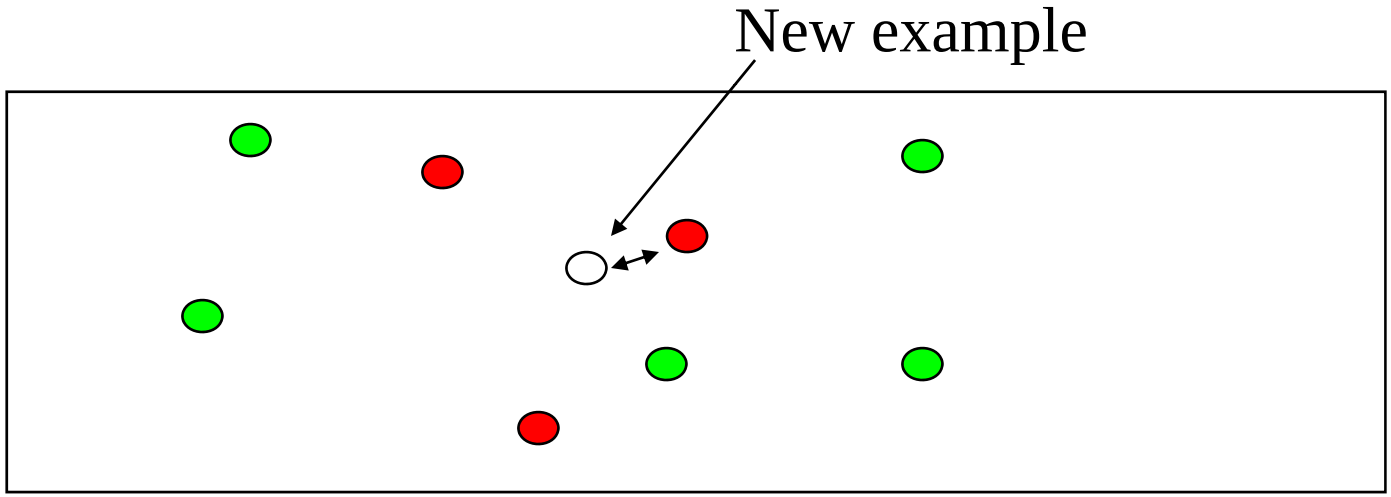
The Nearest Neighbor Algorithm

- A **lazy learning** algorithm
  - The “learning” does not occur until the test example is given
  - In contrast to so called “eager learning” algorithms (which carries out learning without knowing the test example, and after learning training examples can be discarded)

Nearest Neighbor Algorithm

- Remember all training examples
- Given a new example **x,** find the its closest training example <$\mathbf{x}^i$, y^i> and predict y^i

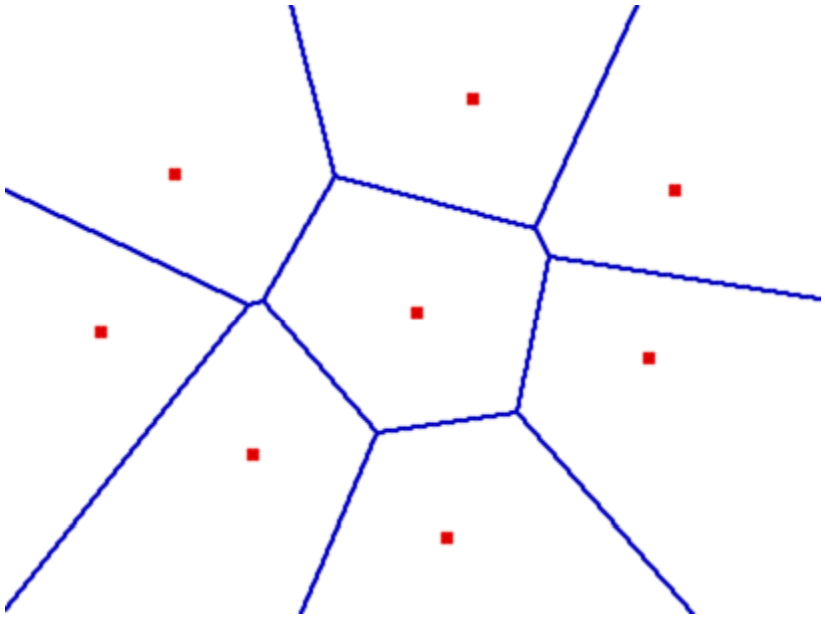


- How to measure distance – Euclidean (squared):

