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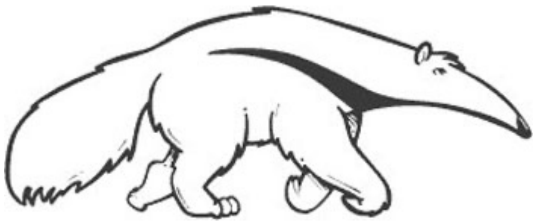
Machine Learning and Data Mining

Complexity & Nearest Neighbor Methods

Prof. Alexander Ihler



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Machine Learning

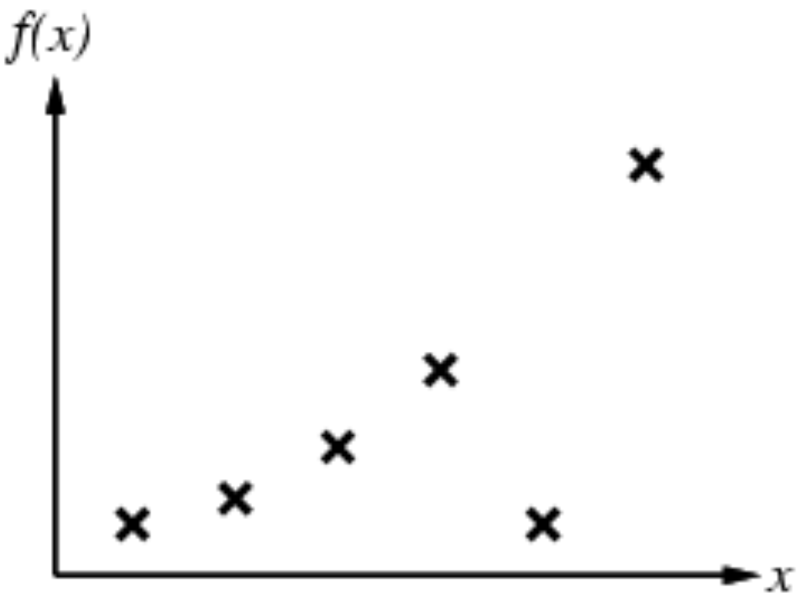
Complexity and Overfitting

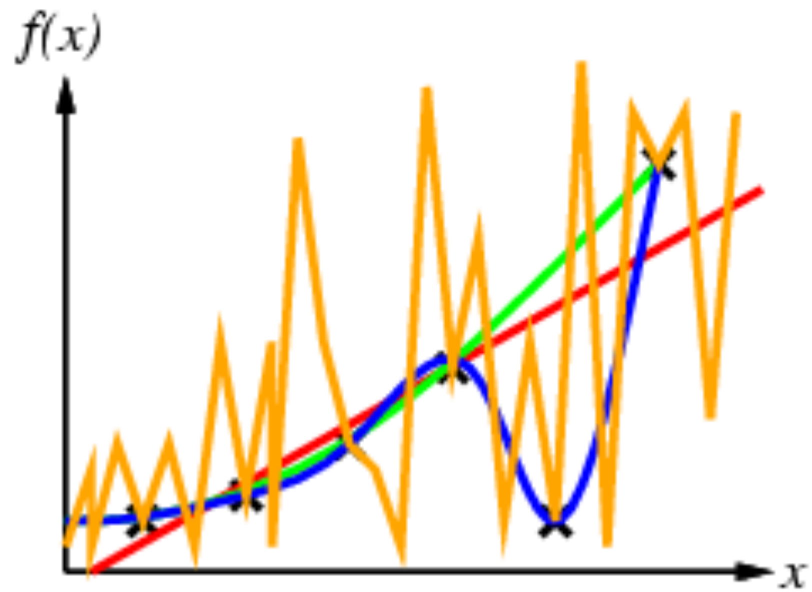
Nearest Neighbors

K-Nearest Neighbors

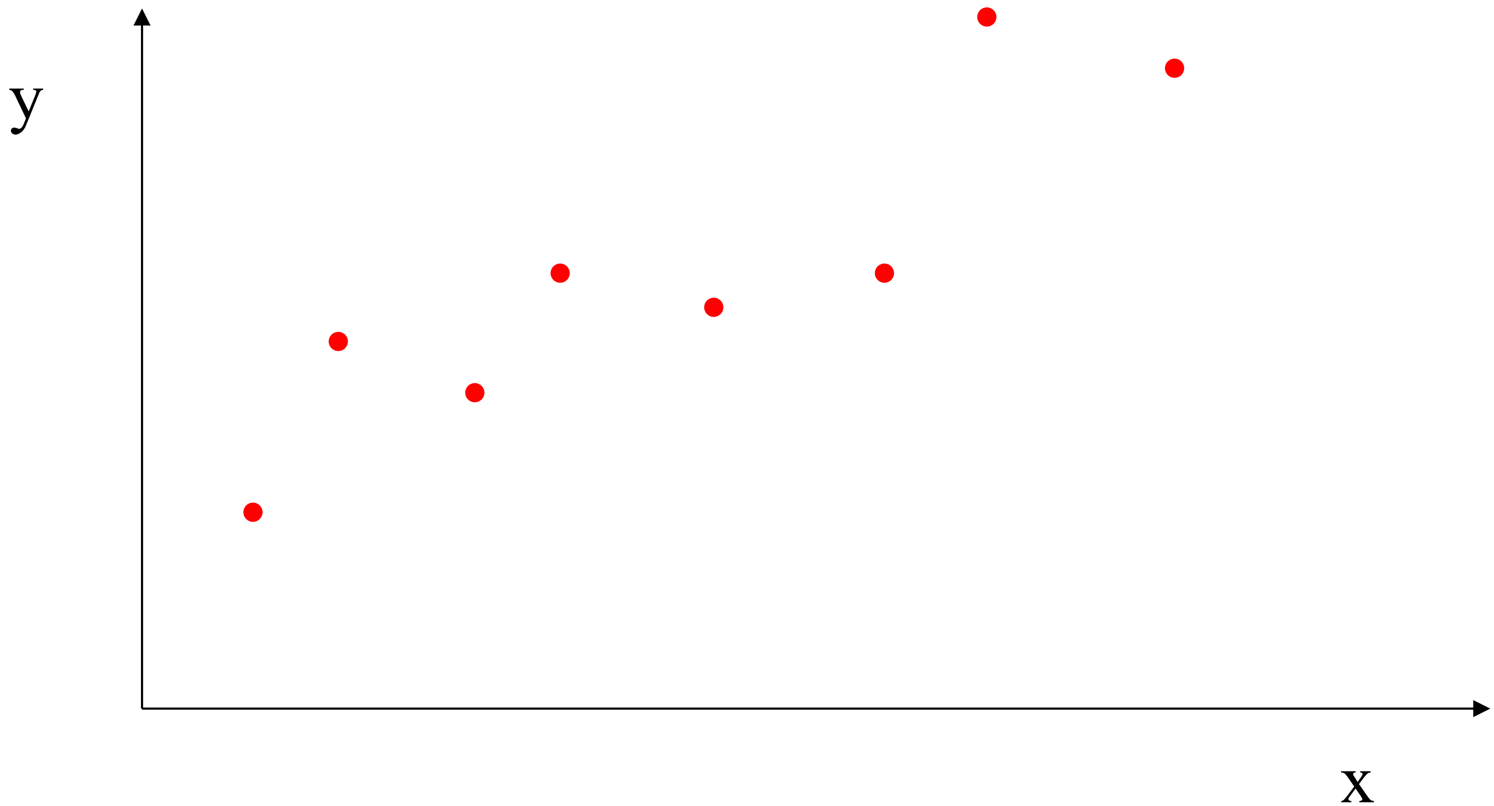
Inductive bias

- “Extend” observed data to unobserved examples
  - “Interpolate” / “extrapolate”
- What kinds of functions to expect? Prefer these (“bias”)
  - Usually, let data pull us away from assumptions only with evidence!



