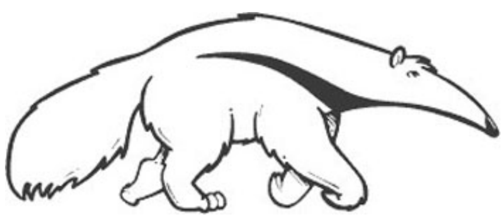
Machine Learning and Data Mining

Nearest neighbor methods

Prof. Alexander Ihler



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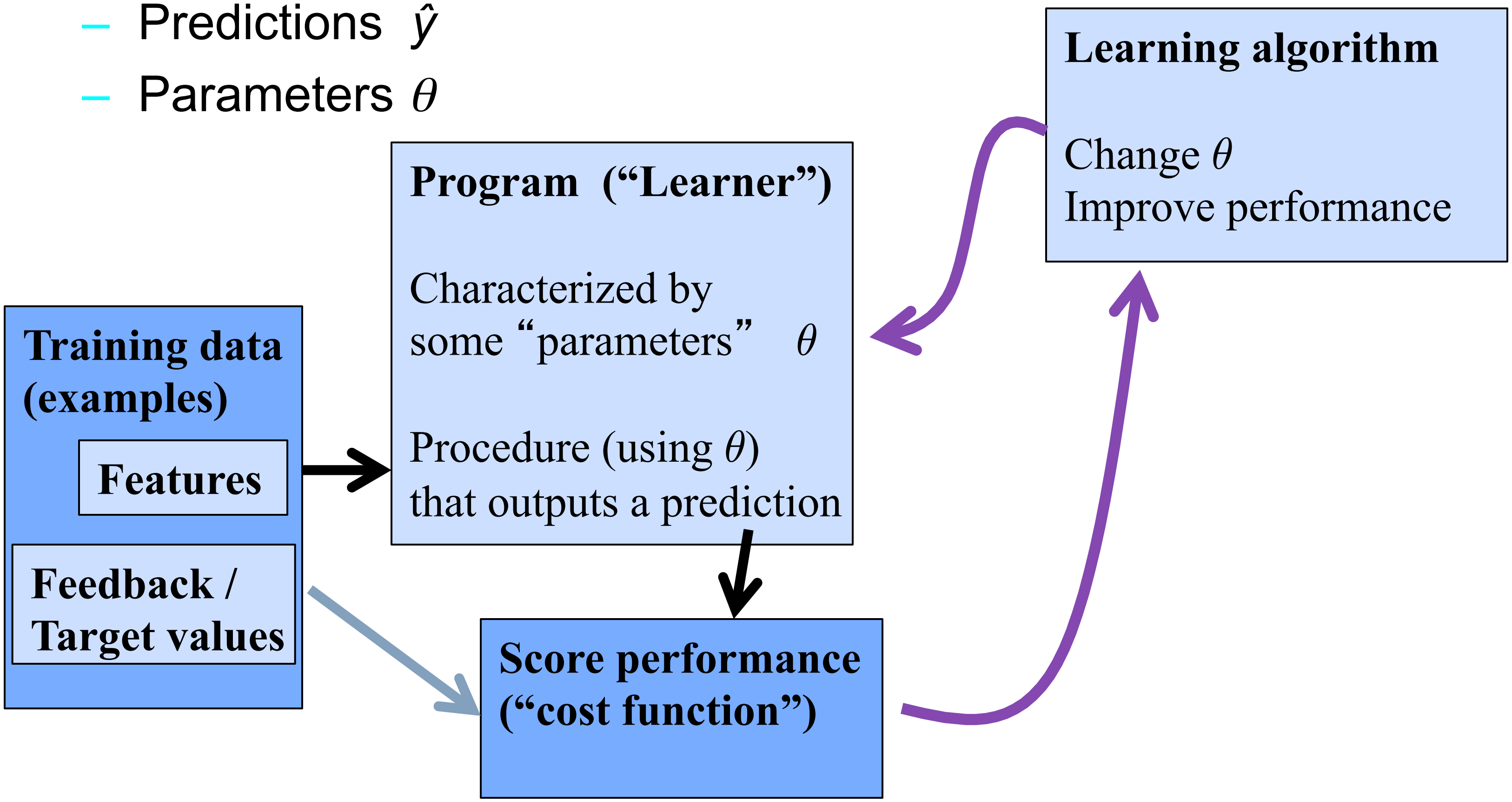
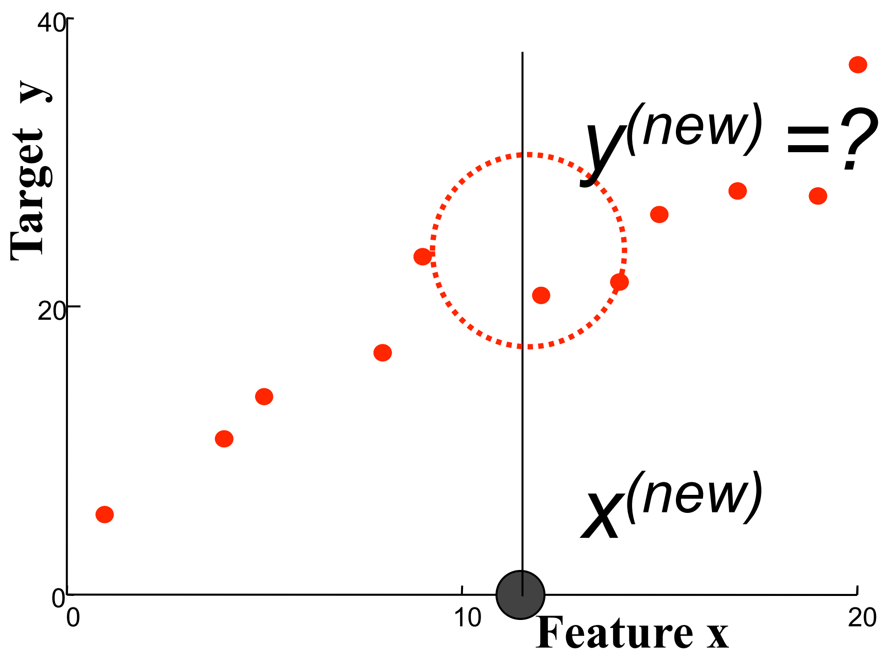
Supervised learning

- Notation
  - Features x
  - Targets y
  - Predictions $\hat{y}$
  - Parameters θ