$$\left\|\mathbf{x}-\mathbf{x}^i\right\|^2=\sum_j(x_j-x_j^i)^2$$

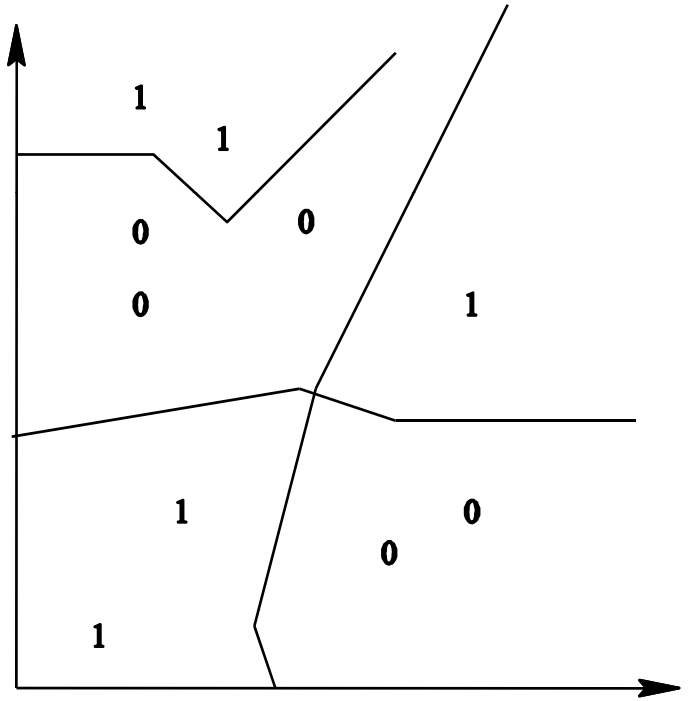
Decision Boundaries: The Voronoi Diagram

- Given a set of points, a **Voronoi diagram** describes the areas that are nearest to any given point.
- These areas can be viewed as zones of control.

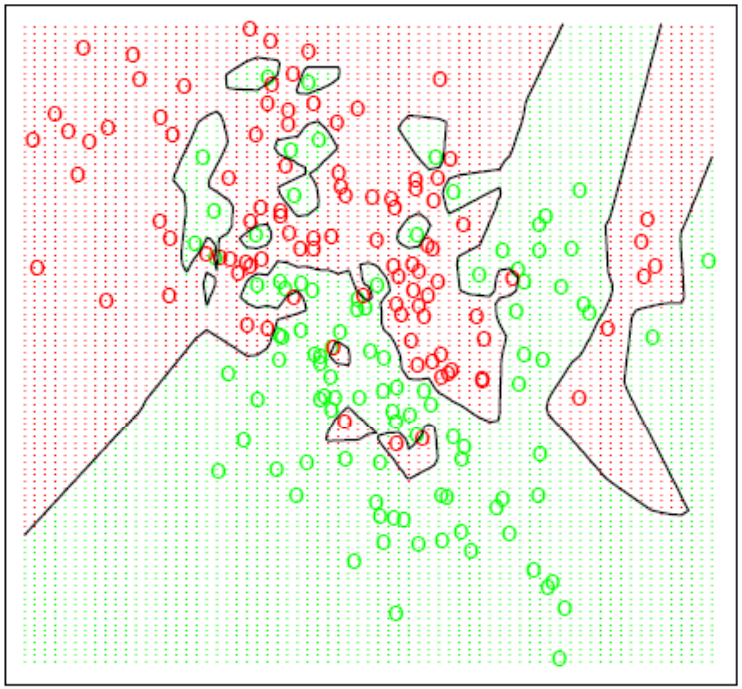


Decision Boundaries: The Voronoi Diagram

- Decision boundaries are formed by a **subset** of the Voronoi diagram of the training data
- Each line segment is equidistant between two points **of opposite class**.
- The more examples that are stored, the more fragmented and complex the decision boundaries can become.



