CSC 461: Machine Learning

Fall 2024

k-Nearest Neighbors

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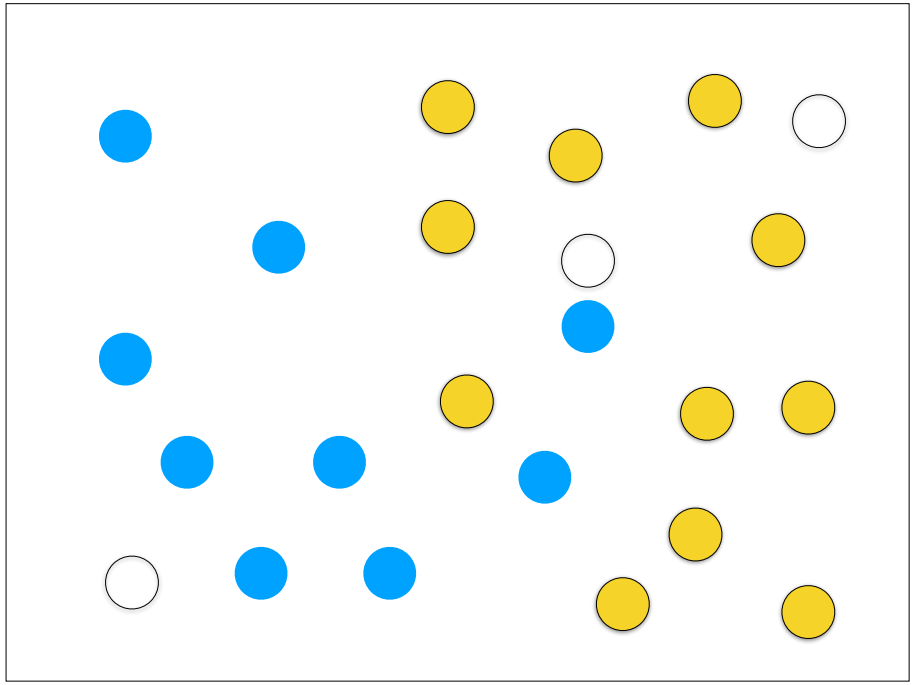
Instance-based learning

- Class of learning methods
  - also called **lazy learning**
- No explicit hypothesis is learned during "training"
- Training/learning phase
  - store instances
- Inference phase
  - computationally intensive



Nearest neighbor classification

- Training examples
  - $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$
  - typically $x_i \in \mathbb{R}^d$ but can work with any data type, given an appropriate distance function
- Learning
  - **store** all training examples, no explicit model is built
- Prediction
  - for a new example, find the closest point in the training set
  - **predict** the label of the new example as the label of the closest point

k-Nearest Neighbors

k-Nearest Neighbors

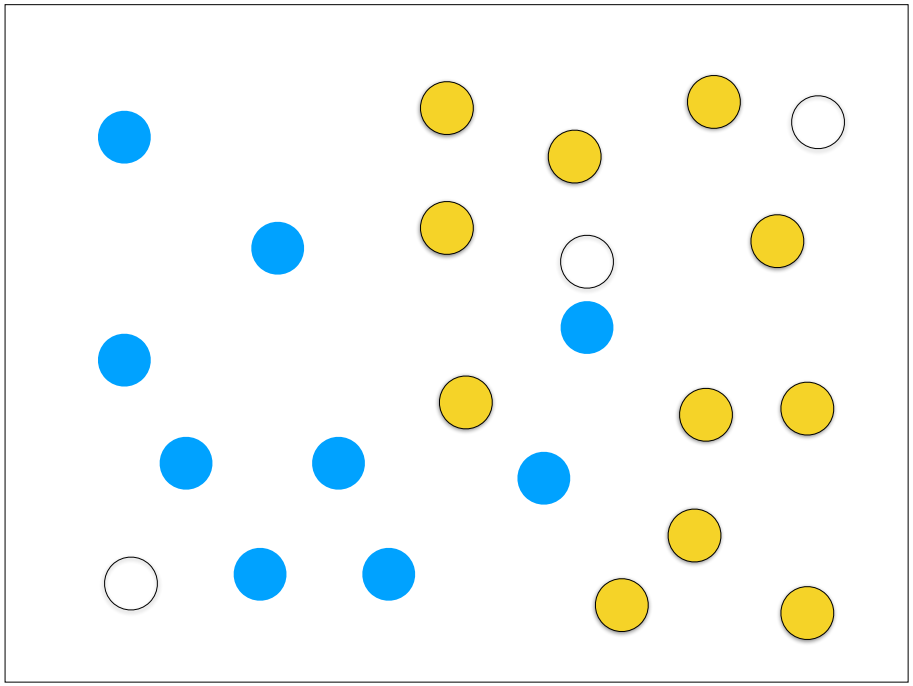
- Prediction for a new example x
  - recover a subset S_x (k **nearest neighbors to** x)

