Nearest Neighbor Methods

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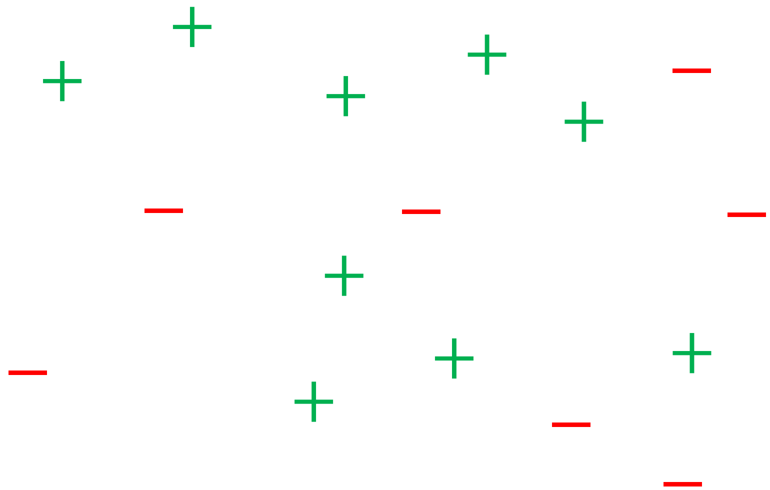
Based on the slides of Vibhav Gogate and David Sontag

Nearest Neighbor Methods

- Learning
  - Store all training examples
- Classifying a new point x'
  - Find the training example $(x^{(i)}, y^{(i)})$ such that $x^{(i)}$is closest (for some notion of close) to x'
  - Classify x' with the label $y^{(i)}$

Nearest Neighbor Methods



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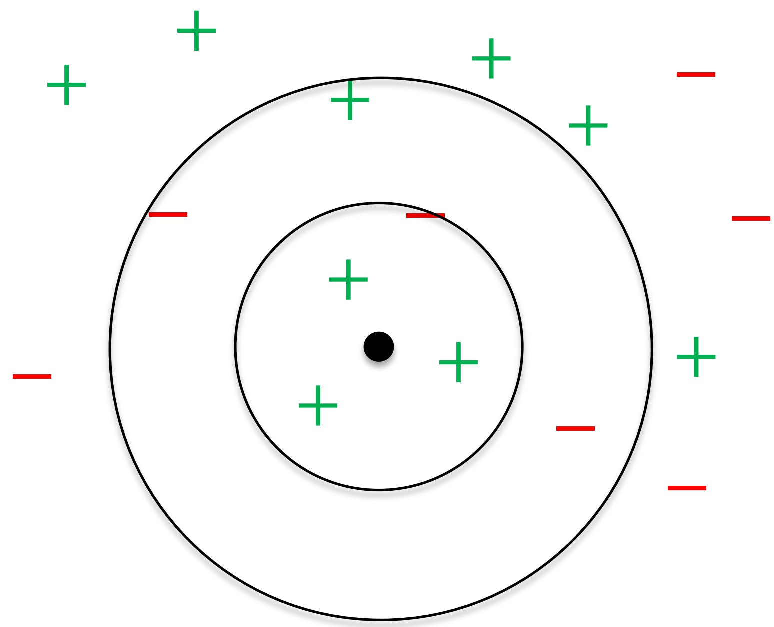

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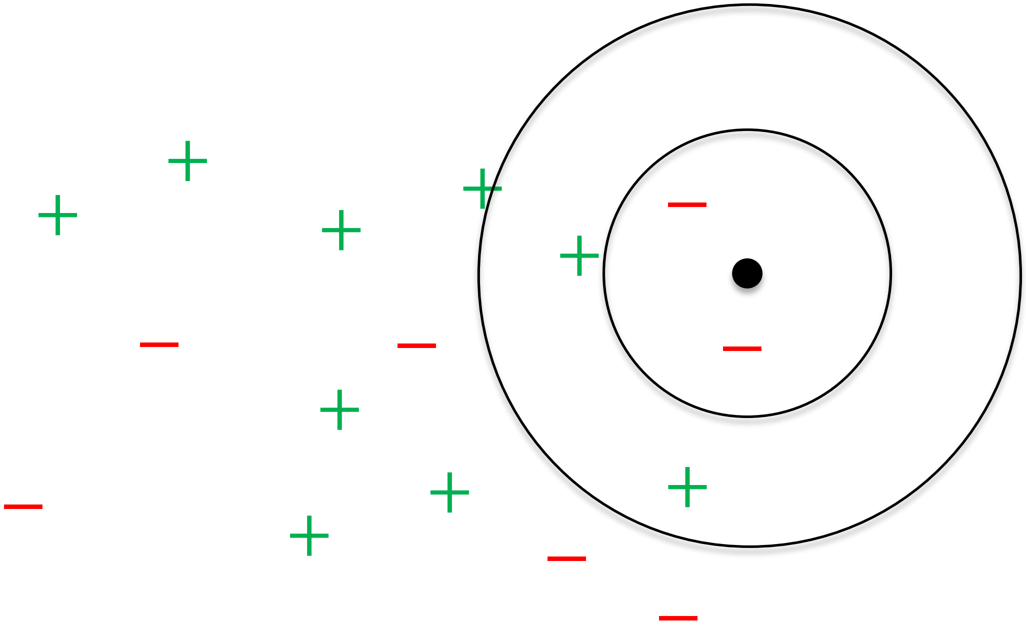

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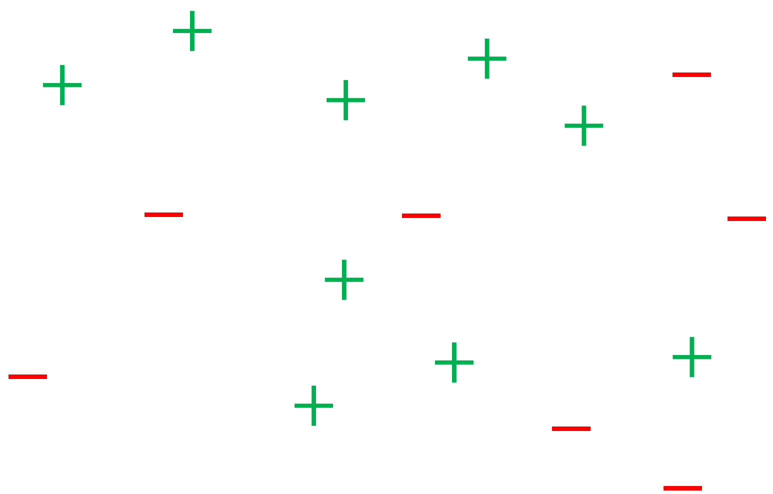