Decision Boundaries

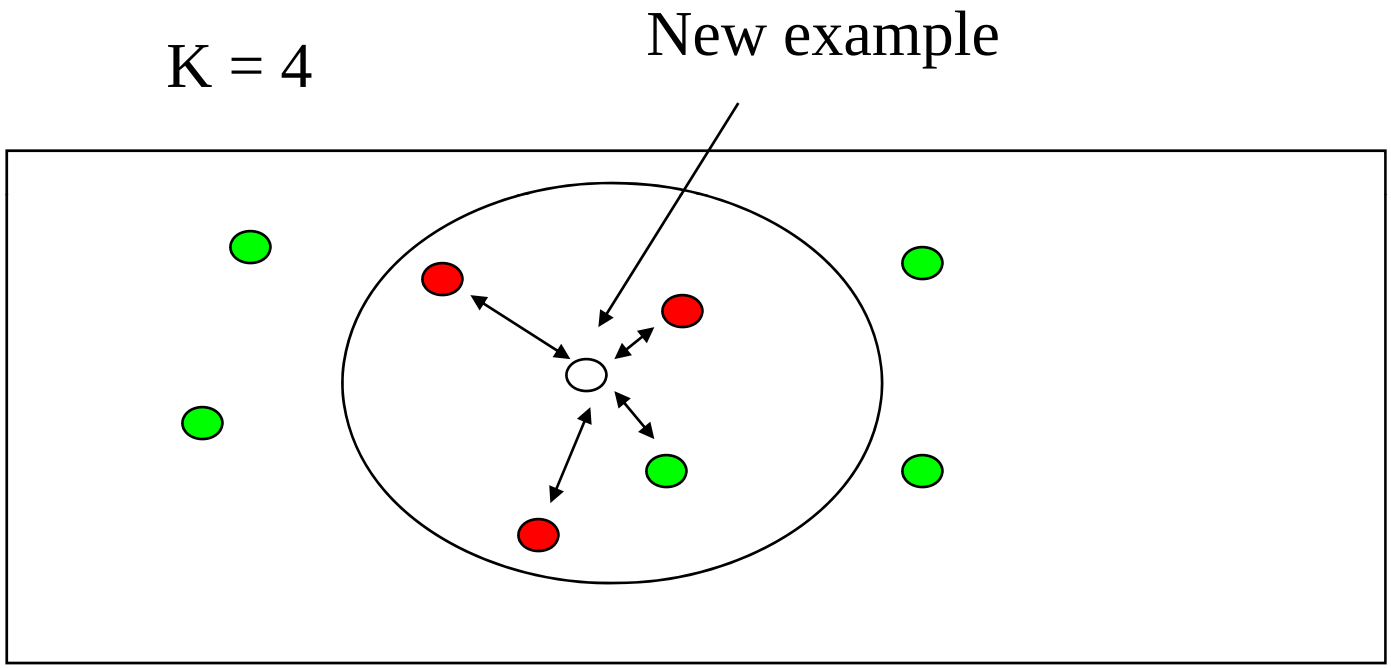


With large number of examples and possible noise in the labels, the decision boundary can become nasty!