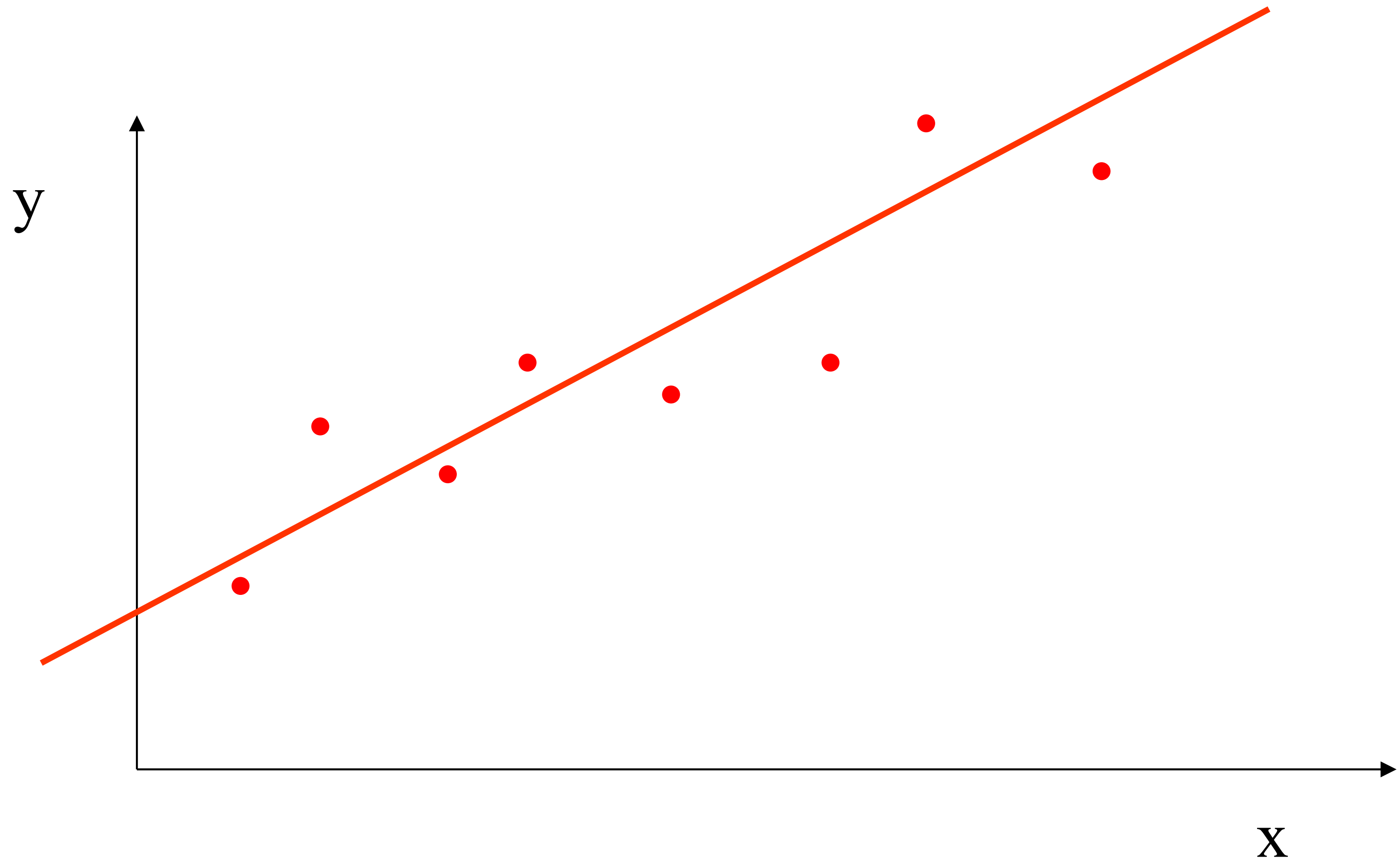


Overfitting and complexity

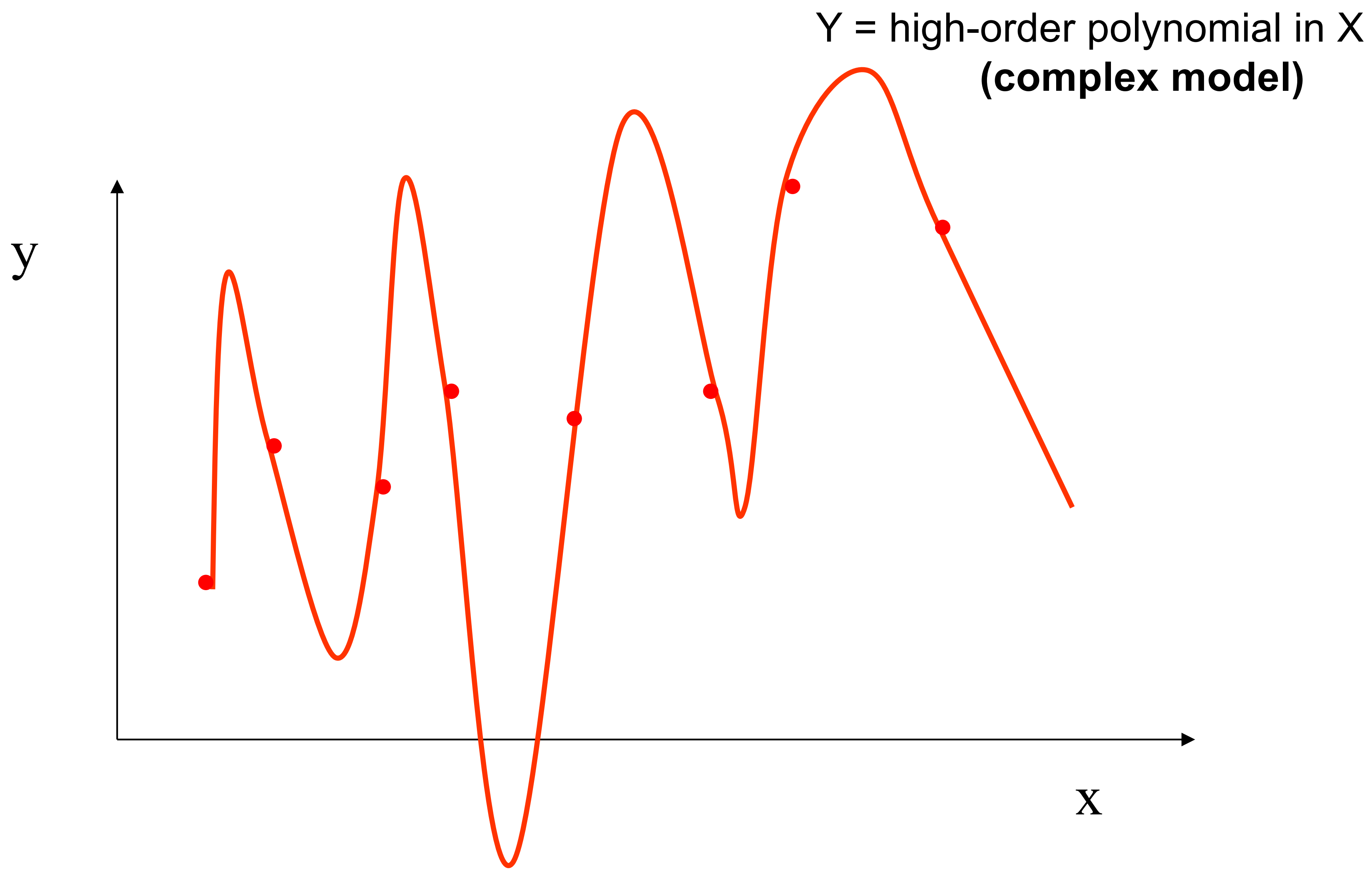


Overfitting and complexity

Simple model: Y= aX + b + e

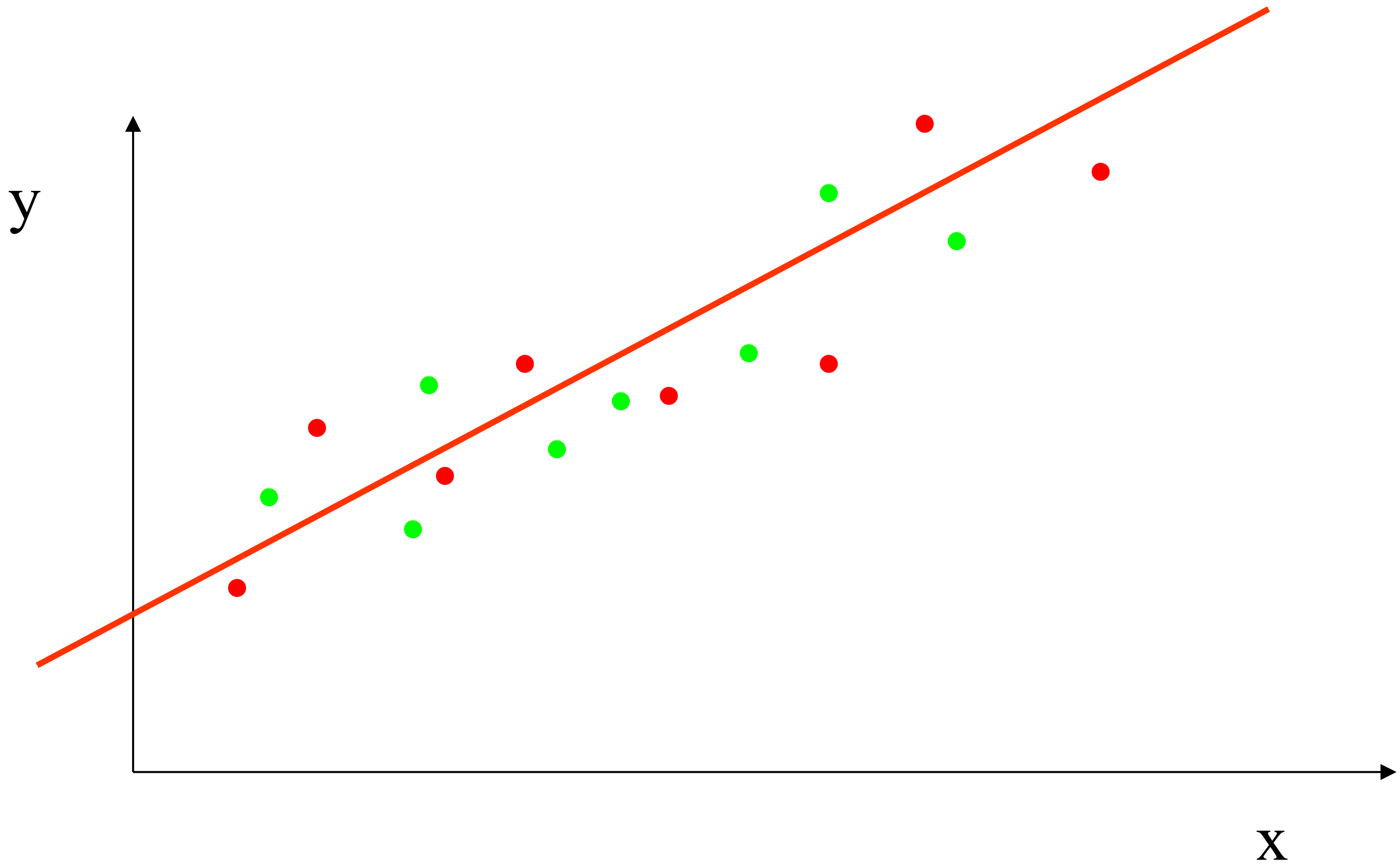


Overfitting and complexity

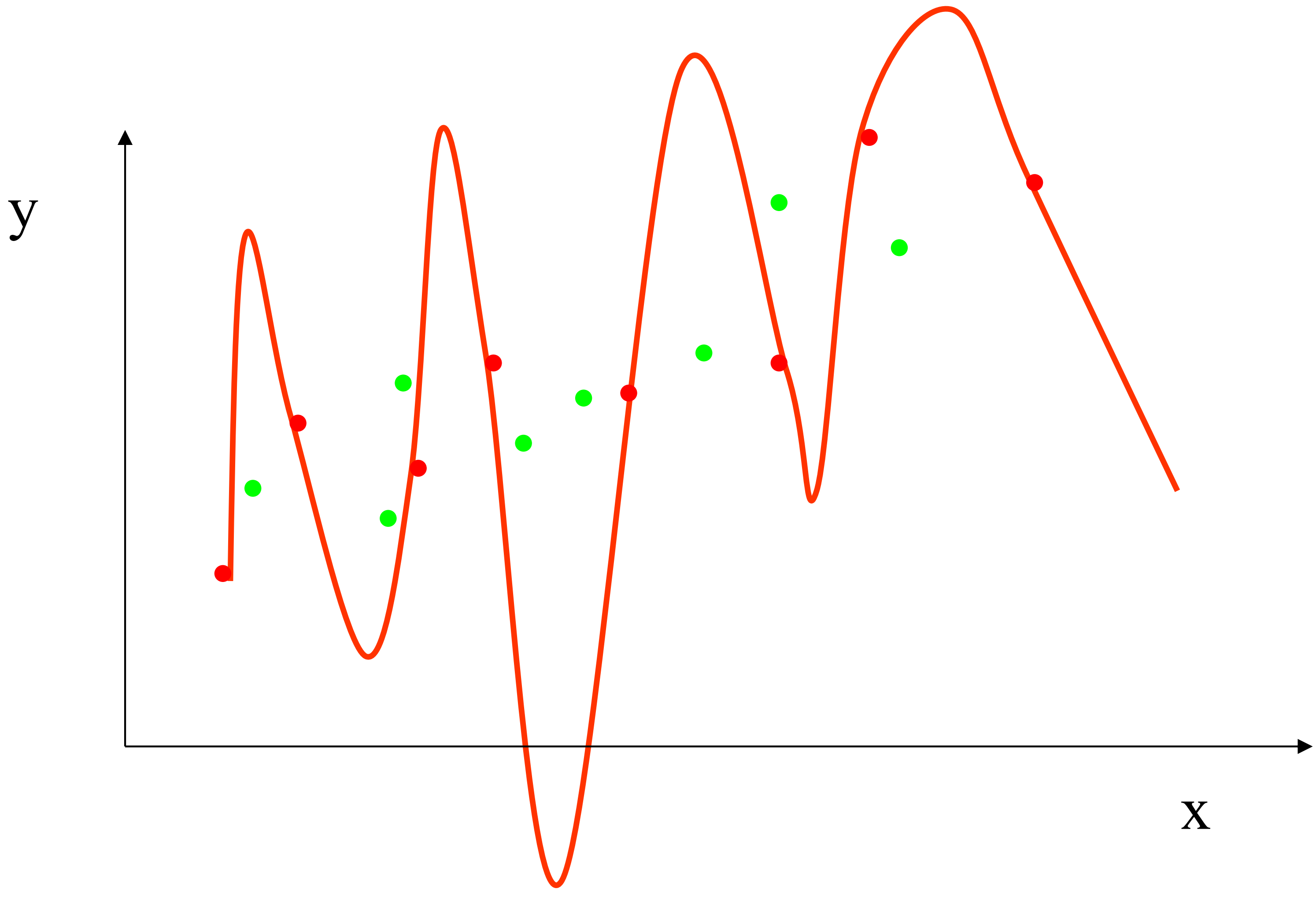


Overfitting and complexity

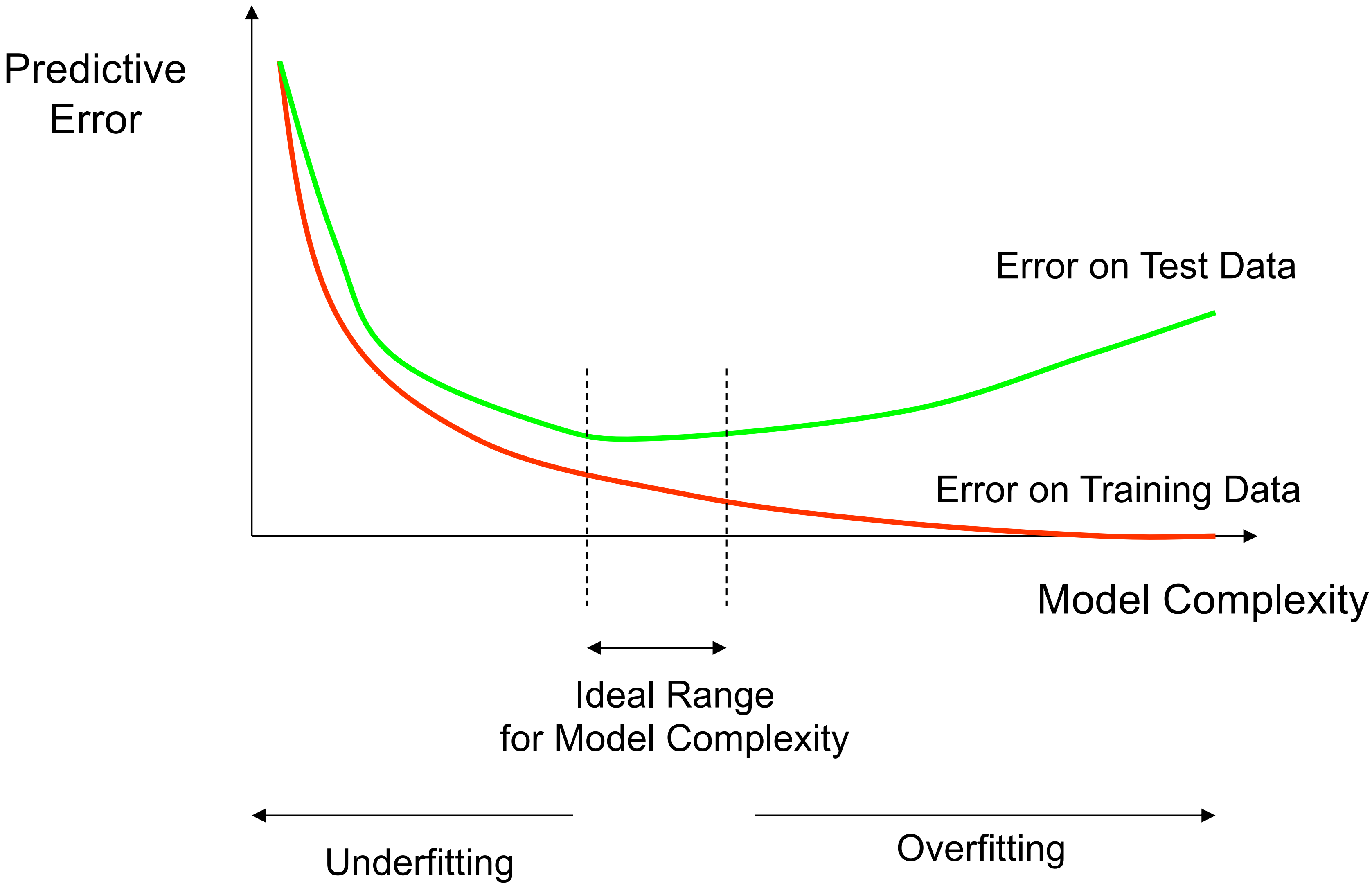
Simple model: Y= aX + b + e



Overfitting and complexity



How Overfitting affects Prediction



Training and Test Data

Data

- Several candidate learning algorithms or models, each of which can be fit to data and used for prediction
- How can we decide which is best?

Approach 1: Split into train and test data