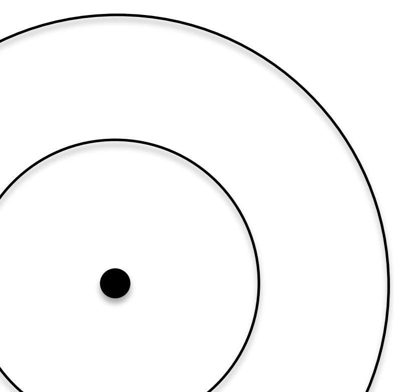

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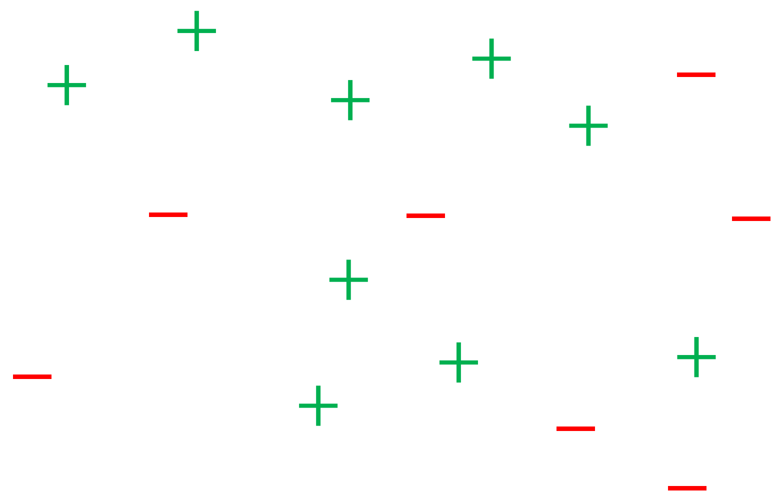
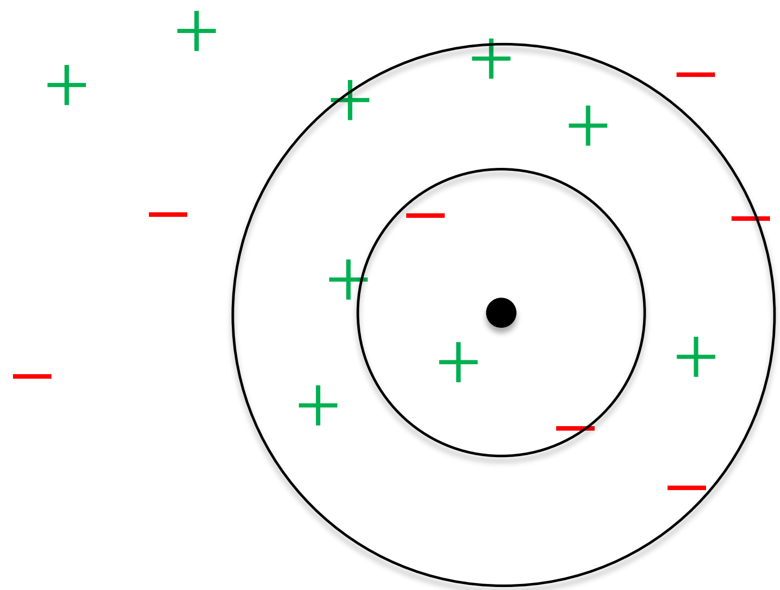


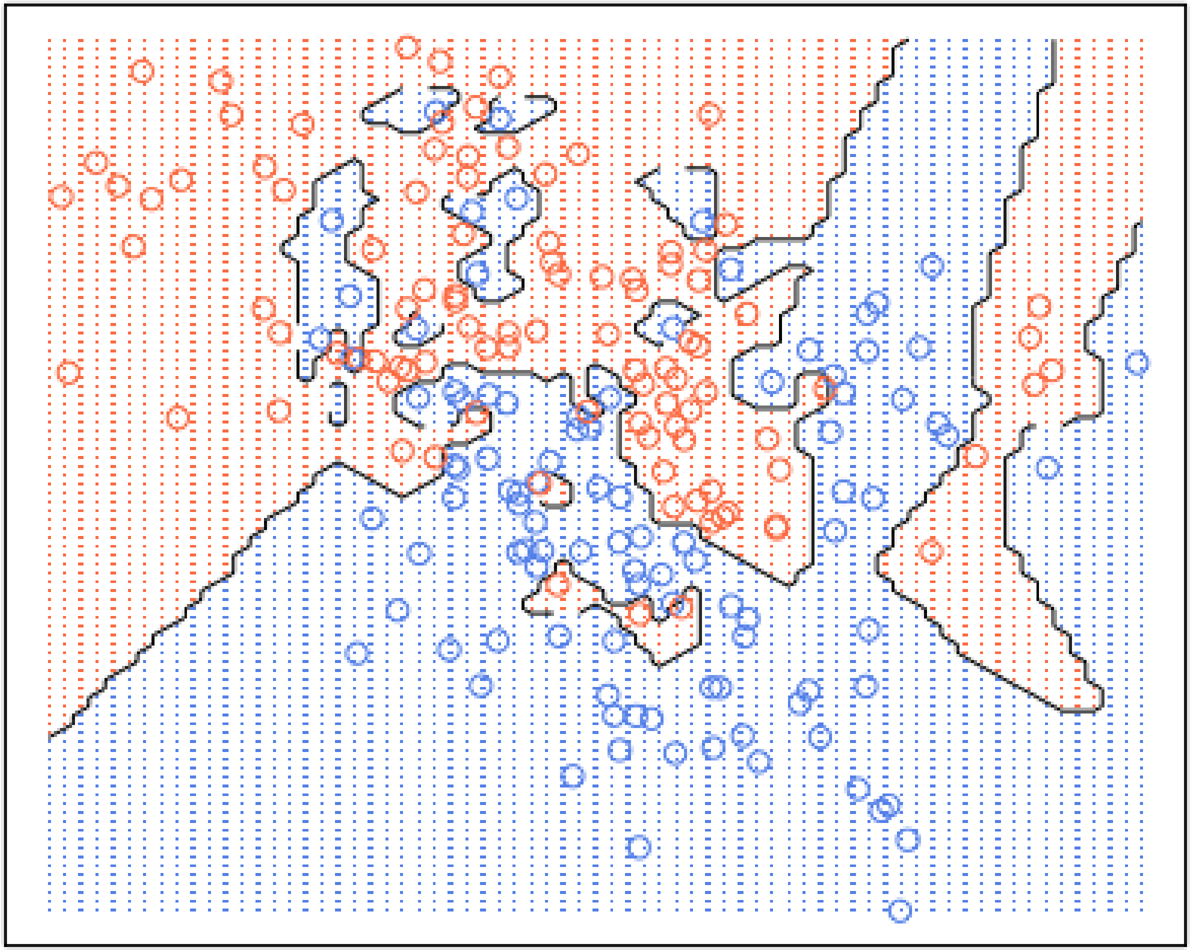
k-nearest neighbor methods look at the k closest points in the training set and take a majority vote (should choose k to be odd)