We end up overfitting the data

K-Nearest Neighbor

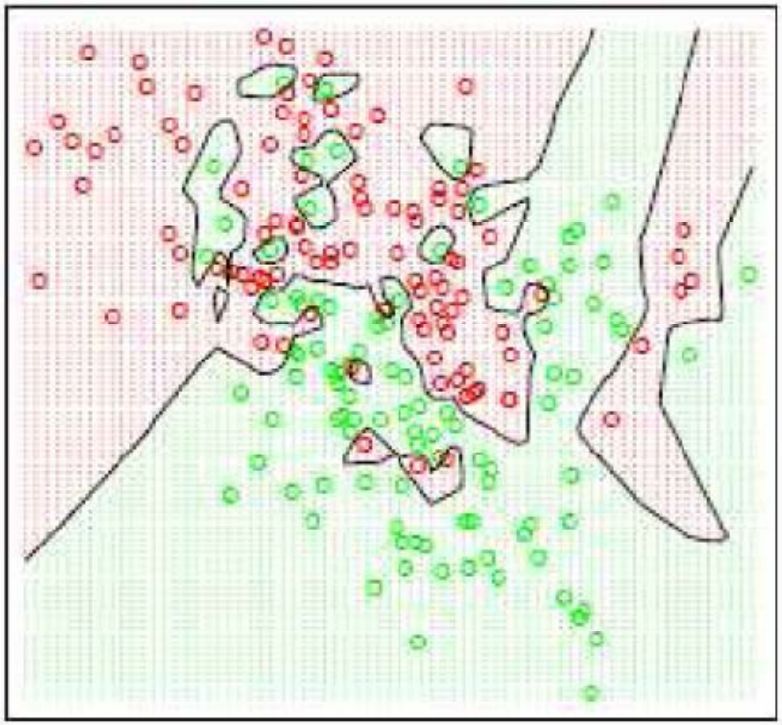
Example:



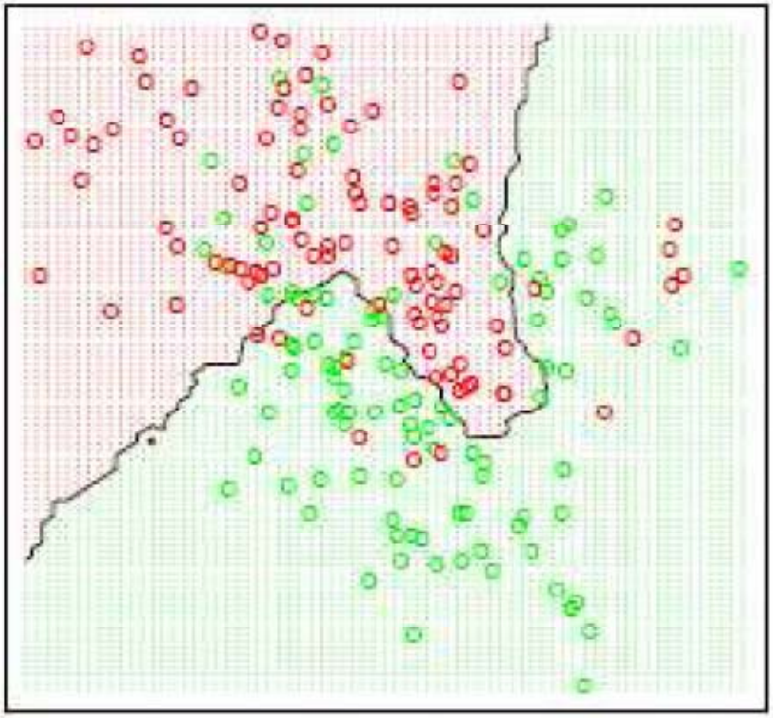
Find the ***k*** nearest neighbors and have them vote. Has a smoothing effect. This is especially good when there is noise in the class labels.