$$S_x \subseteq \mathcal{D} \text{ s.t. } |S_x| = k$$

$$\forall (x', y') \in \mathcal{D} \setminus S_x$$

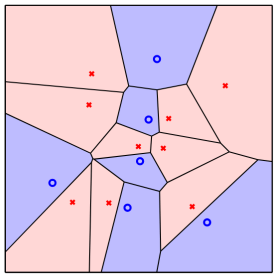
$$D(x, x') \geq \max_{(x'', y'') \in S_x} D(x, x'')$$

  - **classification**: predict the majority label in S_x
  - **regression**: predict the average of labels in S_x



Decision boundary

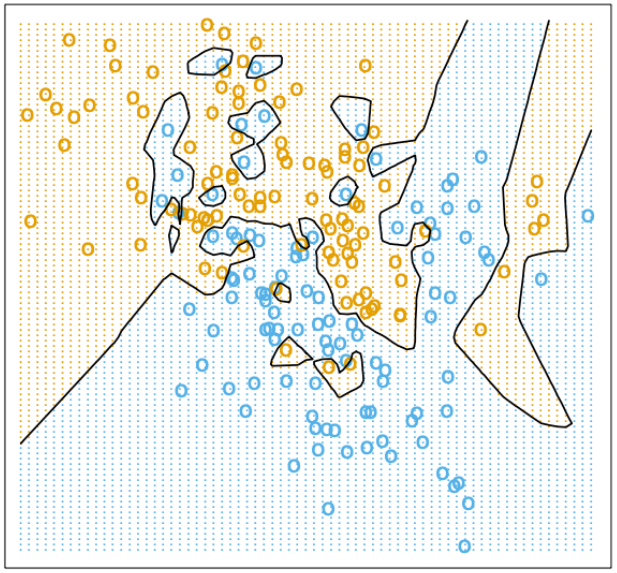
- Is k-NN building an explicit decision boundary?
  - k-NN does not explicitly construct a decision boundary
  - decision boundary is implicitly defined by the training data



Nearest neighbor Voronoi tesselation

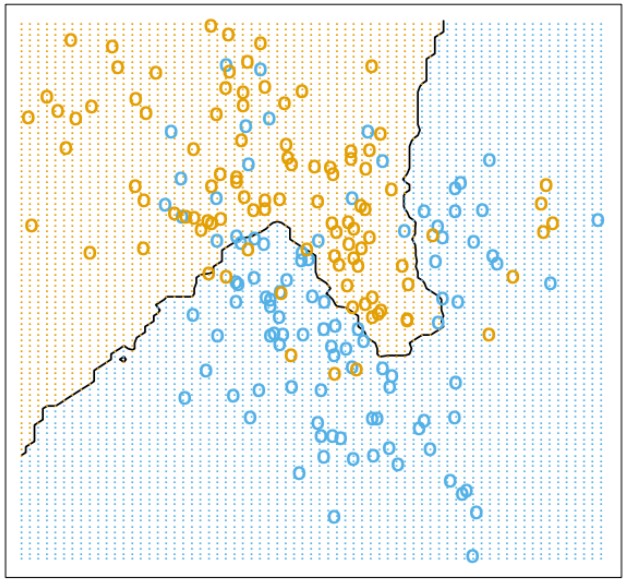
http://www.cs.rpi.edu/~magdon/courses/LFD-Slides/SlidesLect16.pdf

1-Nearest Neighbor Classifier



Elements of Statistical Learning (2nd Ed.) c Hastie, Tibshirani & Friedman 2009 Chap 2

