Lecture 6 – KNN and Decision Trees

CS 335

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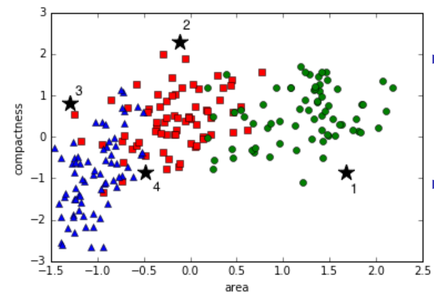
Nearest Neighbor Classification

Seed classification by area and compactness



- What should we predict for unlabeled test points (stars)?
- Nearest neighbor classification: predict label of nearest training example
- k-nearest neighbor: predict consensus of k nearest training examples

k-Nearest Neighbor Classification

- **Training**: store the training data (trivial!)

$$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}, \ldots (\mathbf{x}^{(m)}, y^{(m)})\}$$

- **Prediction**: for a new instance $\mathbf{x}$, predict label that is **most frequent** among k training examples **closest** to $\mathbf{x}$
- KNN can work with any distance function and any value of k. We need to choose these.

Distance and Similarity

- KNN can use any **distance function** to determine k nearest neighbors. A distance function $d(\mathbf{x}, \mathbf{x}')$ takes two data points and returns a distance. It should satisfy
  - $d(\mathbf{x}, \mathbf{x}') \geq 0$ (non-negativity)
  - $d(\mathbf{x}, \mathbf{x}') = 0$ (distance from a point to itself is zero)
- Or you can use a *similarity function*
  - $s(\mathbf{x}, \mathbf{x}') \geq 0$
  - $s(\mathbf{x}, \mathbf{x}) \geq s(\mathbf{x}, \mathbf{x}')$ for all other $\mathbf{x}'$ ($\mathbf{x}$ is more similar to itself than any other point)

Euclidean Distance

- We've already seen one distance function, the **Euclidean distance**:

$$d(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|$$

  - Length of straight line between $\mathbf{x}$ and $\mathbf{x}'$ (= vector norm of $\mathbf{x} - \mathbf{x}'$)

Minkowski Distance

- A more general class of distance functions come from **Minkowski Distance**

$$d_p(\mathbf{x}, \mathbf{x}') := \|\mathbf{x} - \mathbf{x}'\|_p$$

$$\|\mathbf{r}\|_p := \left(\sum_{i=1}^{n} |r_i|^p\right)^{1/p}$$

  - $p = 2$ is Euclidean distance (verify on own)
  - $p = 1$ is called the "Manhattan distance"

Examples

- Jupyter Demo 1: different distance functions

KNN Implementation

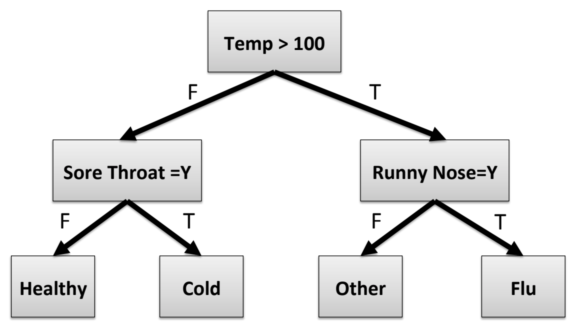
- The "brute force" version of KNN is very straightforward:
  - Given test point $\mathbf{x}$, compute distances $d^{(i)} := d(\mathbf{x}, \mathbf{x}^{(i)})$ to each training example
  - Sort training examples by distance
  - k-nearest neighbors = first k examples in this sorted list.
  - Now, making the prediction is straightforward.
  - **Running time**: $O(m \log m)$ for *one* prediction
- In practice, clever data structures (e.g., KD-trees) can be constructed to find k nearest neighbors and make predictions more quickly.

KNN Trade-Offs

- Strengths
  - Simple
  - Converges to the correct decision surface as data goes to infinity
- Weaknesses
  - Lots of variability in the decision surface when amount of data is low
  - Curse of dimensionality: everything is far from everything else in high dimensions
  - Running time and memory usage: store all training data and perform neighbor search for every prediction → use a lot of memory / time
- Jupyter Demo 2: KNN in action
  - Effect of k
  - KNN convergence as data goes to infinity

Decision Trees

Example: Flu decision tree



Decision Trees

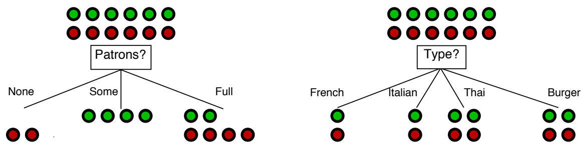
- Classical model for making a decision or classfication using "splitting rules" organized into tree data structure
- Data instance $\mathbf{x}$ is routed from the root to leaf
  - Nodes = "splitting rules"
    - Continuous variables: test if $(x_j < c)$ or $(x_j \geq c)$ (2 branches)
    - Discrete variables: test $(x_j = 1), (x_j = 2), \ldots$ for k possible values of x_j (k branches)
  - $\mathbf{x}$ goes down branch corresponding to result of test
  - Leaf nodes are assigned labels → prediction for $\mathbf{x}$

Decision Tree Intution

- Board work
  - Geometric illustration of decision tree: recursive axis-aligned partitioning
  - Intuition for how to partition to fit a dataset (= learning a decision tree)

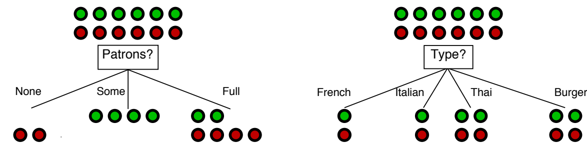
Decision Tree Learning

- How do we fit a decision tree to training data? We won't give details here, just some intuition...
- **Idea**: recursive splitting of training set



  - Start with all training examples at root of tree
  - Find "best" splitting rule at root
  - Recurse on each branch

Decision Tree Learning



- "Best" splitting rule? Which of these is better?
  - Ideally, split the examples into subsets that are all the same class
  - Design heuristics based on this principle to choose the best split
- When to stop? Recusively split training examples until:
  - All examples have same class
  - Too few data training examples
  - Maximum depth exceeded

Decision Tree Learning

- Jupyter Demo 3: visualize decision trees to fit to seeds dataset

Decision Tree Trade-Offs

- Strengths
  - **Interpretability**: the learned model is easy to understand
  - **Running time for predictions**: shallow trees can be extremely fast classifiers
- Weaknessees
  - **Running time for learning**: finding the optimal trees is computationally intractable (NP-complete), so we need to design greedy heuristics.
  - **Representation**: we may need very large trees to accurately model geometry of our problem with axis-aligned splits
- General advice: decision trees are very competitive "out-of-the-box" machine learning models for lots of problems!