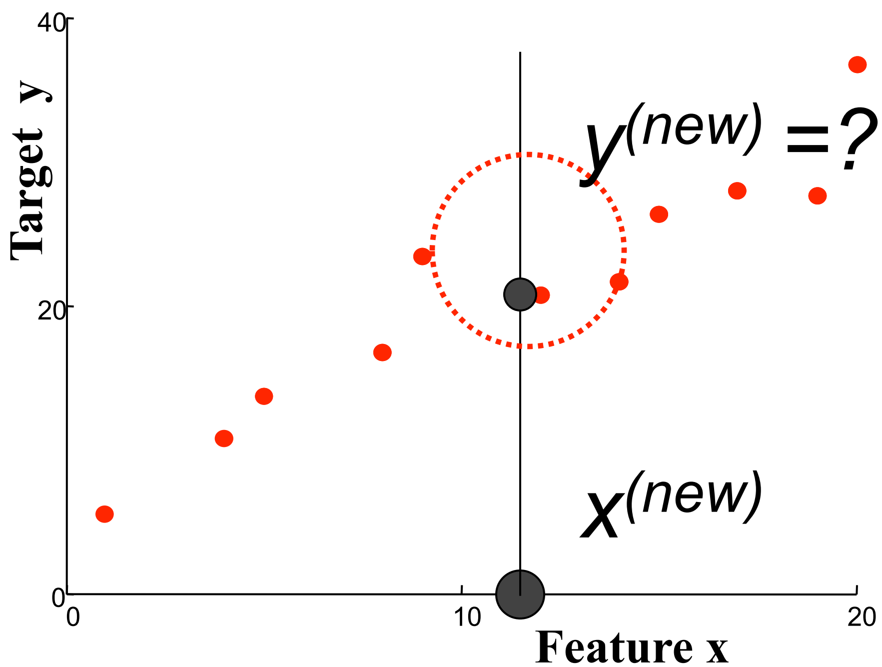


Regression; Scatter plots



- Suggests a relationship between x and y
- Regression: given new observed $x^{(new)}$, estimate $y^{(new)}$

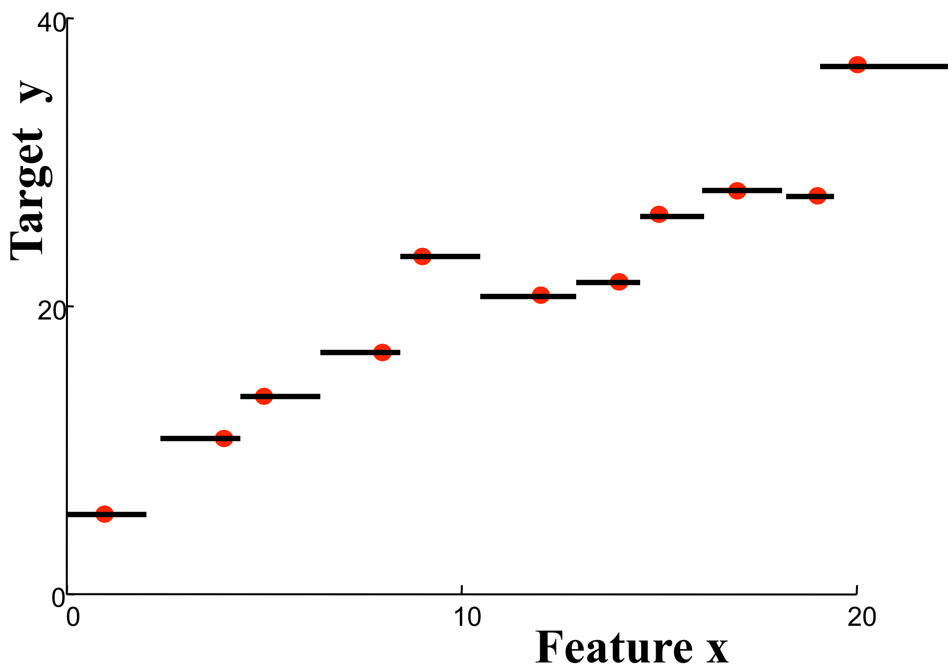
Nearest neighbor regression



"Predictor":
Given new features:
Find nearest example
Return its value

- Find training datum $x^{(i)}$ closest to $x^{(new)}$; predict $y^{(i)}$

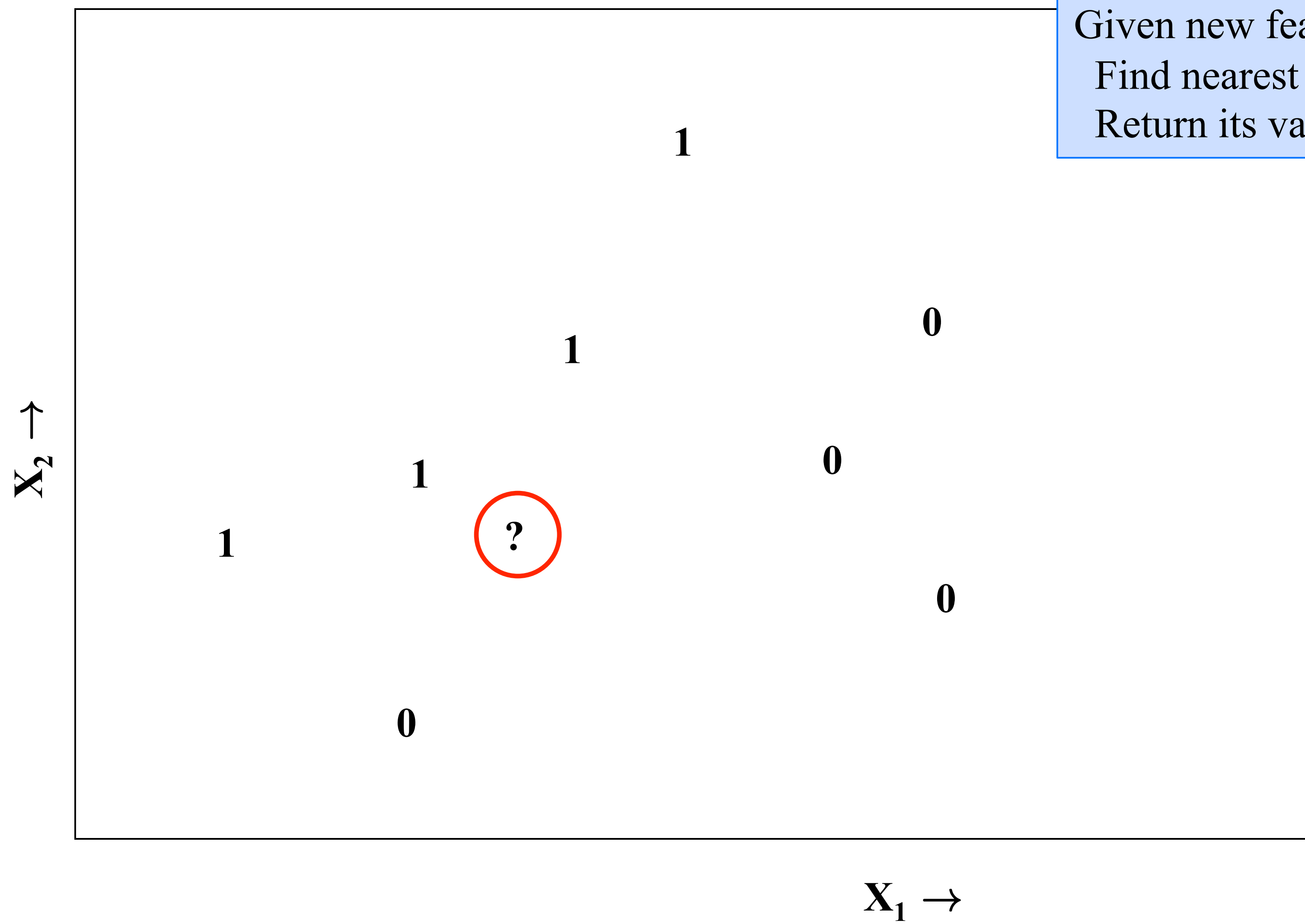
Nearest neighbor regression



"Predictor":
Given new features:
Find nearest example
Return its value

- Find training datum $x^{(i)}$ closest to $x^{(new)}$; predict $y^{(i)}$
- Defines an (implict) function f(x)
- "Form" is piecewise constant