Nearest Neighbor Methods



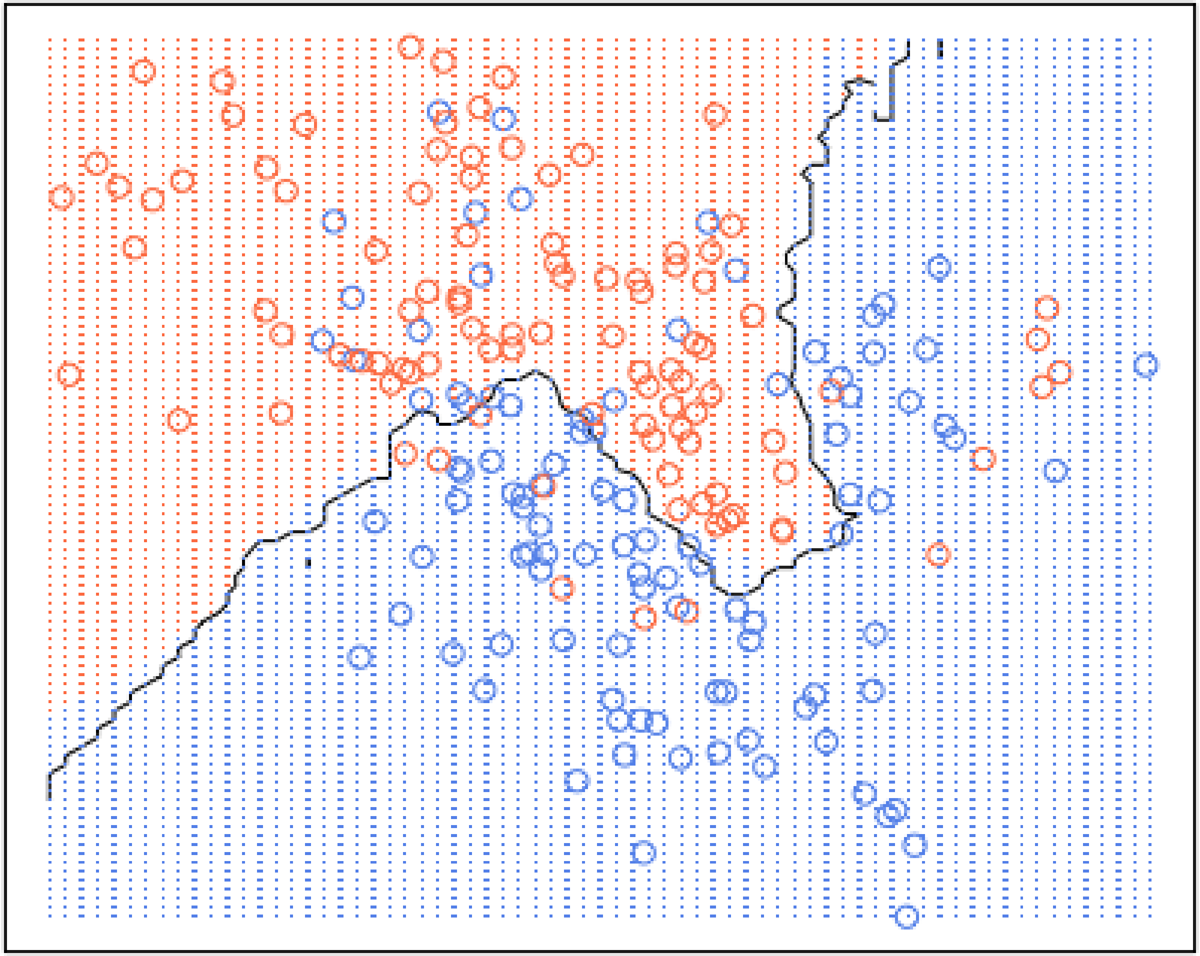
k-nearest neighbor methods look at the k closest points in the training set and take a majority vote (should choose k to be odd)

1-NN Example



[Kevin Zakka]

20-NN Example



[Kevin Zakka]

Nearest Neighbor Methods

- Applies to data sets with points in $\mathbb{R}^d$
  - Best for large data sets with only a few (< 20) attributes
- Advantages
  - Learning is easy
  - Can learn complicated decision boundaries
- Disadvantages
  - Classification is slow (need to keep the entire training set around)
  - Easily fooled by irrelevant attributes

Practical Challenges

- How to choose the right measure of closeness?
  - Euclidean distance is popular, but many other possibilities
- How to pick k?
  - Too small and the estimates are noisy, too large and the accuracy suffers
- What if the nearest neighbor is really far away?