15-Nearest Neighbor Classifier



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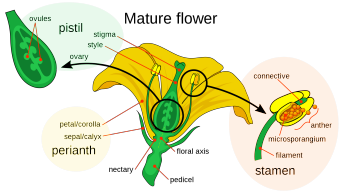
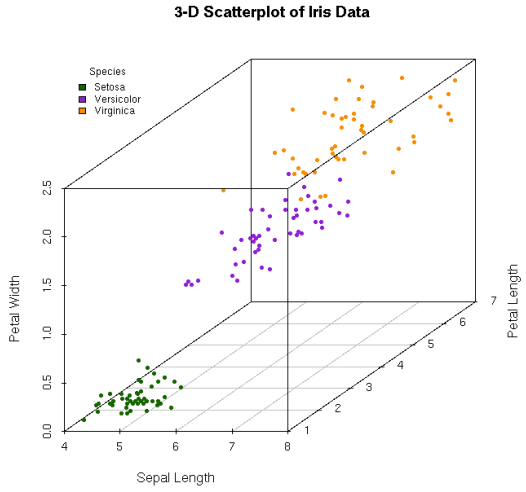
Iris dataset (example)

```
In [25]: from sklearn.datasets import load_iris

In [26]: data = load_iris()
In [30]: data.data.shape
Out[30]: (150, 4)

In [27]: idx = np.random.choice(np.arange(len(data.target)), 10)

In [28]: data.target[idx]
Out[28]: array([1, 0, 0, 1, 1, 1, 2, 0, 0, 2])

In [29]: data.data[idx]
Out[29]:
array([[6.6, 3. , 4.4, 1.4],
       [5. , 3.3, 1.4, 0.2],
       [4.7, 3.2, 1.3, 0.2],
       [5.7, 2.8, 4.1, 1.3],
       [6.1, 2.9, 4.7, 1.4],
       [6.3, 2.5, 4.9, 1.5],
       [6.3, 2.7, 4.9, 1.8],
       [5.4, 3.4, 1.7, 0.2],
       [4.6, 3.6, 1. , 0.2],
       [6.3, 2.9, 5.6, 1.8]])
```

sepal length, sepal width, petal length, petal width



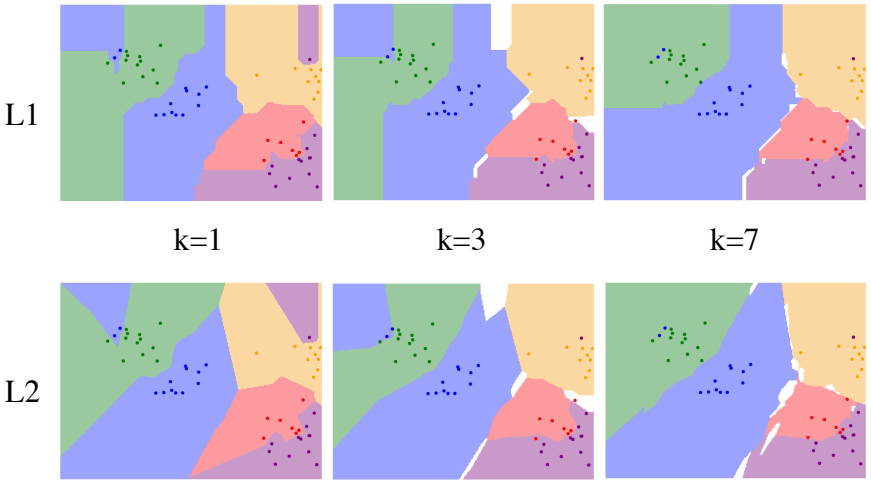
Iris dataset (example)



Hyperparameters

- The number of neighbors (K)
  - if too small, sensitive to noise
  - if too large, may include points from other classes
- Distance function
  - e.g., euclidean, manhattan, etc.
- How to find a value that may **generalize** better?
  - try multiple values and evaluate performance using an evaluation metric

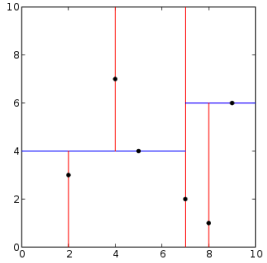
Different hyperparameters

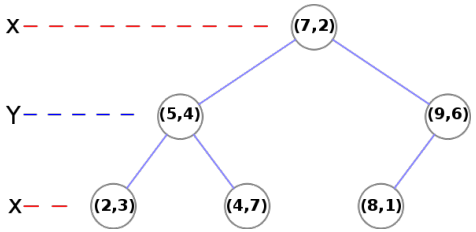


http://vision.stanford.edu/teaching/cs231n-demos/knn

Computational cost

- Calculating the nearest neighbors is expensive
  - does not scale well to large and/or high-dimensional datasets
- Can use advanced data structures and algorithms
  - insert the data (during learning/training) into a sophisticated data structure
  - perform search on the three more efficiently
  - e.g., kd-trees, ball trees