Effect of K

K=1



K=15



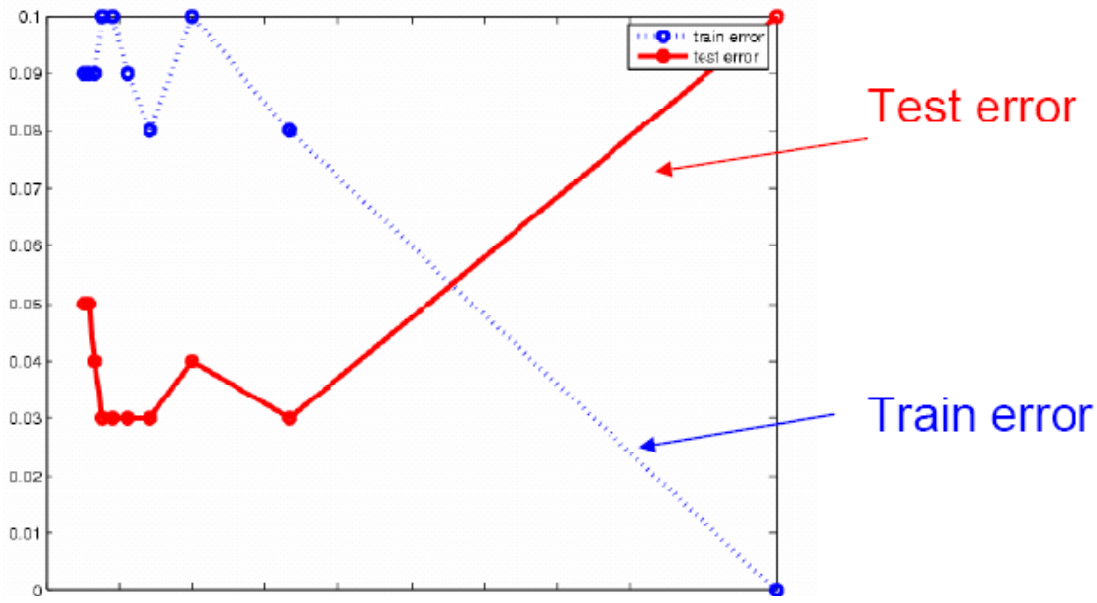
Figures from Hastie, Tibshirani and Friedman (Elements of Statistical Learning)

Larger k produces smoother boundary effect and can reduce the impact of class label noise.

But when K = N, we always predict the majority class

Question: how to choose k?

- Can we choose k to minimize the mistakes that we make on training examples (*training error*)?



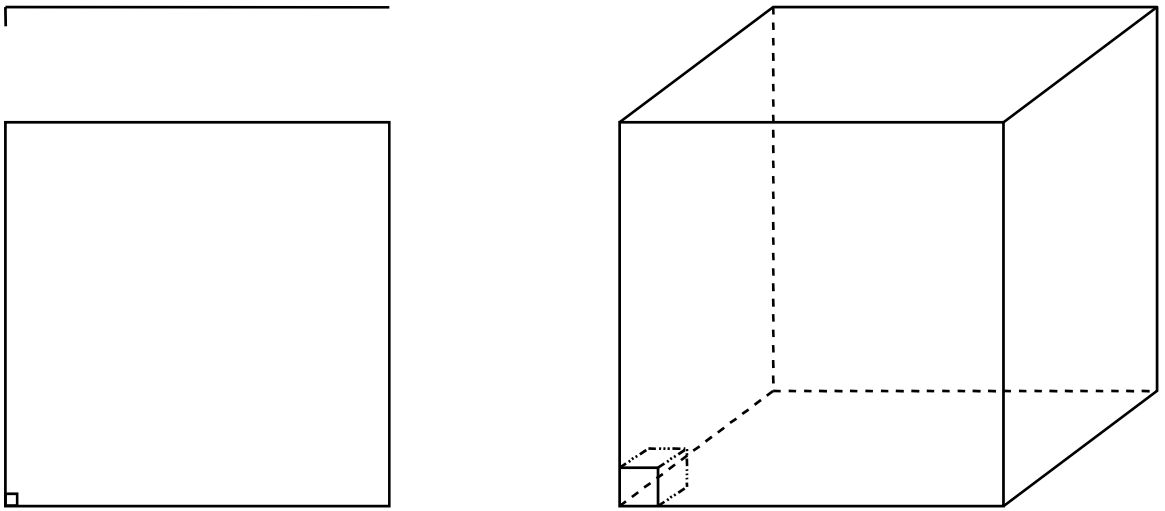
A model selection problem that we will study later