Choosing the Distance

- Euclidean distance makes sense when each of the features is roughly on the same scale
  - If the features are very different (e.g., height and age), then Euclidean distance makes less sense as height would be less significant than age simply because age has a larger range of possible values
  - To correct for this, feature vectors are often scaled by the standard deviation over the training set

Normalization

- Sample mean

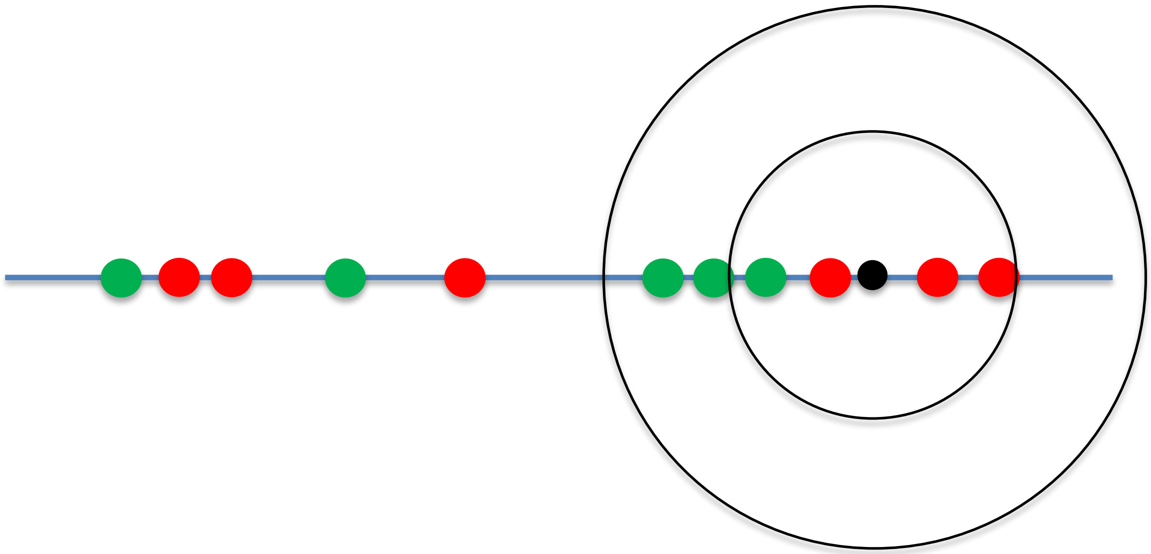
$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x^{(i)}$$

- Sample variance

$$\hat{\sigma}_k^2 = \frac{1}{n}\sum_{i=1}^{n} \left(x_k^{(i)} - \bar{x}_k\right)^2$$

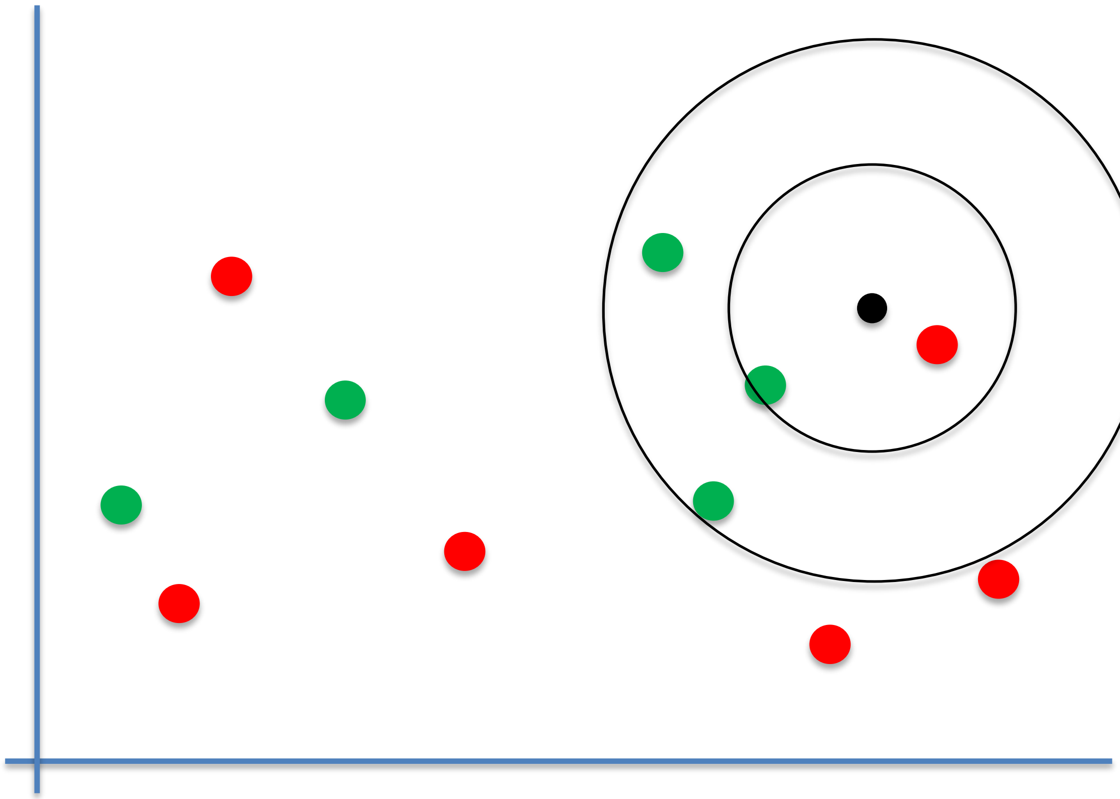
Irrelevant Attributes

Consider the nearest neighbor problem in one dimension



Irrelevant Attributes

Now, add a new attribute that is just random noise...