Nearest neighbor classifier



"Predictor":
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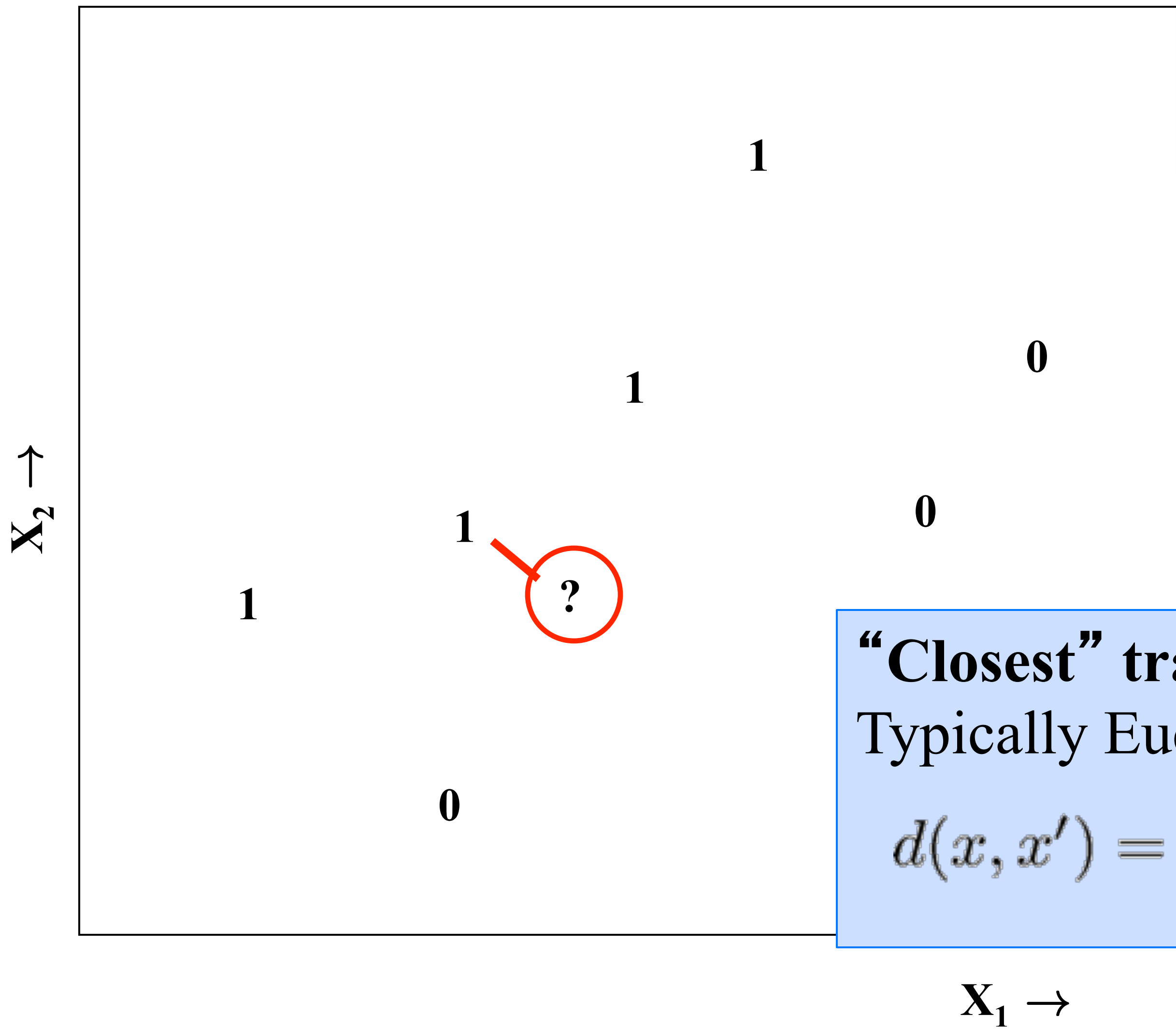
Nearest neighbor classifier

