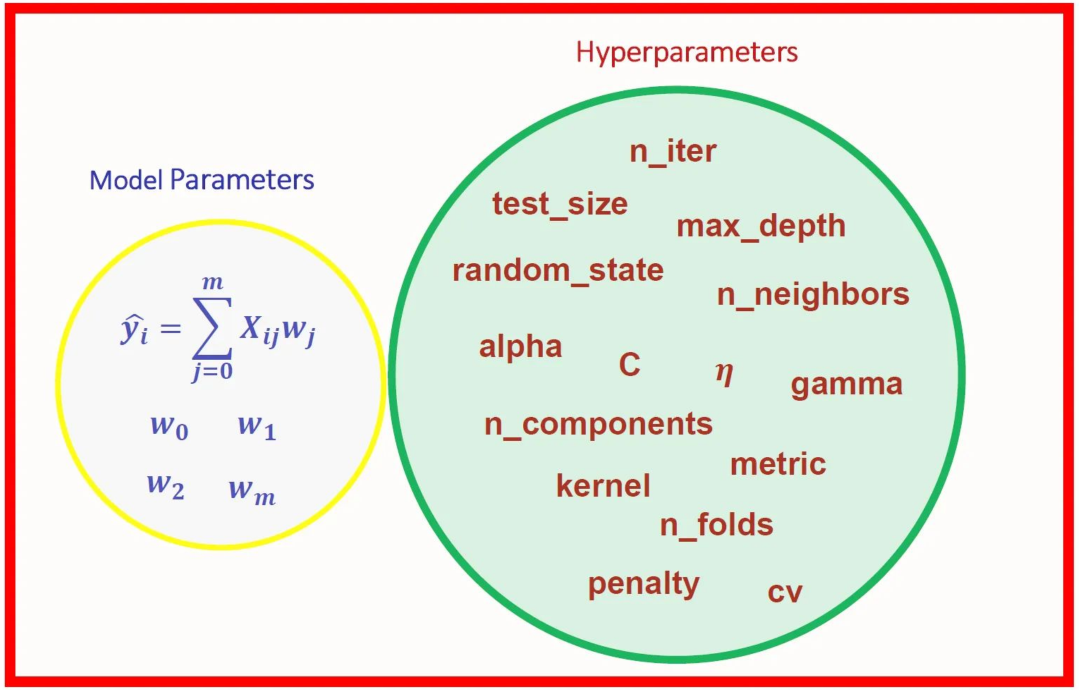
Model Selection / Assessment

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.

Hyperparameters vs Parameters



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

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

Tuning hyperparameters

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.