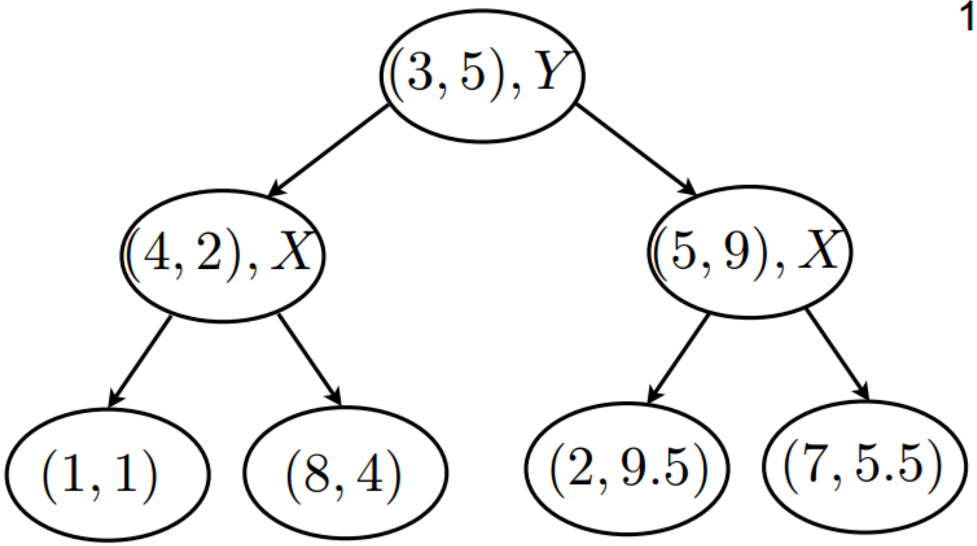
K-Dimensional Trees

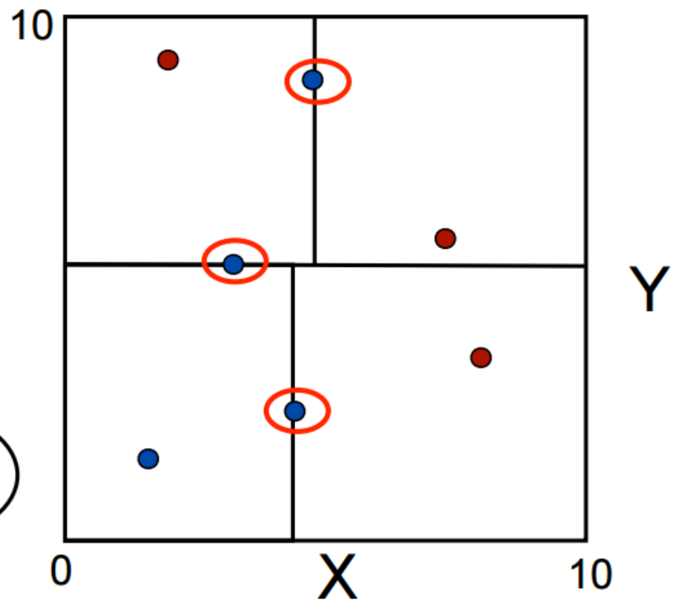
- In order to do classification, we can compute the distances between all points in the training set and the point we are trying to classify
  - With m data points in n-dimensional space, this takes $O(mn)$ time for Euclidean distance
  - It is possible to do better if we do some preprocessing on the training data

K-Dimensional Trees

- k-d trees provide a data structure that can help simplify the classification task by constructing a tree that partitions the search space
  - Starting with the entire training set, choose some dimension, i
  - Select an element of the training data whose i^{th} dimension has the median value among all elements of the training set
  - Divide the training set into two pieces: depending on whether their i^{th} attribute is smaller or larger than the median
  - Repeat this partitioning process on each of the two new pieces separately

K-Dimensional Trees



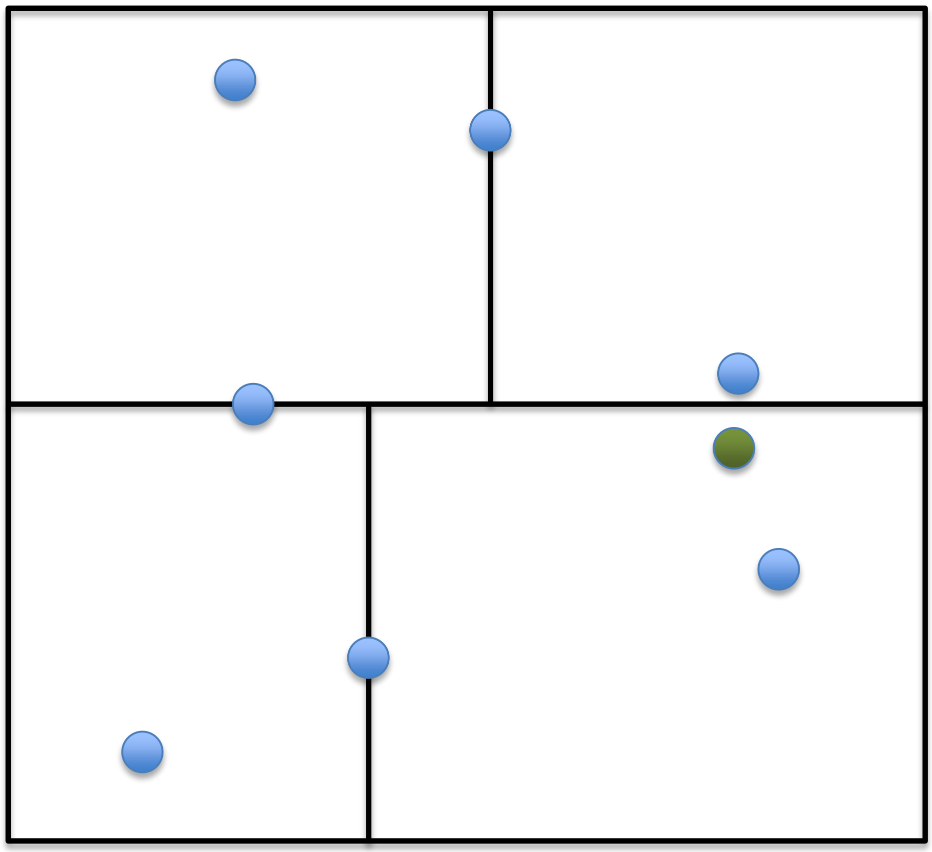


[Images from slides by Mehyrar Mohri]

K-Dimensional Trees

- Start at the top of the k-d tree and traverse it to a leaf of the tree based on where the point to classify should fall
- Once a leaf node is reached, it is selected to be the current closest point to x'
- Follow the path, in the opposite direction, from the leaf to the root
  - If the current node along the path is closer to x' than the selected closest point it becomes the new closest point
  - Before moving up the tree, the algorithm checks if there could be any points in the opposite partition that are closer to x' than the current closest point
    - If so, then closest point in that subtree is computed recursively
    - Otherwise, the parent of the current node along the path becomes the new current node