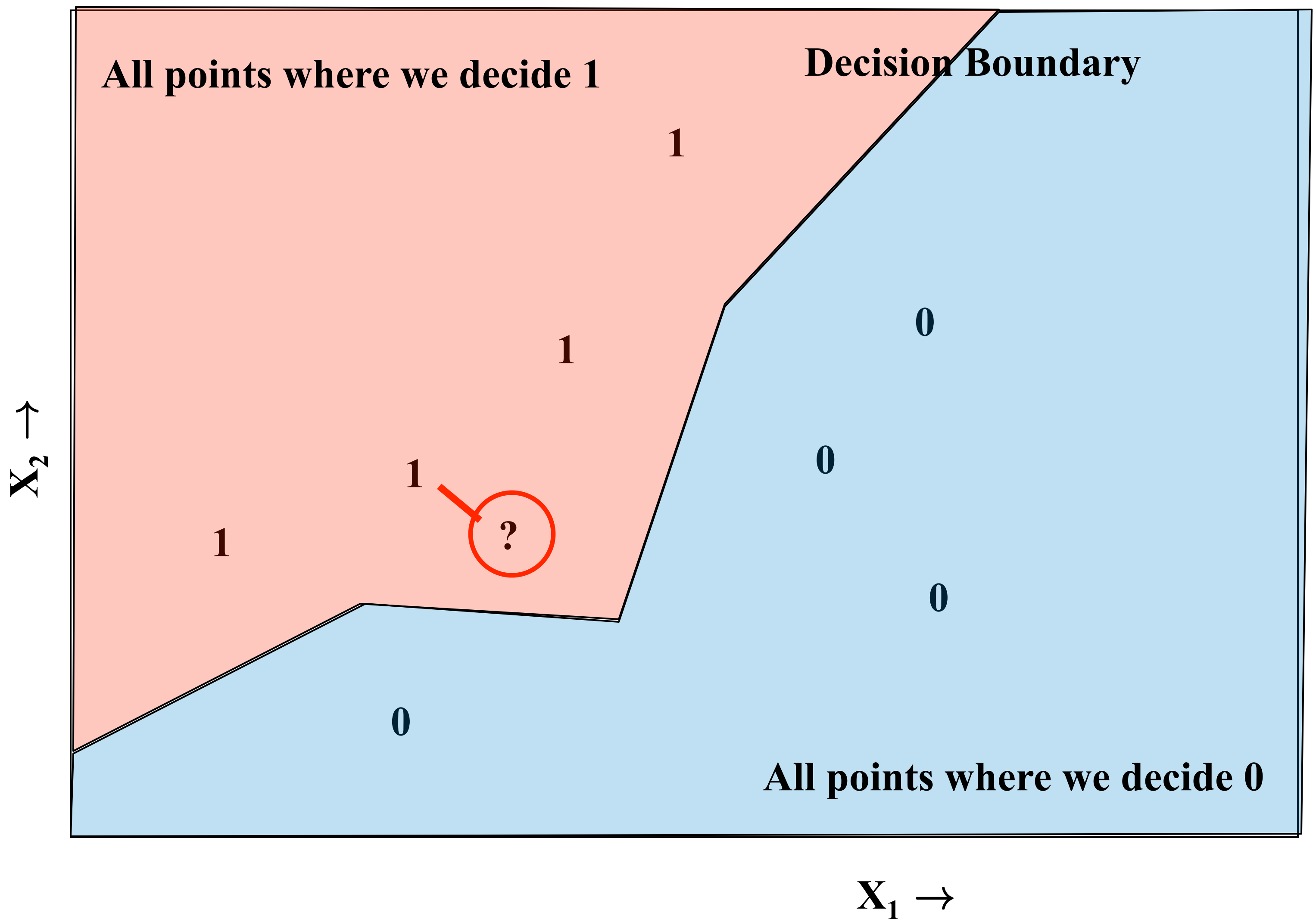


"Predictor":
Given new features:
Find nearest example
Return its value

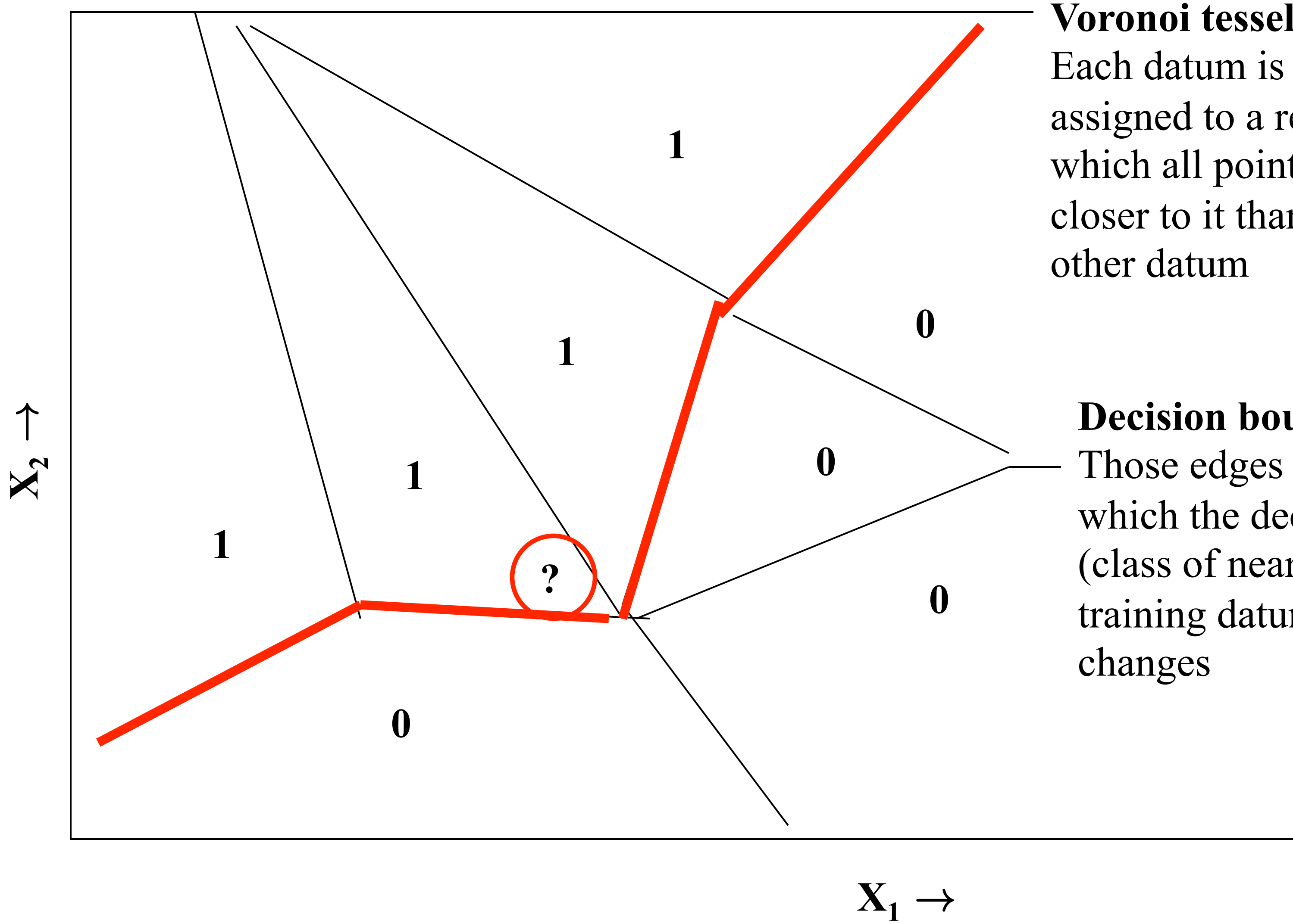
"Closest" training x?
Typically Euclidean distance:

$$d(x, x') = \sqrt{\sum_i (x_i - x'_i)^2}$$

Nearest neighbor classifier



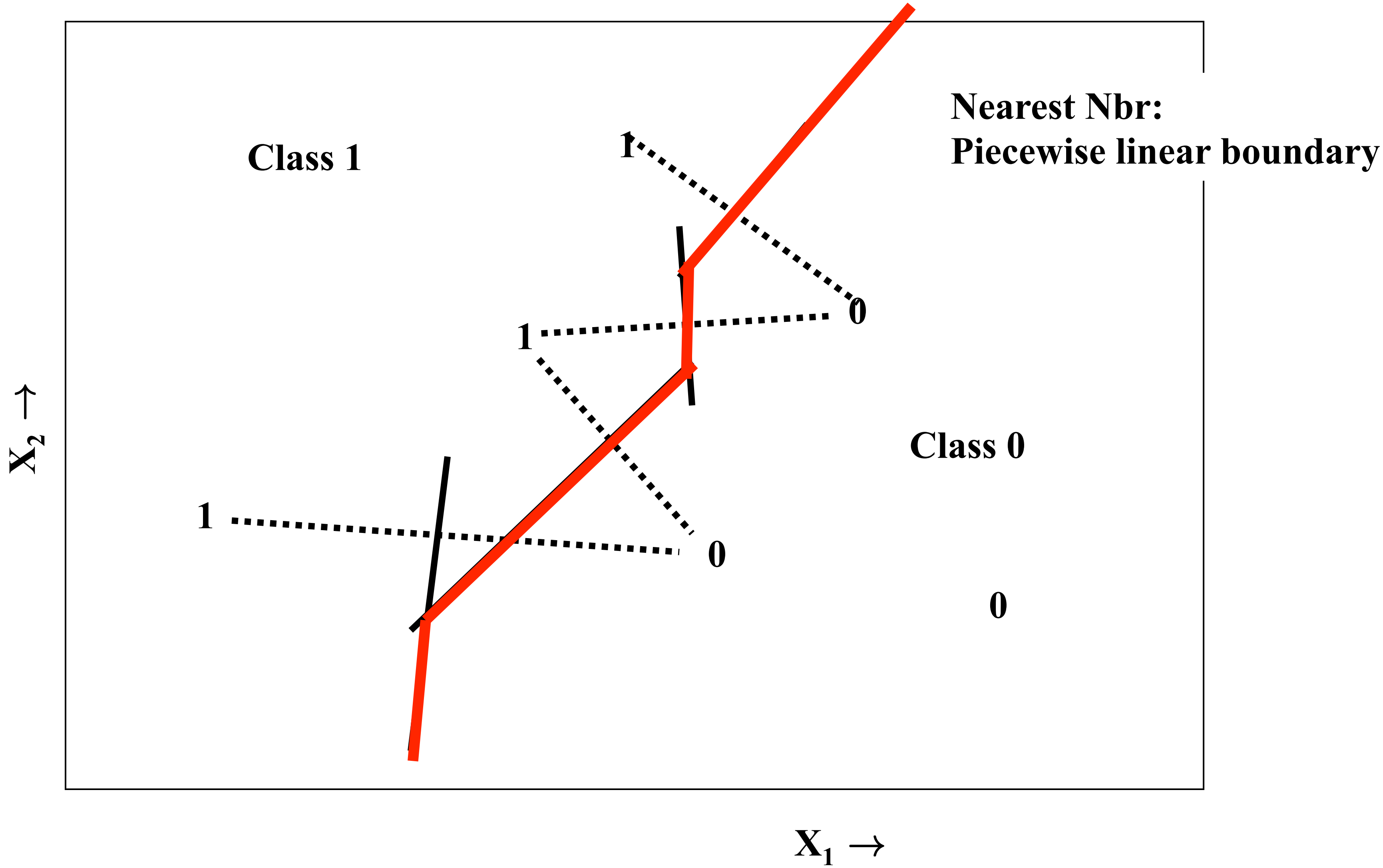
Nearest neighbor classifier



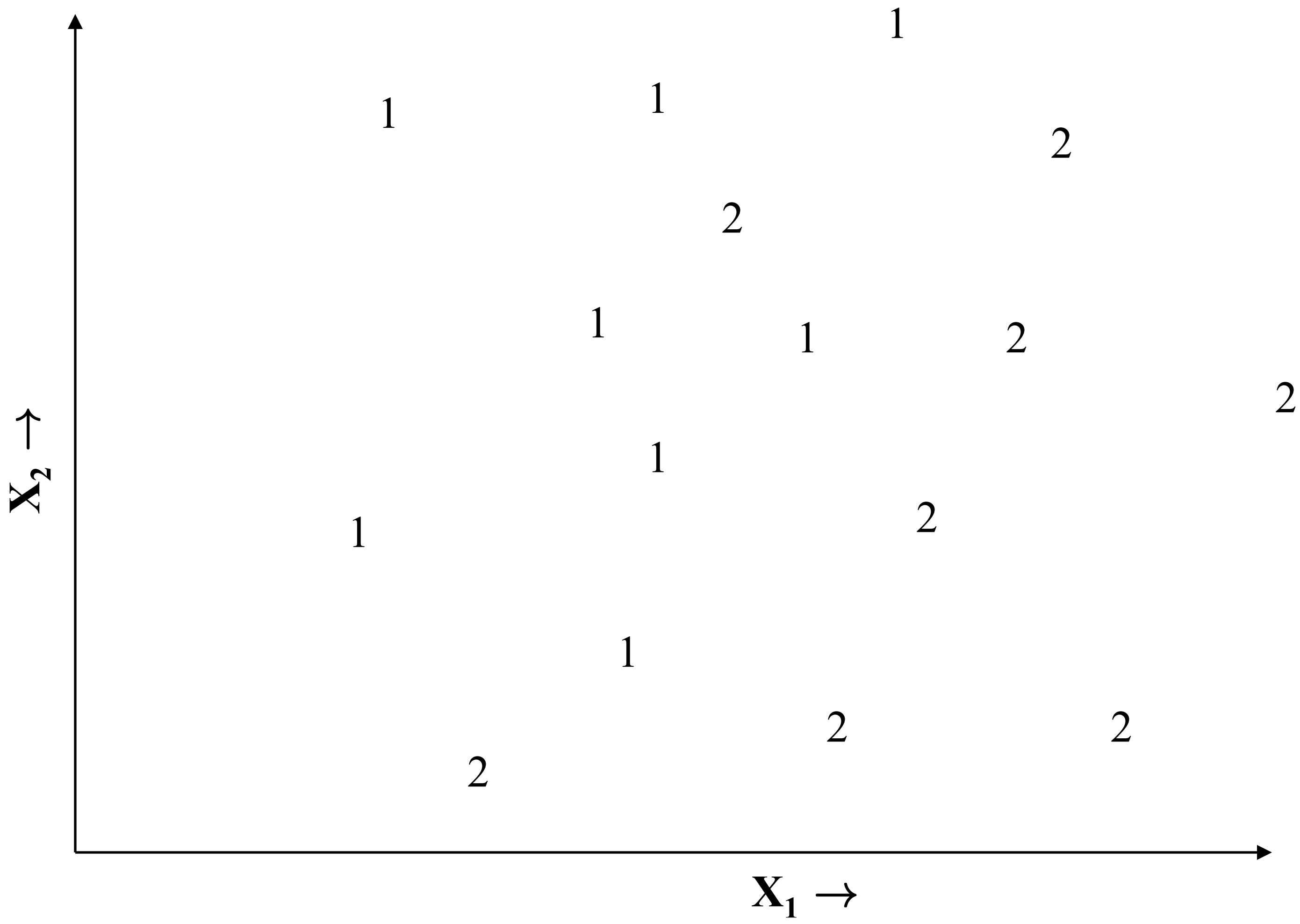
Voronoi tessellation: Each datum is assigned to a region, in which all points are closer to it than any other datum

Decision boundary: Those edges across which the decision (class of nearest training datum) changes