Training Data	Test Data

- Learn parameters of each model from training data
- Evaluate all models on test data, and pick best performer

Problem:

- Over-estimates test performance ("lucky" model)
- Learning algorithms should *never* have access to test data

Training, Validation, and Test Data

Data

- Several candidate learning algorithms or models, each of which can be fit to data and used for prediction
- How can we decide which is best?

Approach 2: Reserve some data for validation

Training Data	Validation	Test Data

- Learn parameters of each model from training data
- Evaluate models on validation data, pick best performer
- Reserve test data to benchmark chosen model

Problem:

- Wasteful of training data (learning can't use validation)
- May bias selection towards overly simple models

Competitions

- Training data
  - Used to build your model(s)
- Validation data
  - Used to assess, select among, or combine models
  - Personal validation; leaderboard; …
- Test data
  - Used to estimate “real world” performance

#	Δ1w	Team Name * in the money	Score	Entries	Last Submission UT
1	-	BrickMover *	1.21251	40	Sat, 31 Aug 2013 23:
2	new	vsu *	1.21552	13	Sat, 31 Aug 2013 20:
3	↑2	Merlion	1.22724	29	Sat, 31 Aug 2013 23:
4	↓2	Sergey	1.22856	15	Sat, 31 Aug 2013 23:
5	new	liuyongqi	1.22980	13	Sat, 31 Aug 2013 13:

Machine Learning

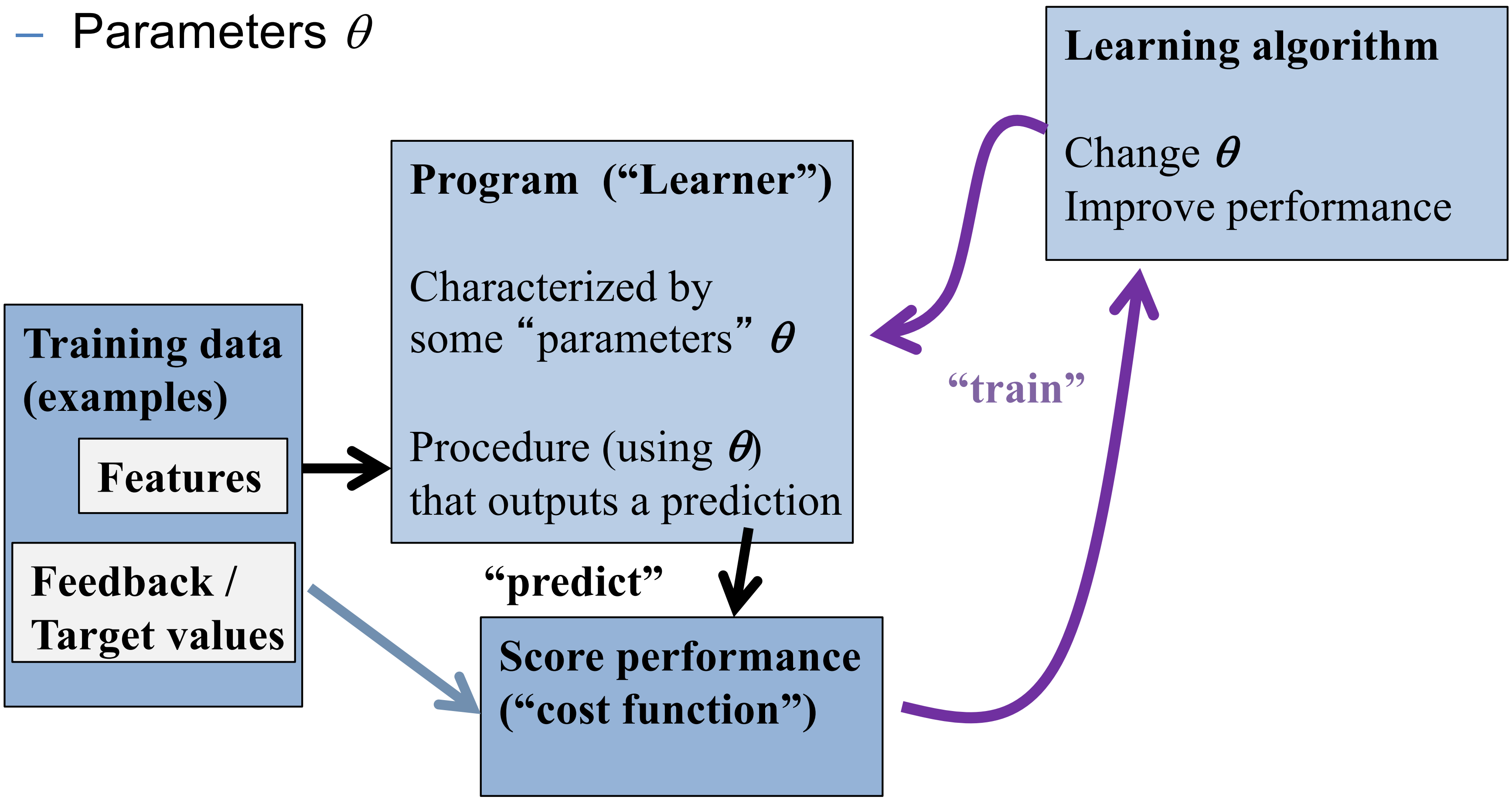
Complexity and Overfitting

Nearest Neighbors

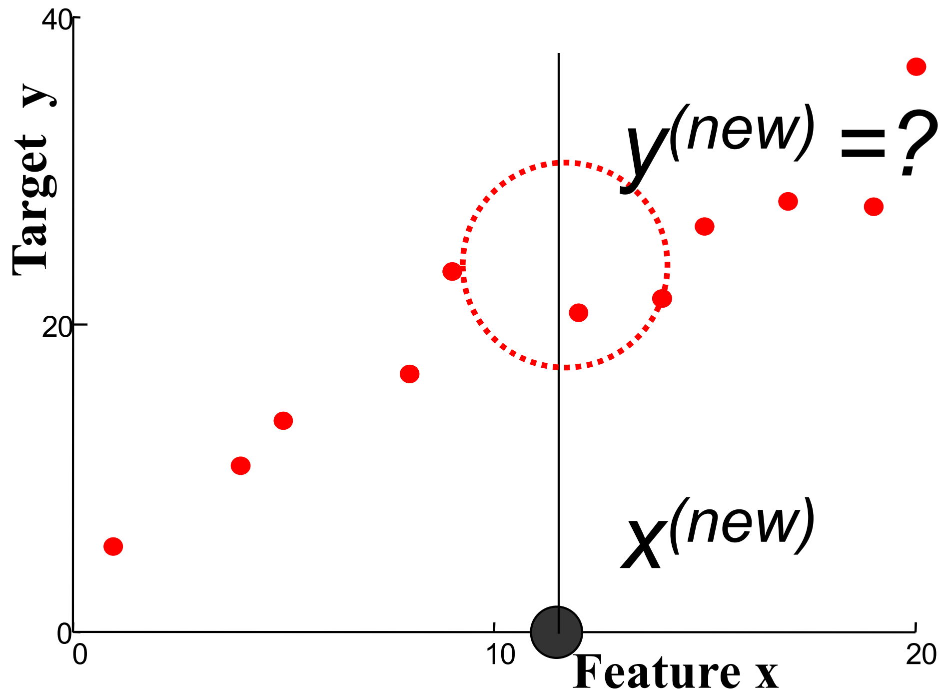
K-Nearest Neighbors

Supervised learning

- Notation
  - Features x
  - Targets y
  - Predictions $\hat{y} = f(x\ ;\ \theta)$
  - Parameters θ