K-Dimensional Trees



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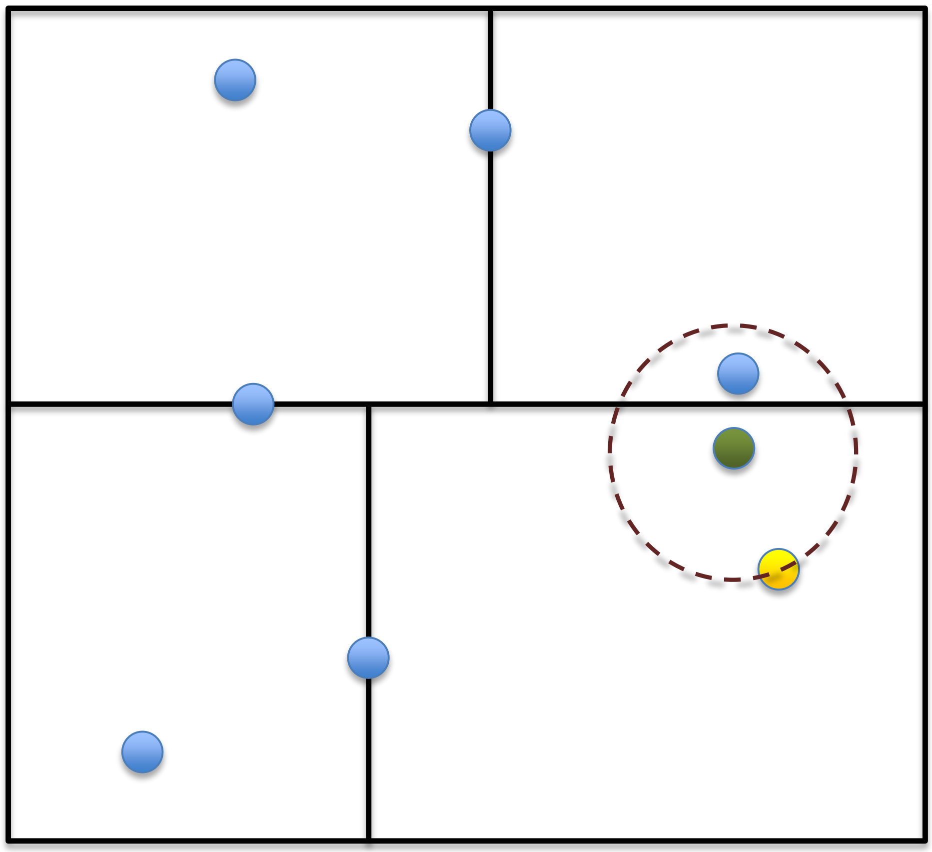

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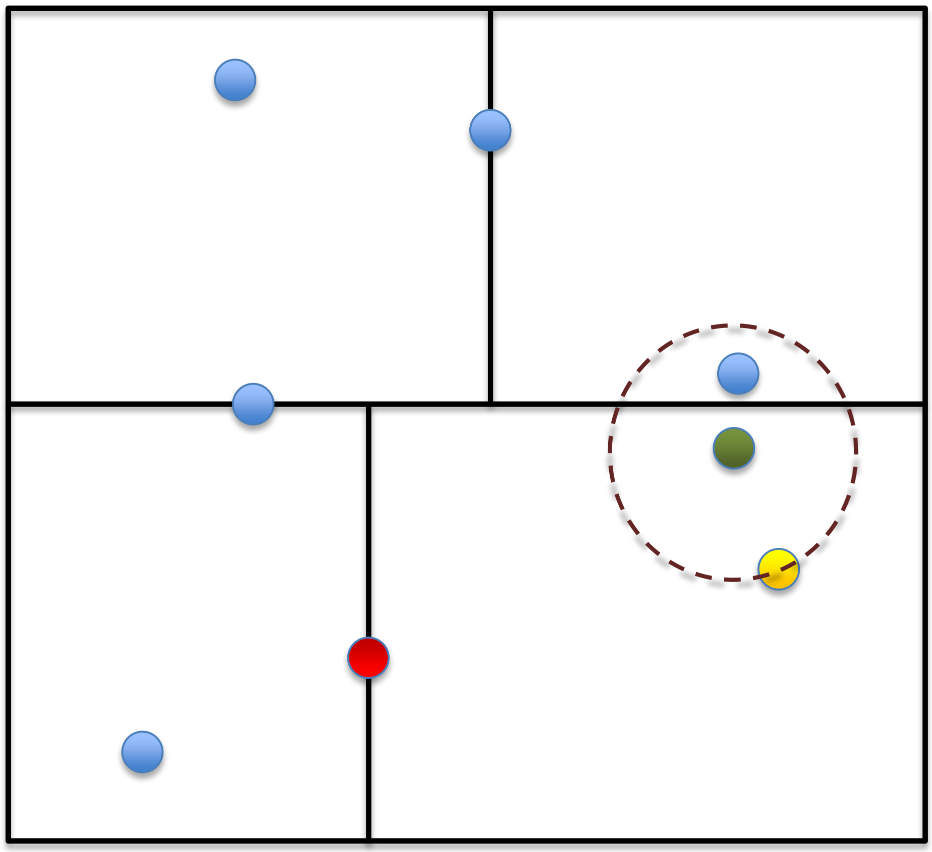