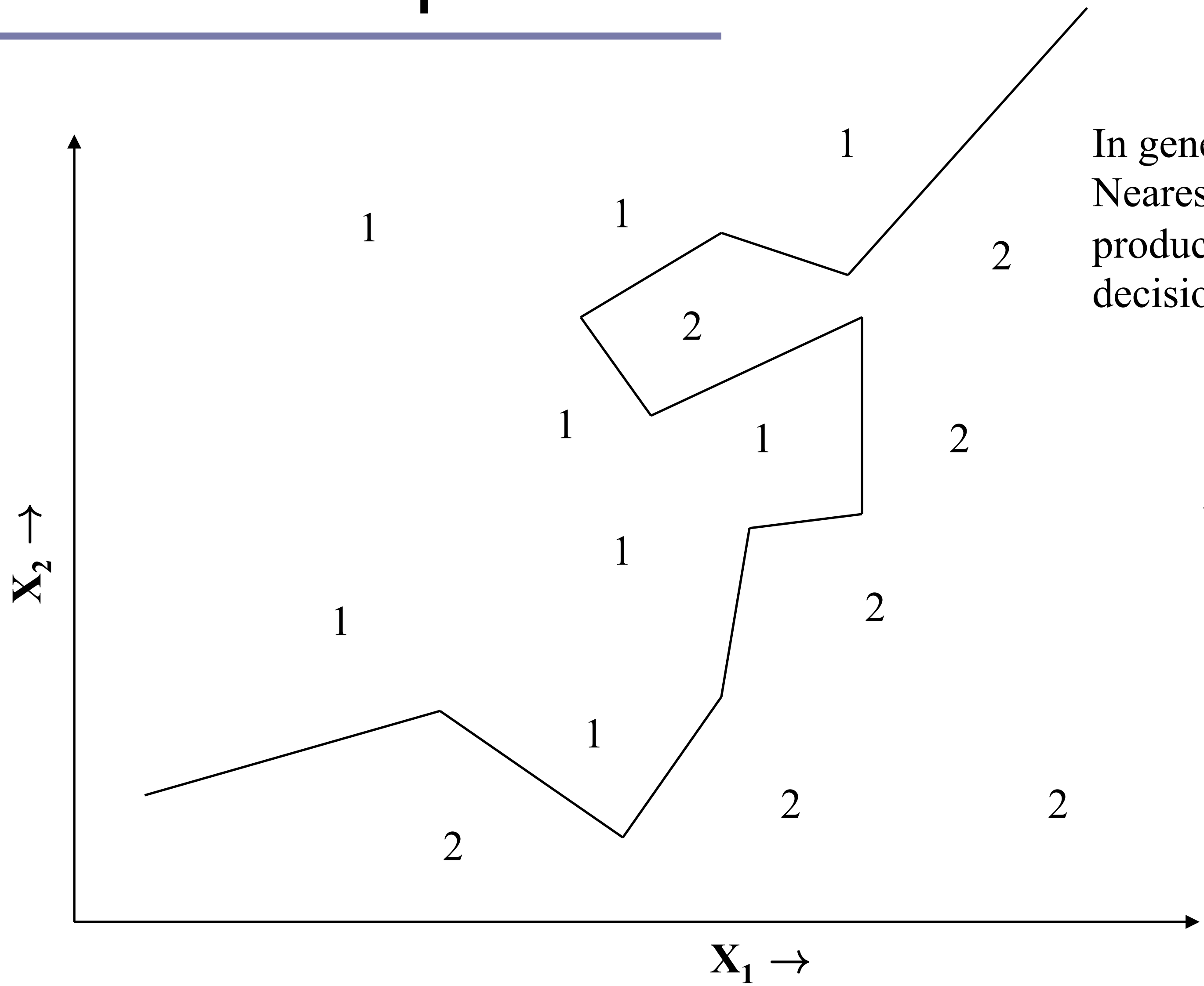
Nearest neighbor classifier



More Data Points



More Complex Decision Boundary



In general:
Nearest-neighbor classifier produces piecewise linear decision boundaries

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Machine Learning and Data Mining

Nearest neighbor methods:
K-Nearest Neighbors

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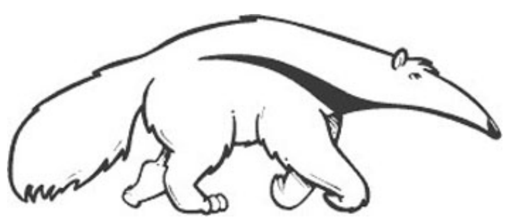

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K-Nearest Neighbor (kNN) Classifier

- Find the k-nearest neighbors to $\underline{x}$ in the data
  - i.e., rank the feature vectors according to Euclidean distance
  - select the k vectors which are have smallest distance to $\underline{x}$

- Regression
  - Usually just average the y-values of the k closest training examples

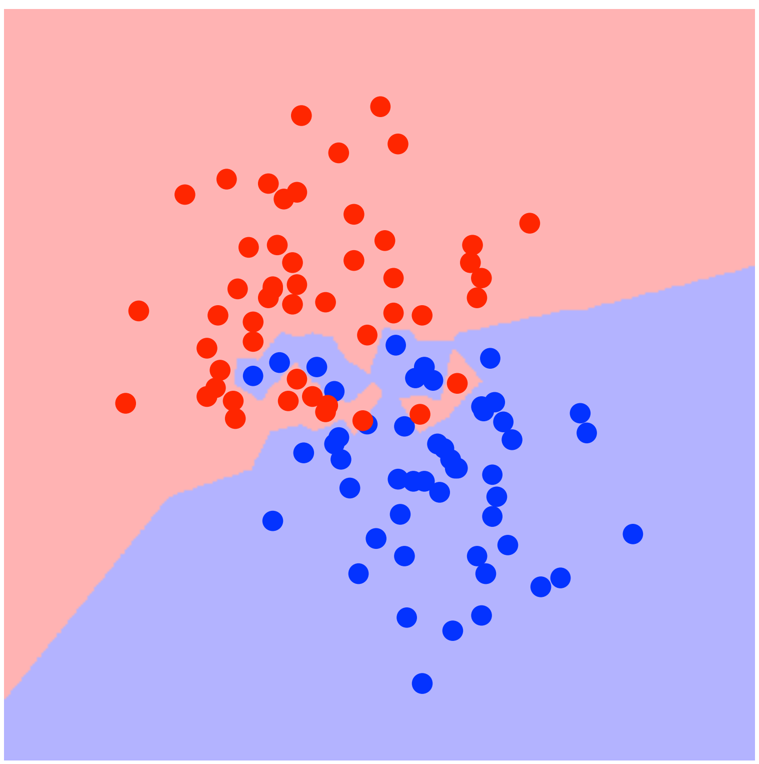
- Classification
  - ranking yields k feature vectors and a set of k class labels
  - pick the class label which is most common in this set ("vote")
  - classify $\underline{x}$ as belonging to this class
  - Note: for two-class problems, if k is odd (k=1, 3, 5, …) there will never be any "ties"

- "Training" is trivial: just use training data as a lookup table, and search to classify a new datum

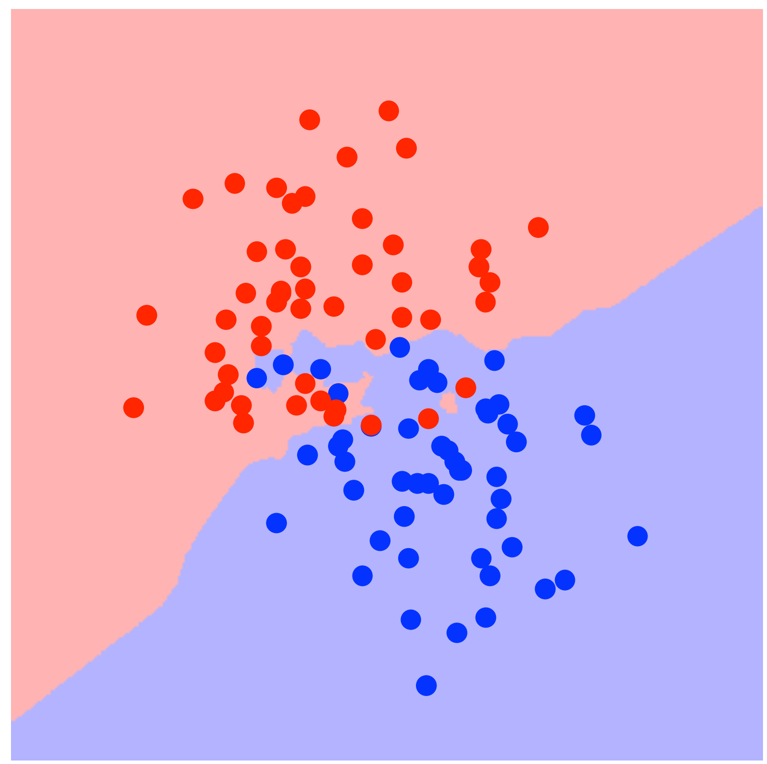
kNN Decision Boundary

- Piecewise linear decision boundary
- Increasing k "simplifies" decision boundary
  – Majority voting means less emphasis on individual points