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, …

Tuning hyperparameters

K-fold cross validation

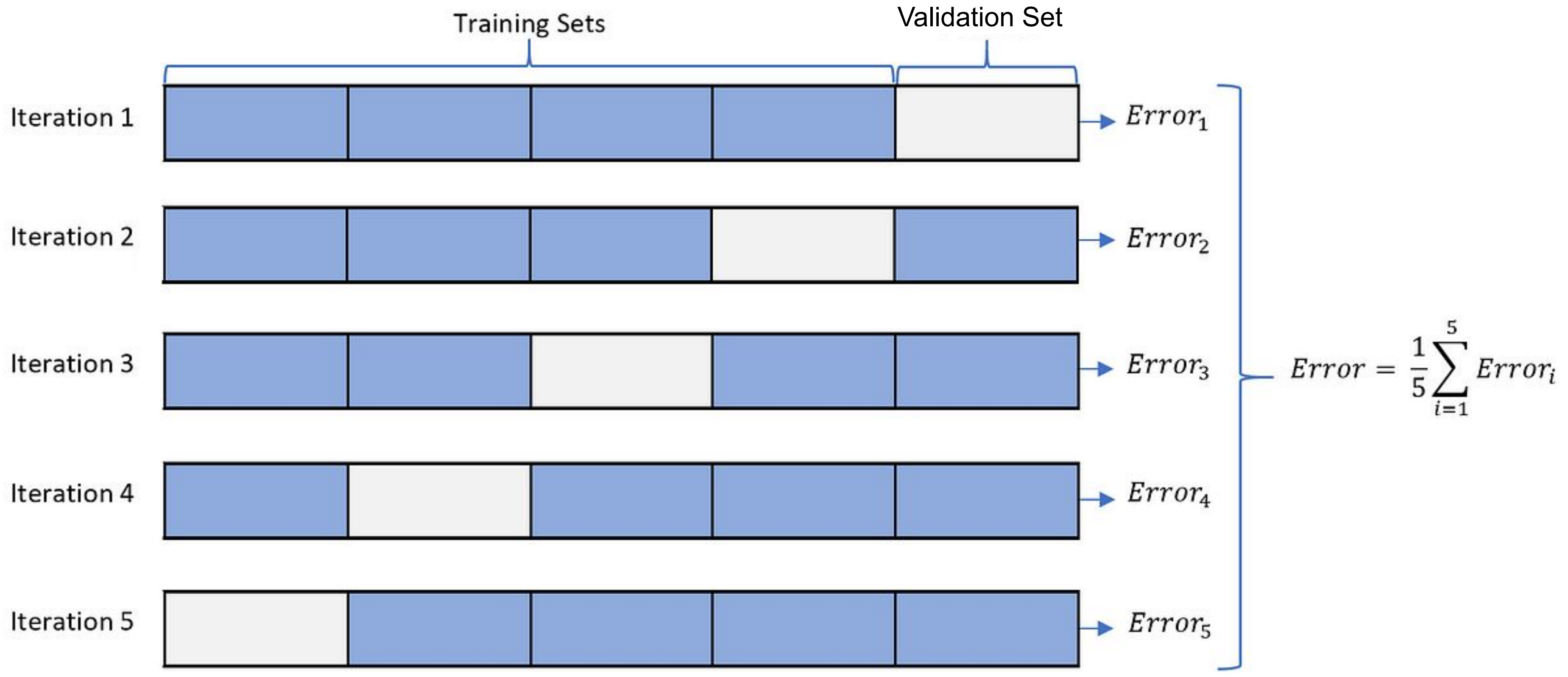
- Randomly partition train set S into K disjoint sets; call them $\mathrm{fold}_1, \dots, \mathrm{fold}_K$
- For each hyperparameter $h \in \{1, \dots, H\}$

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

  - For each $k \in \{1, \dots, K\}$
    - train $\hat{f}_k^h$ with $S \setminus \mathrm{fold}_\mathrm{k}$
    - 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.

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

5-fold cross validation



Scikit-Learn

Python library for machine learning. Install using Anaconda:

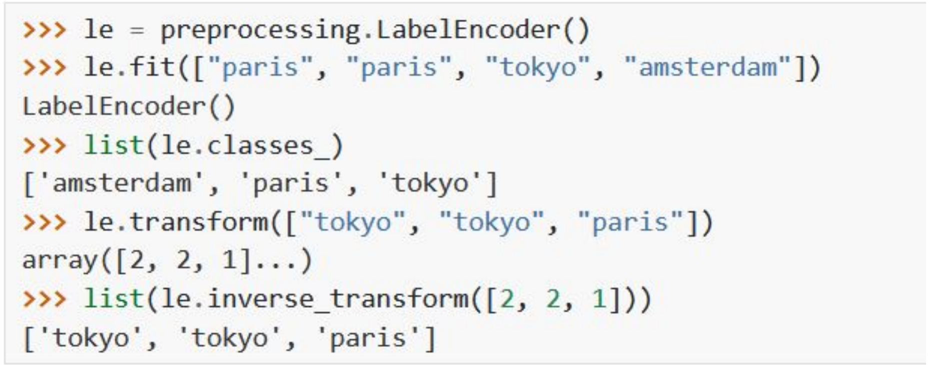
```
$ conda install -c conda-forge scikit-learn
```

Or using PyPi:

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

Preprocessing : Encoding Labels

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']
```

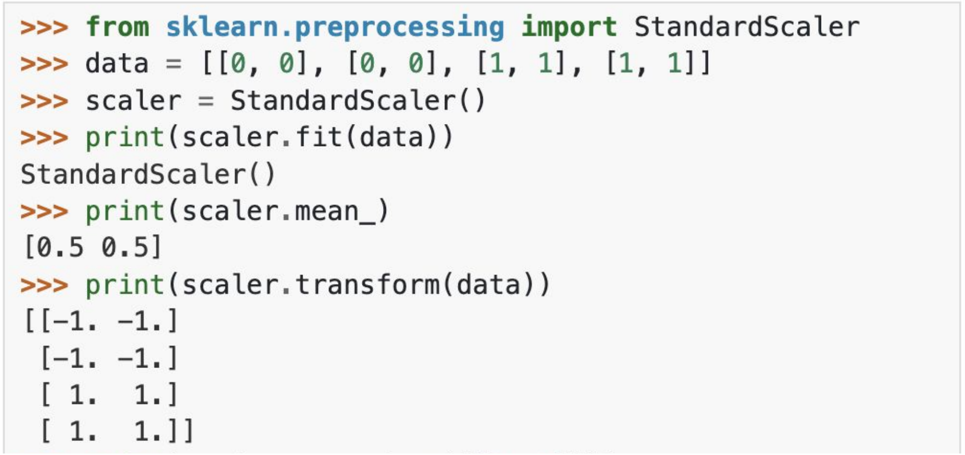
`LabelEncoder` transforms these into integer values, e.g. for categorical distributions

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

Preprocessing : Z-Score

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)

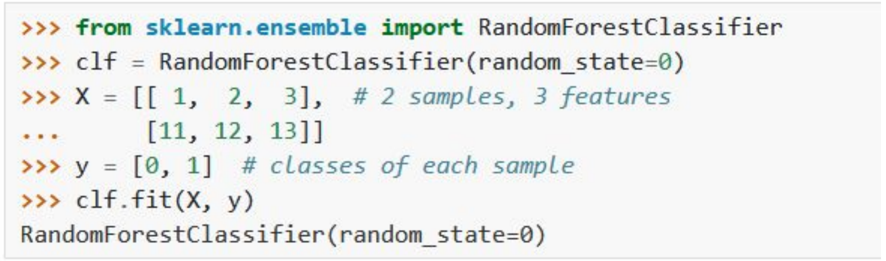
Cross-Validation

Easily do cross validation for model selection / evaluation…

```
from sklearn.model_selection import cross_val_score
import numpy as np

#create a new KNN model
knn_cv = KNeighborsClassifier(n_neighbors=3)

#train model with cv of 5
cv_scores = cross_val_score(knn_cv, X, y, cv=5)

#print each cv score (accuracy) and average them
print(cv_scores)
print('cv_scores mean:{}'.format(np.mean(cv_scores)))
```

Scikit-Learn

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

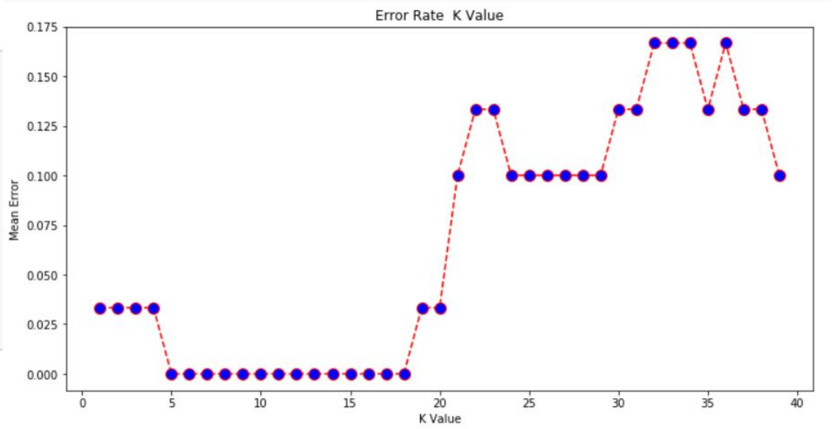
k-Nearest Neighbors

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')
```