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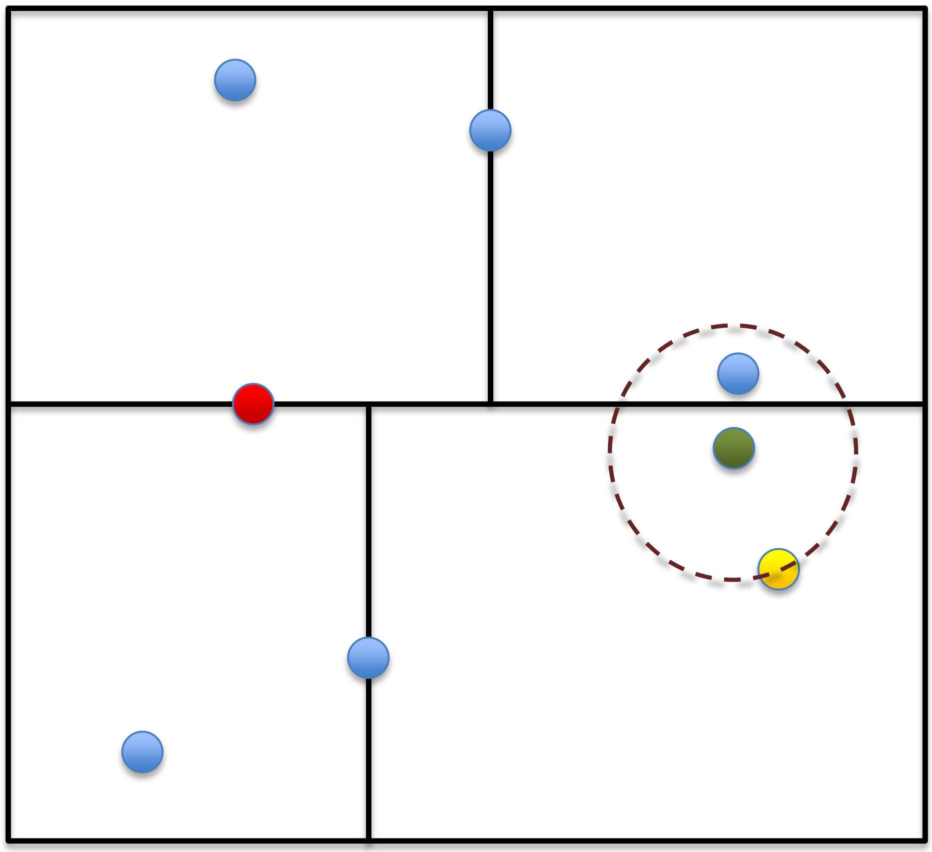

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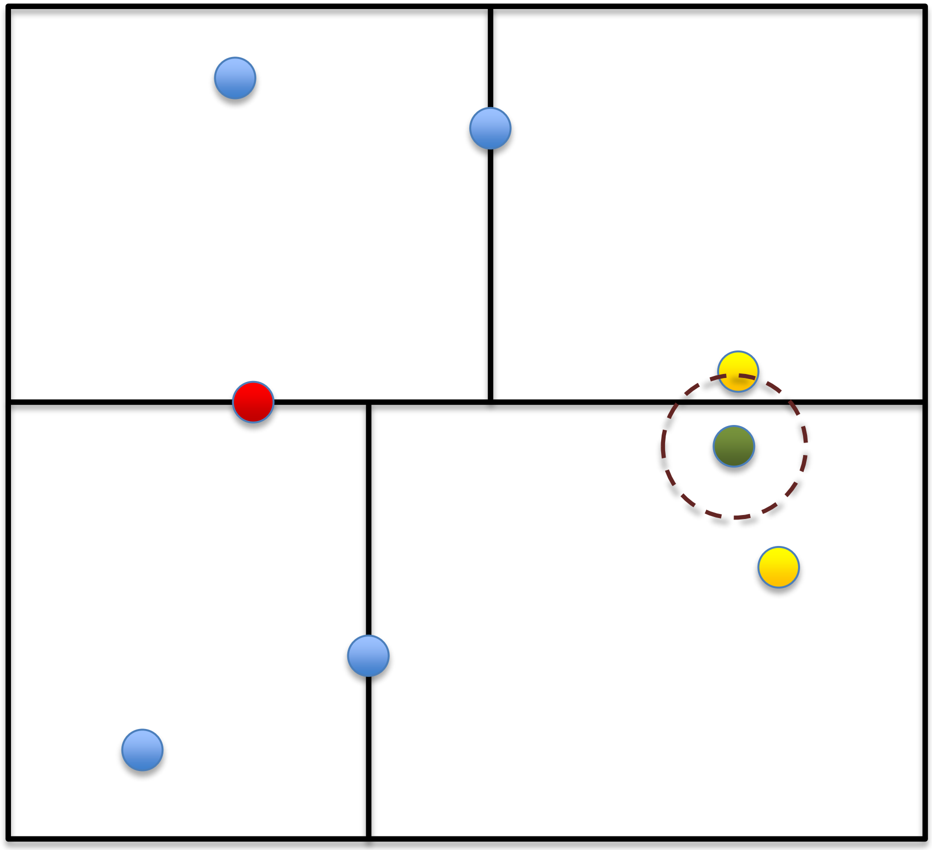

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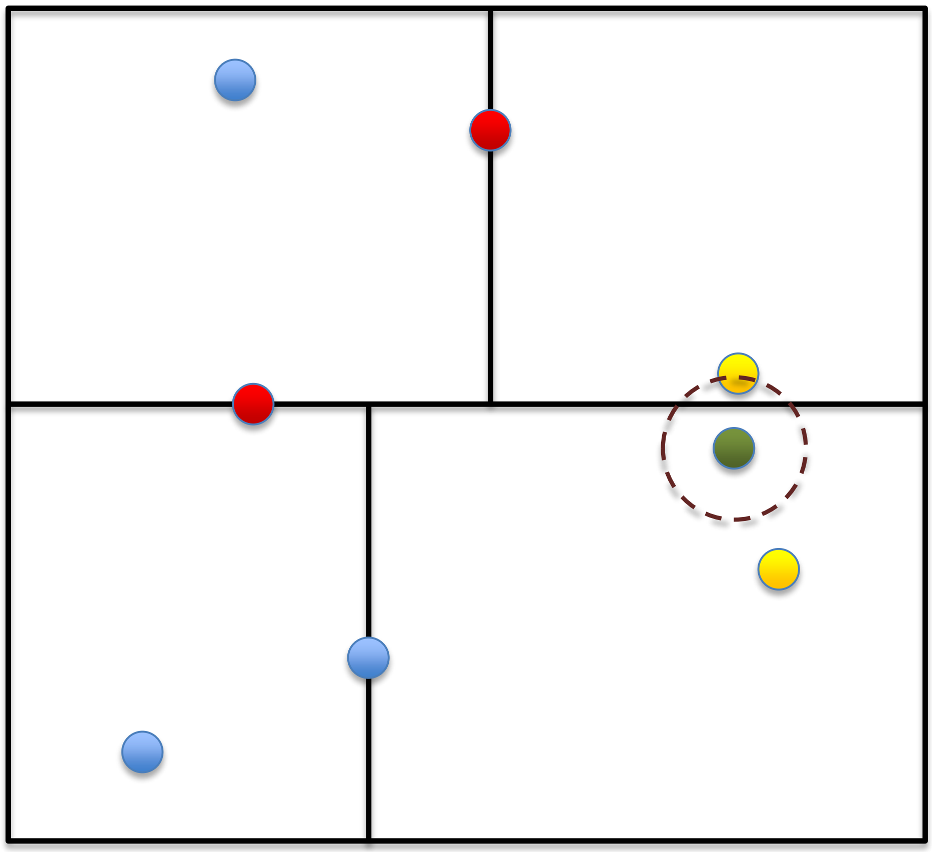