K = 1



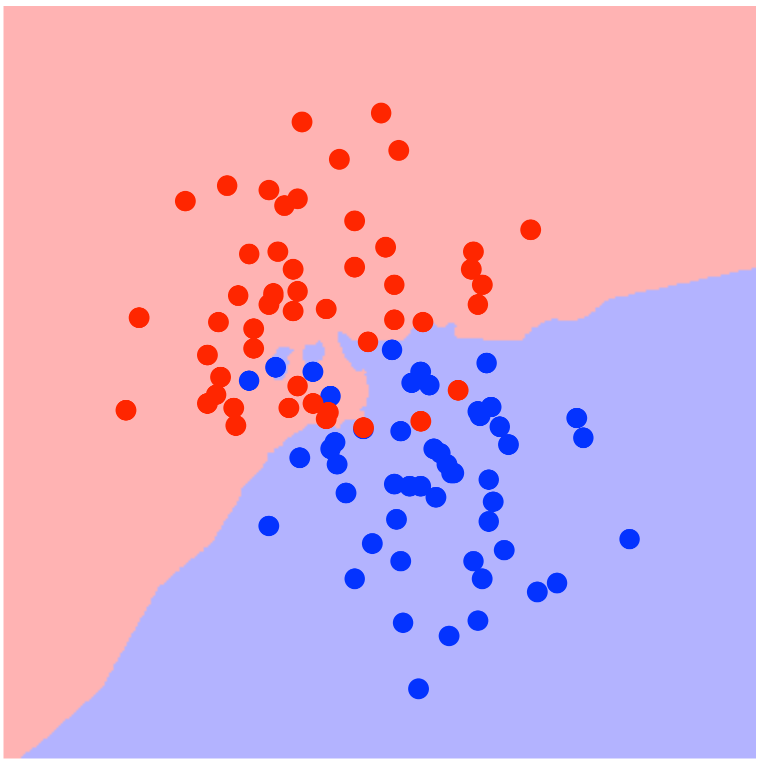
K = 3



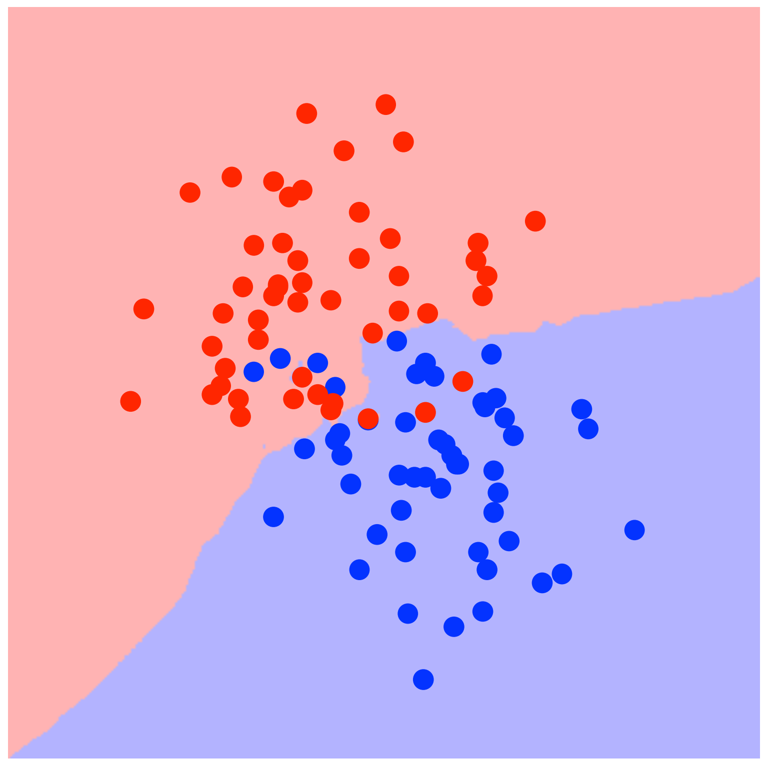
kNN Decision Boundary

- Recall: piecewise linear decision boundary
- Increasing k “simplifies” decision boundary
  – Majority voting means less emphasis on individual points