Distance Weighted Nearest Neighbor

- It makes sense to weight the contribution of each example according to the distance to the new query example
  - Weight varies inversely with the distance, such that examples closer to the query points get higher weight
- Instead of only k examples, we could allow all training examples to contribute
  - Shepard's method (Shepard 1968)

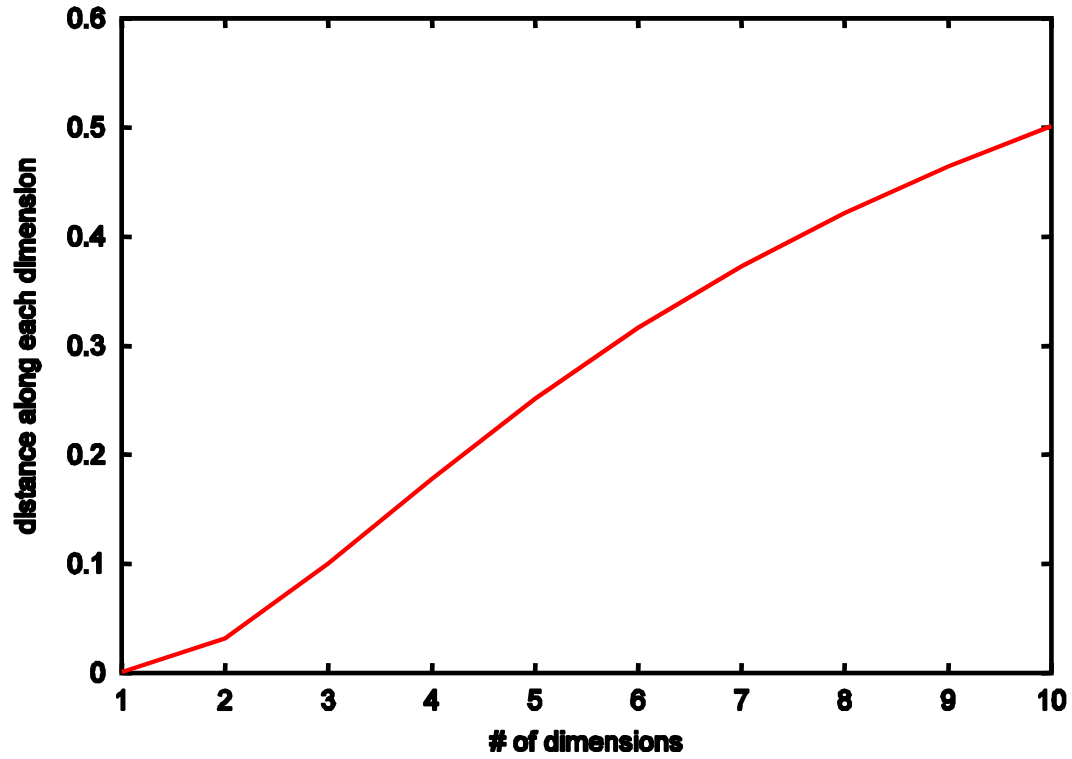
Curse of Dimensionality

- *k*NN breaks down in high-dimensional space
  - "Neighborhood" becomes very large.
- Assume 5000 points uniformly distributed in the unit hypercube and we want to apply 5-nn. Suppose our query point is at the origin.
  - In 1-dimension, we must go a distance of 5/5000 = 0.001 on the average to capture 5 nearest neighbors
  - In 2 dimensions, we must go $\sqrt{0.001}$ to get a square that contains 0.001 of the volume.
  - In d dimensions, we must go $(0.001)^{1/d}$