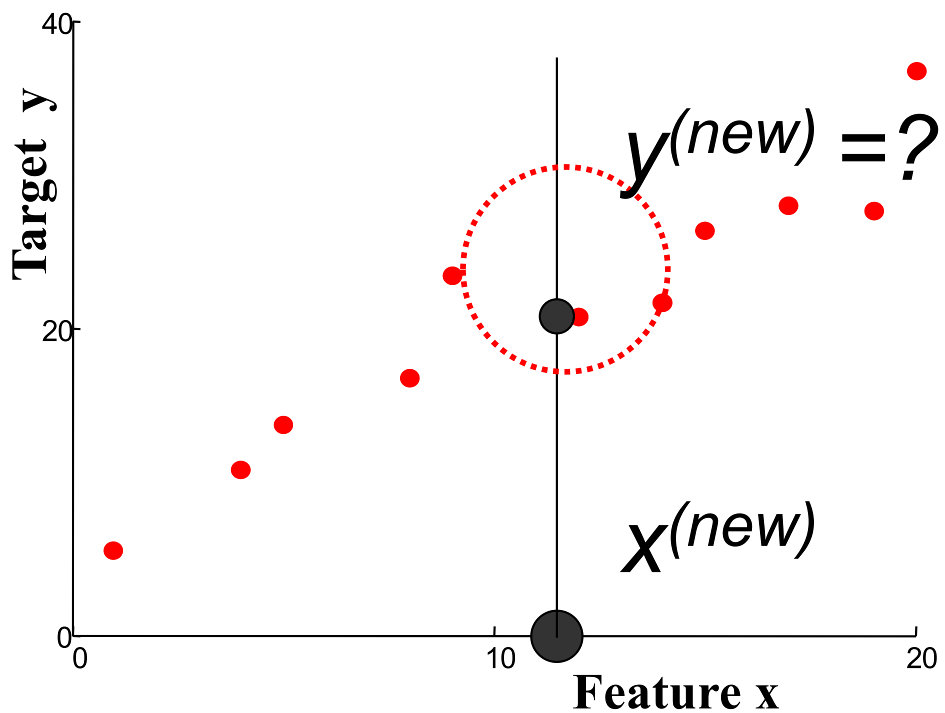


Regression; Scatter plots



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

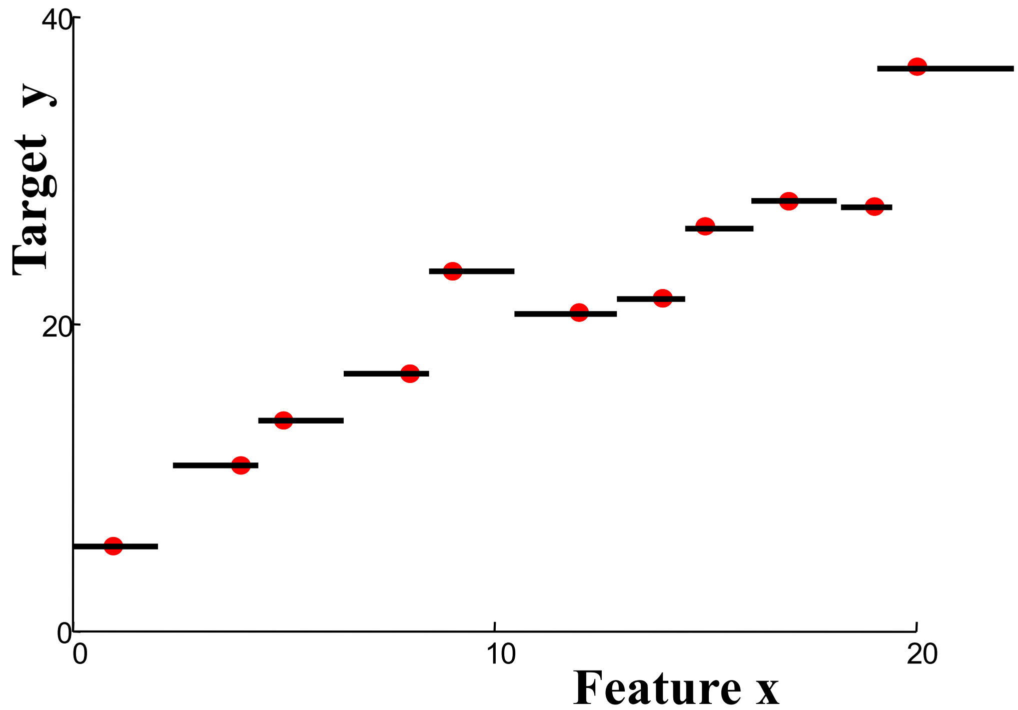
Nearest neighbor regression



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