K = 5

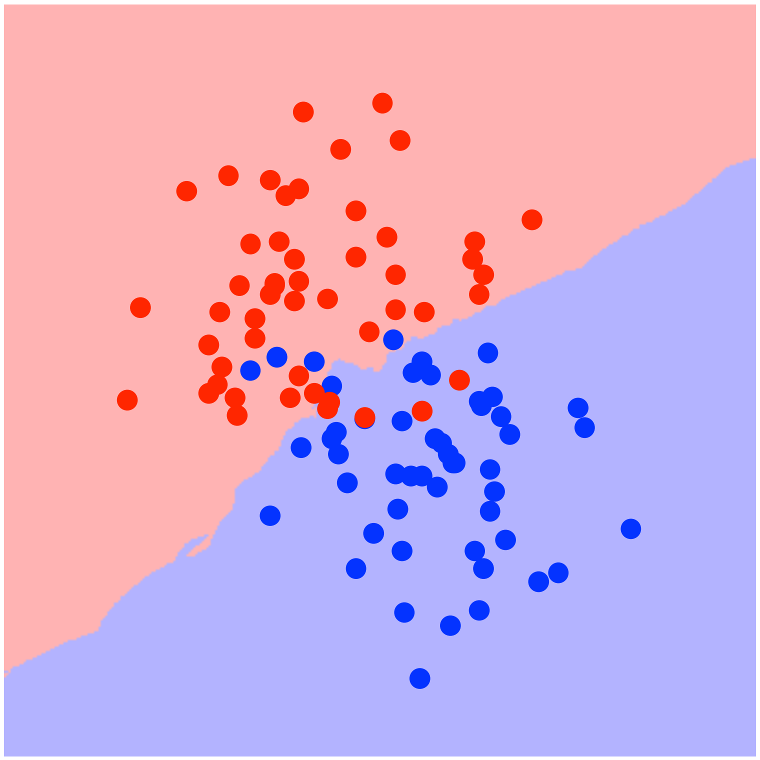


K = 7

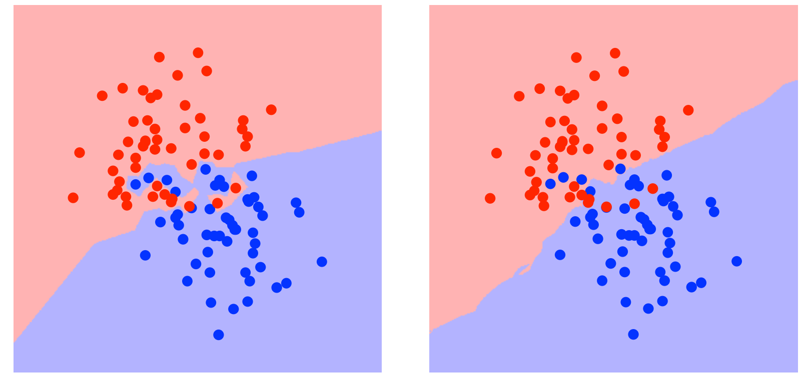


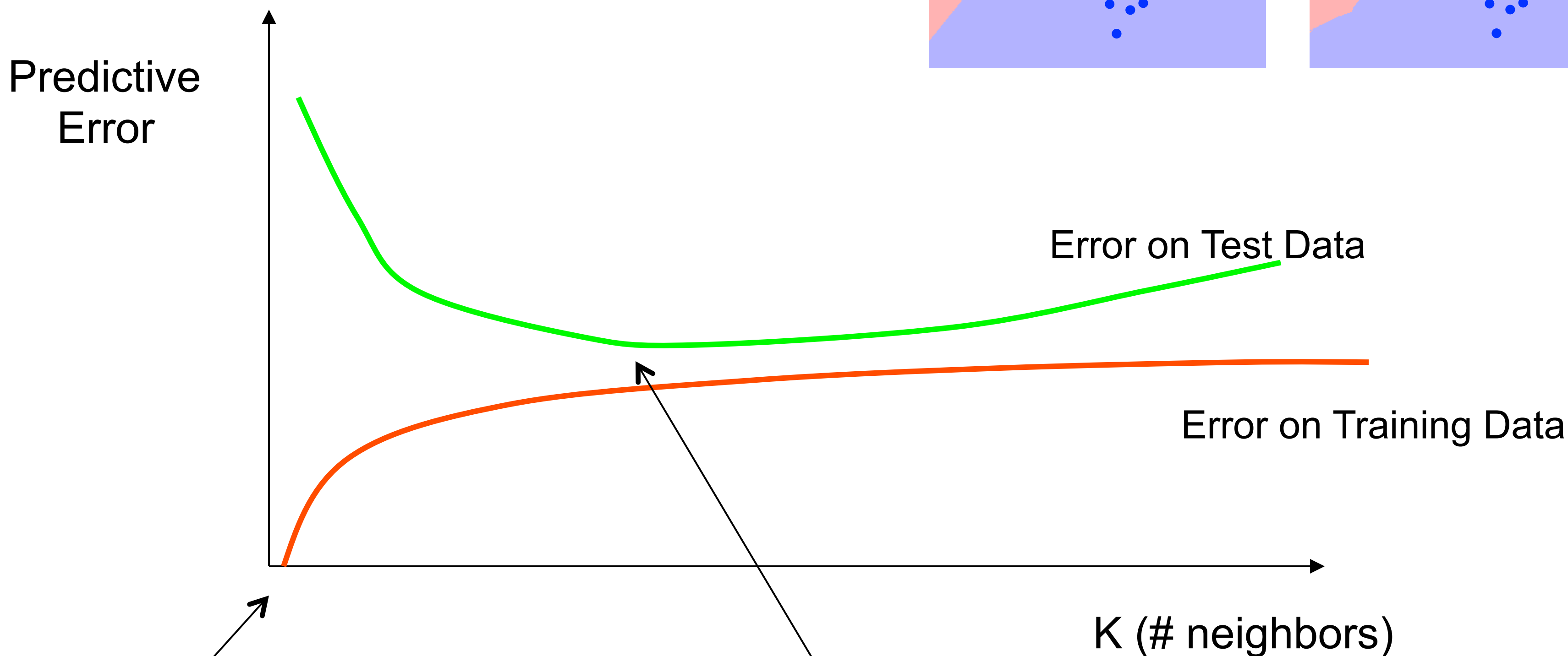
kNN Decision Boundary

- Recall: piecewise linear decision boundary
- Increasing k “simplifies” decision boundary
  - Majority voting means less emphasis on individual points



Error rates and K



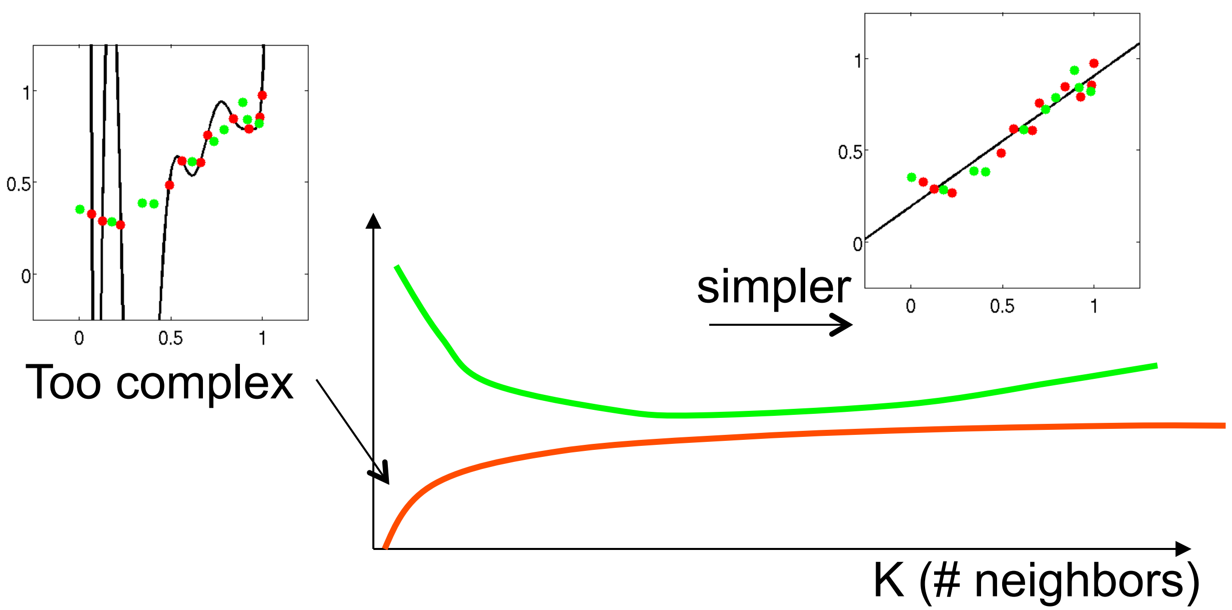


K=1? Zero error!
Training data have been memorized...

Best value of K

Complexity & Overfitting

- Complex model predicts all training points well
- Doesn't generalize to new data points
- K=1 : perfect memorization of examples (complex)
- K=M : always predict majority class in dataset (simple)
- Can select K using validation data, etc.



K-Nearest Neighbor (kNN) Classifier

- Theoretical Considerations
  - as k increases
    - we are averaging over more neighbors
    - the effective decision boundary is more "smooth"
  - as N increases, the optimal k value tends to increase
  - k=1, m increasing to infinity : error < 2x optimal

- Extensions of the Nearest Neighbor classifier
  - weighted distances
    - e.g., if some of the features are more important
    - e.g., if features are irrelevant

$$d(x, x') = \sqrt{\sum_i w_i (x_i - x'_i)^2}$$

  - fast search techniques (indexing) to find k-nearest neighbors in d-space

Summary

- K-nearest neighbor models
  - Classification (vote)
  - Regression (average or weighted average)

- Piecewise linear decision boundary
  - How to calculate

- Test data and overfitting
  - Model “complexity” for knn
  - Use validation data to estimate test error rates & select k