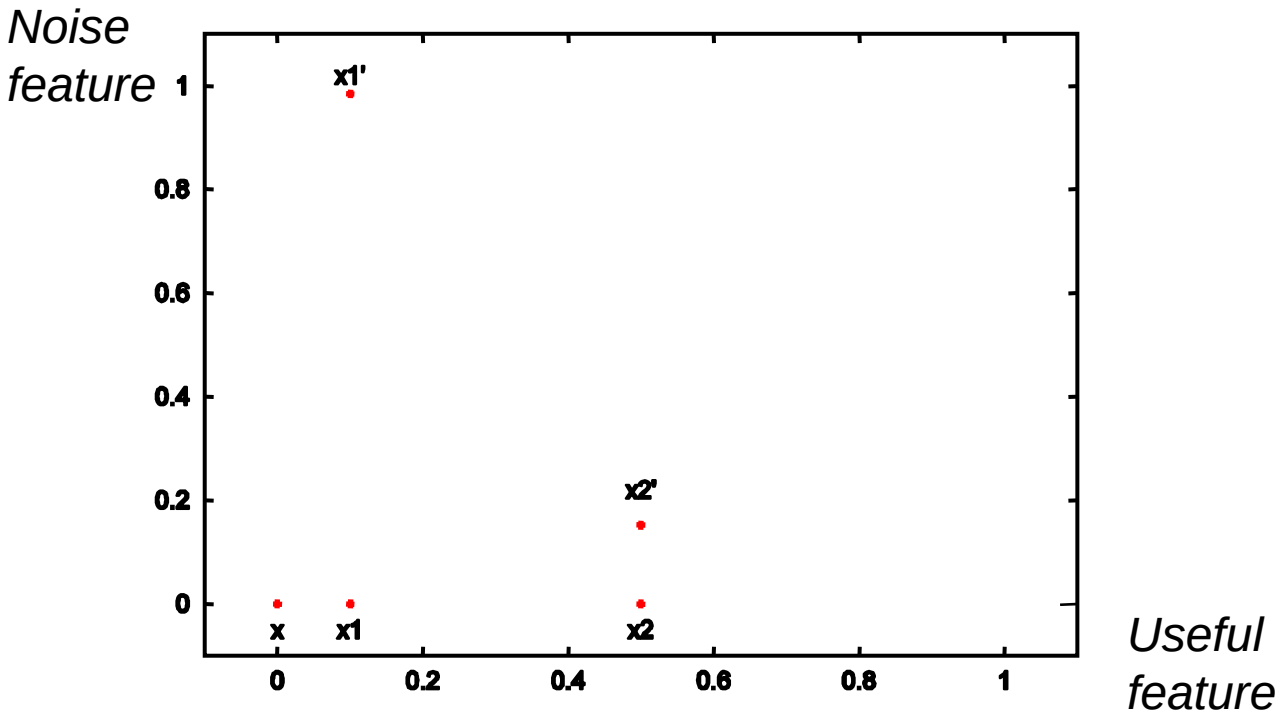
The Curse of Dimensionality: Illustration

- With 5000 points in 10 dimensions, we must go 0.501 distance along each dimension in order to find the 5 nearest neighbors