Additional remarks

Data normalization/scaling

- k-NN is sensitive to feature scales
  - e.g., using the euclidean distance

$$D(\mathbf{a}, \mathbf{b}) = \sqrt{\sum_{i=1}^{d} (a_i - b_i)^2}$$

- Solution: preprocess the data
  - e.g., standardize to zero mean and unit variance

$$x'_j = \frac{x_j - \mu_j}{\sigma_j}$$

apply this formula to all columns (features)

For certain datasets, the scale may be important

Data normalization/scaling

- Be careful …
  - must **calculate normalization parameters using training data** then apply same transformation to validation/test data

```
from sklearn import preprocessing
import numpy as np

# define the scaler object
scaler = preprocessing.StandardScaler()

# fit training data
scaler.fit(X_train)

# apply to training and test data
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

`sklearn.preprocessing`: Preprocessing and Normalization

The `sklearn.preprocessing` module includes scaling, centering, normalization, binarization methods.

User guide: See the Preprocessing data section for further details.

`preprocessing.Binarizer`(*[, threshold, copy])	Binarize data (set feature values to 0 or 1) according to a threshold.
`preprocessing.FunctionTransformer`([func, ...])	Constructs a transformer from an arbitrary callable.
`preprocessing.KBinsDiscretizer`([n_bins, ...])	Bin continuous data into intervals.
`preprocessing.KernelCenterer`()	Center an arbitrary kernel matrix K.
`preprocessing.LabelBinarizer`(*[, neg_label, ...])	Binarize labels in a one-vs-all fashion.
`preprocessing.LabelEncoder`()	Encode target labels with value between 0 and n_classes-1.
`preprocessing.MultiLabelBinarizer`(*[, ...])	Transform between iterable of iterables and a multilabel format.
`preprocessing.MaxAbsScaler`(*[, copy])	Scale each feature by its maximum absolute value.
`preprocessing.MinMaxScaler`([feature_range, ...])	Transform features by scaling each feature to a given range.
`preprocessing.Normalizer`([norm, copy])	Normalize samples individually to unit norm.
`preprocessing.OneHotEncoder`(*[, categories, ...])	Encode categorical features as a one-hot numeric array.
`preprocessing.OrdinalEncoder`(*[, ...])	Encode categorical features as an integer array.
`preprocessing.PolynomialFeatures`([degree, ...])	Generate polynomial and interaction features.
`preprocessing.PowerTransformer`([method, ...])	Apply a power transform featurewise to make data more Gaussian-like.
`preprocessing.QuantileTransformer`(*[, ...])	Transform features using quantiles information.
`preprocessing.RobustScaler`(*[, ...])	Scale features using statistics that are robust to outliers.
`preprocessing.SplineTransformer`([n_knots, ...])	Generate univariate B-spline bases for features.
`preprocessing.StandardScaler`(*[, copy, ...])	Standardize features by removing the mean and scaling to unit variance.

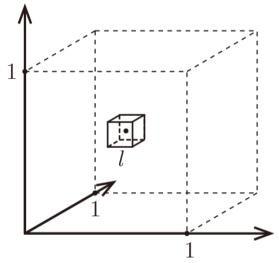
https://scikit-learn.org/stable/modules/classes.html#module-sklearn.preprocessing

kNN regression

- Prediction
  - find the k nearest neighbors
  - return the average label of the k nearest neighbors

Curse of dimensionality

- In high-dimensional spaces, the concept of distance starts to lose its meaning



Assume **n** points are **uniformly distributed** and we are looking for the **k** nearest neighbors in **d** dimensions

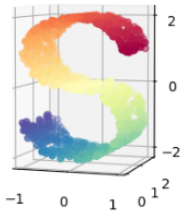
Now think about the volume of the minimal enclosing box for the set of **k** nearest neighbors

$$l^d \approx \frac{k}{n}$$

`Solve for l and play with different values for d`

Why k-NN might work?

- Data is not always uniformly distributed over *d* dimensions
  - data distribution *P* may be lying on a low-dimensional subspace (low intrinsic dimensionality) or on an underlying manifold
  - local distances (such as nearest neighbors) work better than global distances



Summary

- No assumptions about data distribution *P*
  - adapts to data density
- Cost of training/learning is zero
  - unless a **kd-tree** or other data structures are used
- Recommended to normalize/scale the data
  - features with larger ranges dominate distances (automatically becoming more important)
  - be careful: sometimes range matters

Summary

- Irrelevant or correlated attributes add noise to distance
  - may want to drop them or use dimensionality reduction
- Prediction is computationally expensive
  - can use **kd-trees** or hashing techniques like **locality sensitive hashing** (LSH)
- Curse of dimensionality
  - data required to generalize grows exponentially with dimensionality
  - distances less meaningful in higher dimensions