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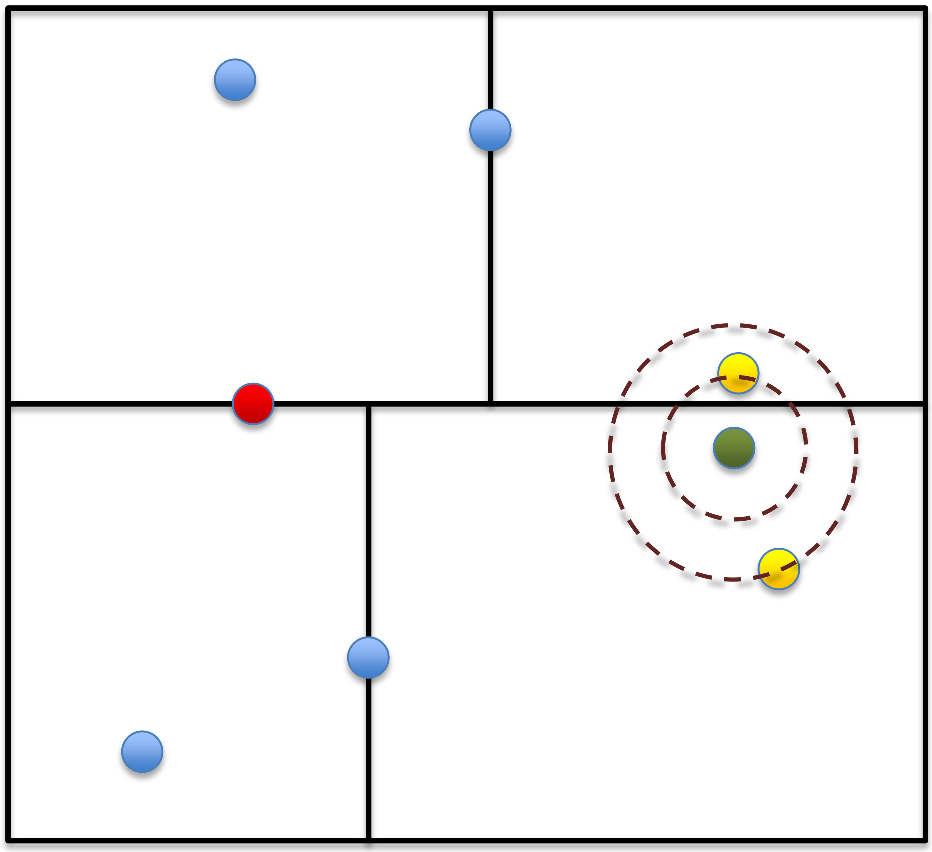

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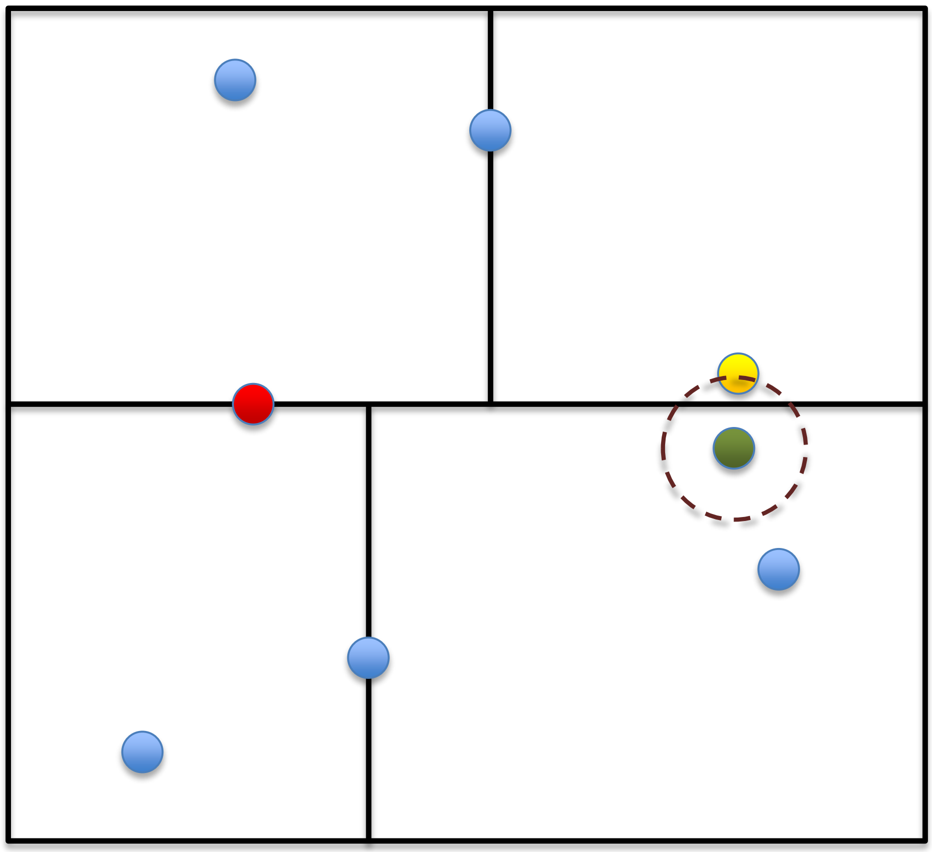

K-Dimensional Trees

- By design, the constructed k-d tree is "bushy"
  - The idea is that if new points to classify are evenly distributed throughout the space, then the expected (amortized) cost of classification is approximately $O(d \log n)$ operations
- Summary
  - k-NN is fast and easy to implement
  - No training required
  - Can be good in practice (where applicable)