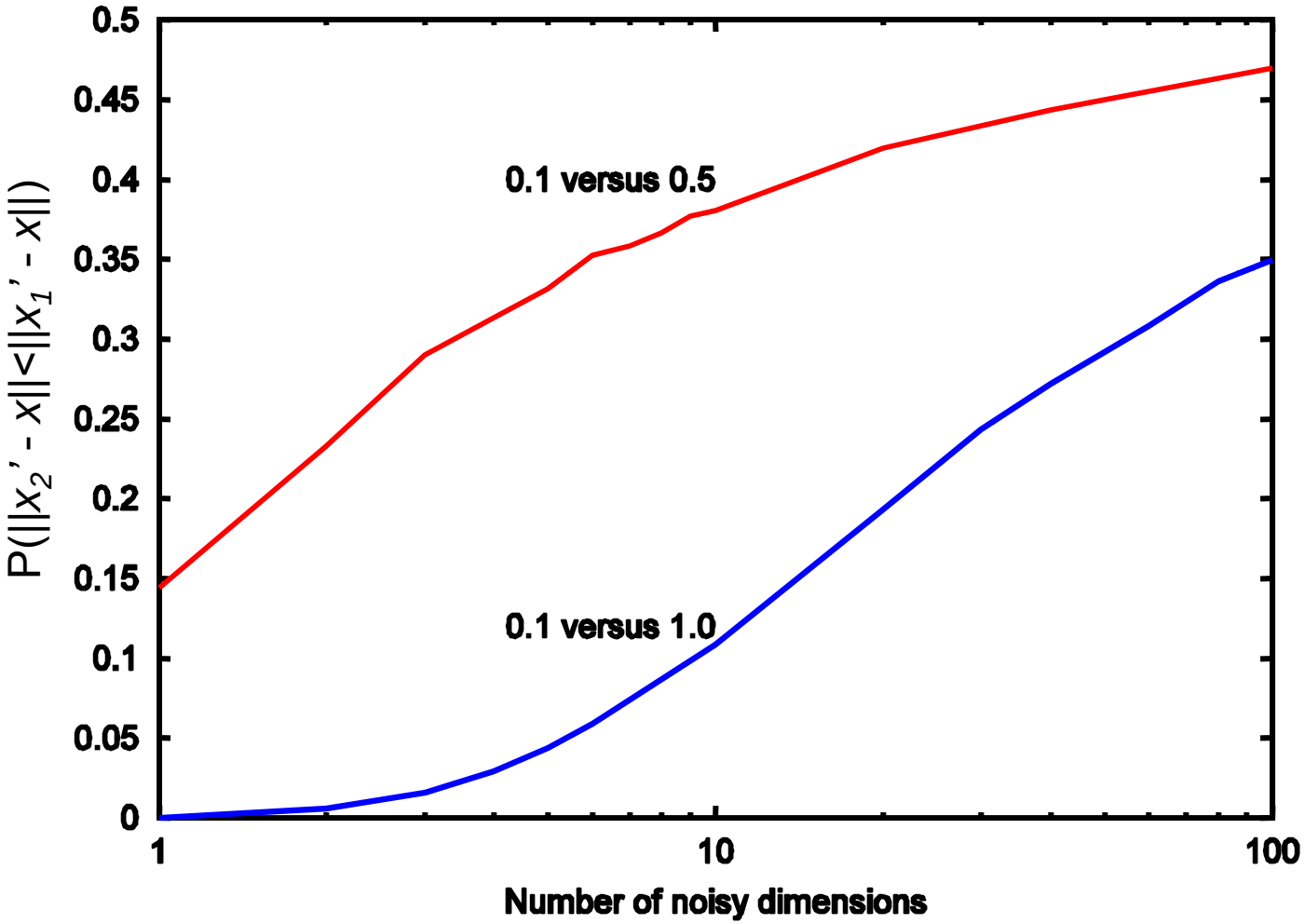
The Curse of Noisy/Irrelevant Features

- NN also breaks down when data contains irrelevant/noisy features.
- Consider a 1-d problem where query x is at the origin, our nearest neighbor is x_1 at 0.1, and our second nearest neighbor is x_2 at 0.5.
- Now add a uniformly random noisy feature.
  - $P(||x_2' - x|| < ||x_1' - x||) \approx 0.15$.



Curse of Noise (2)

Location of x_1 versus x_2



Problems of k-NN

- Nearest neighbor is easily misled by noisy/irrelevant features

- One approach: Learn a distance metric:
  - that weights each feature by its ability to minimize the prediction error, e.g., its mutual information with the class.
  - that weights each feature differently or only use a subset of features and use cross validation to select the weights or feature subsets
  - Learning distance function is an active research area

Nearest Neighbor Summary

- Advantages
  - Learning is extremely simple and intuitive,
  - Very flexible decision boundaries
  - Variable-sized hypothesis space
- Disadvantages
  - distance function must be carefully chosen or tuned
  - irrelevant or correlated features have high impact and must be eliminated
  - typically cannot handle high dimensionality
  - computational costs: memory and classification-time computation
    - To reduce the cost of finding nearest neighbors, use data structure such as kd-tree