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

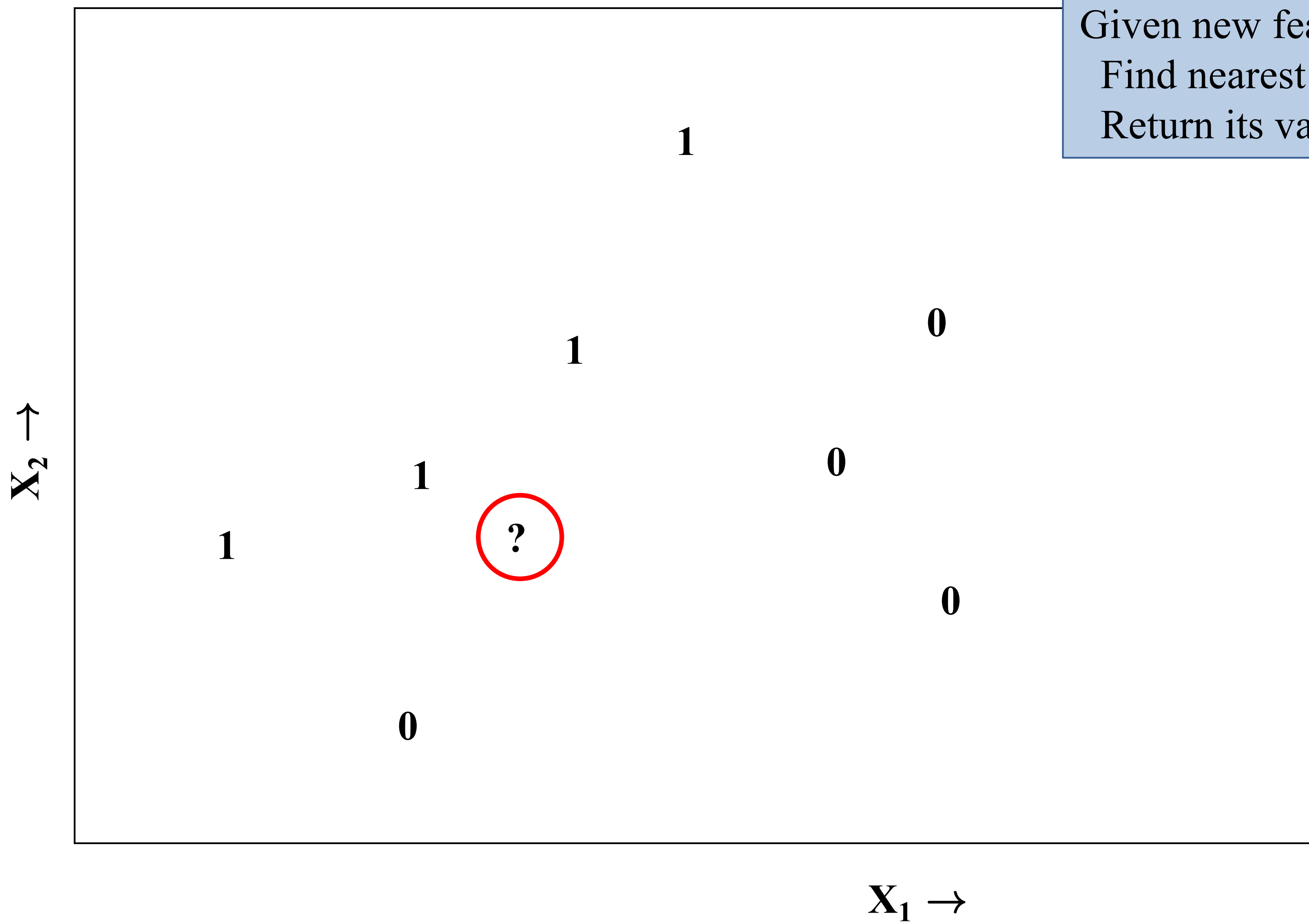
Nearest neighbor regression



"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”:
Given new features:
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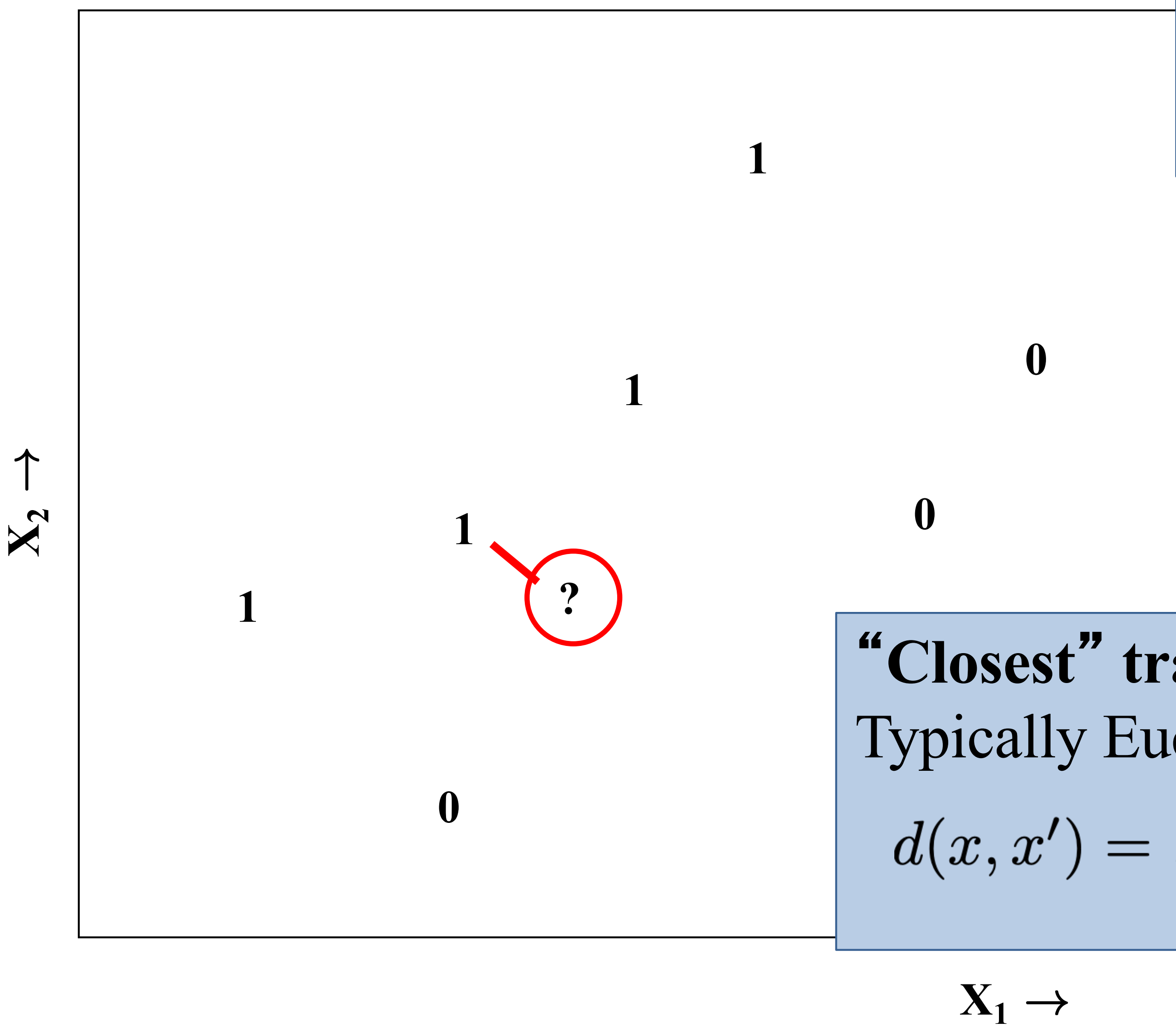
Nearest neighbor classifier

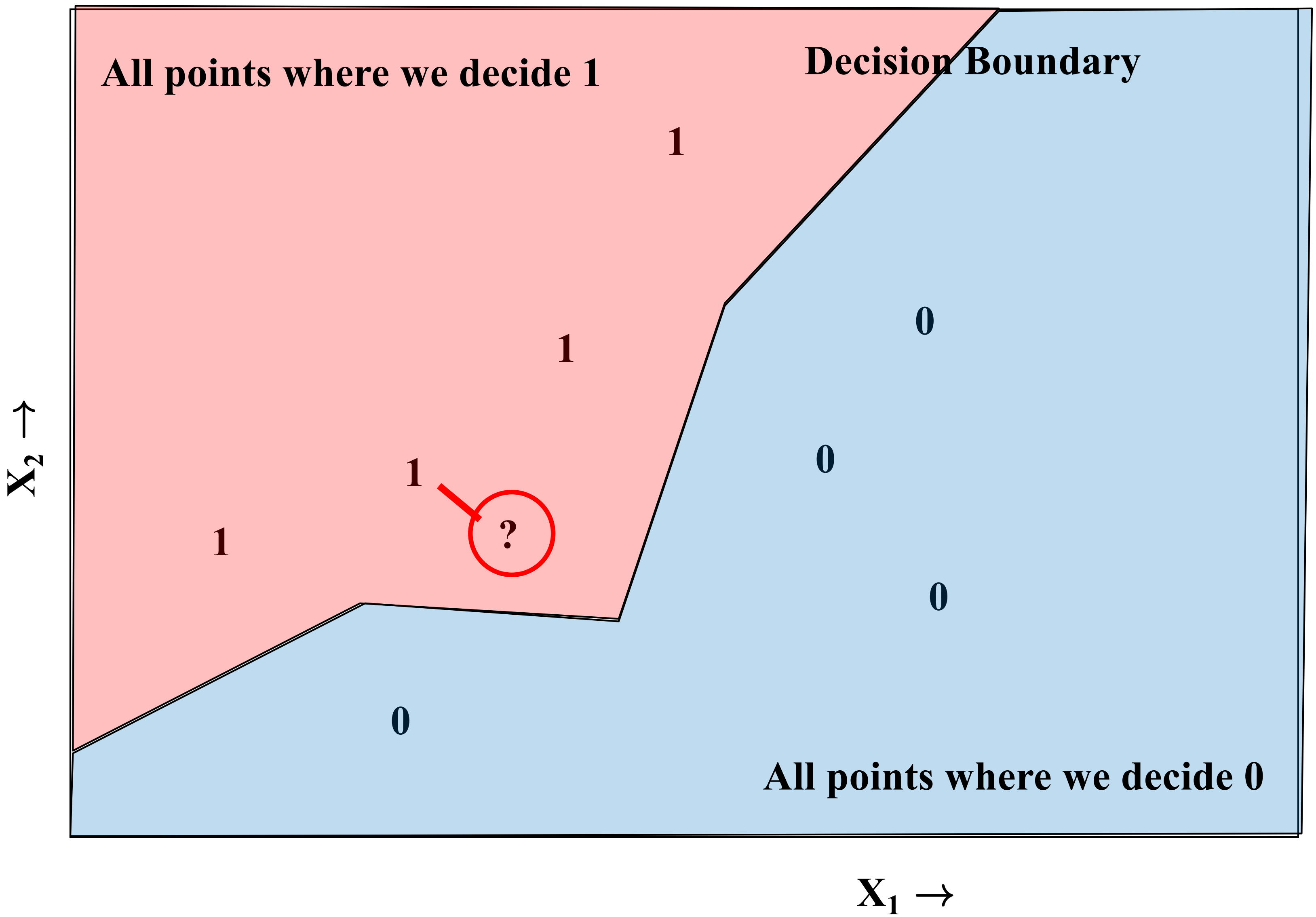


"Predictor":
Given new features:
Find nearest example
Return its value

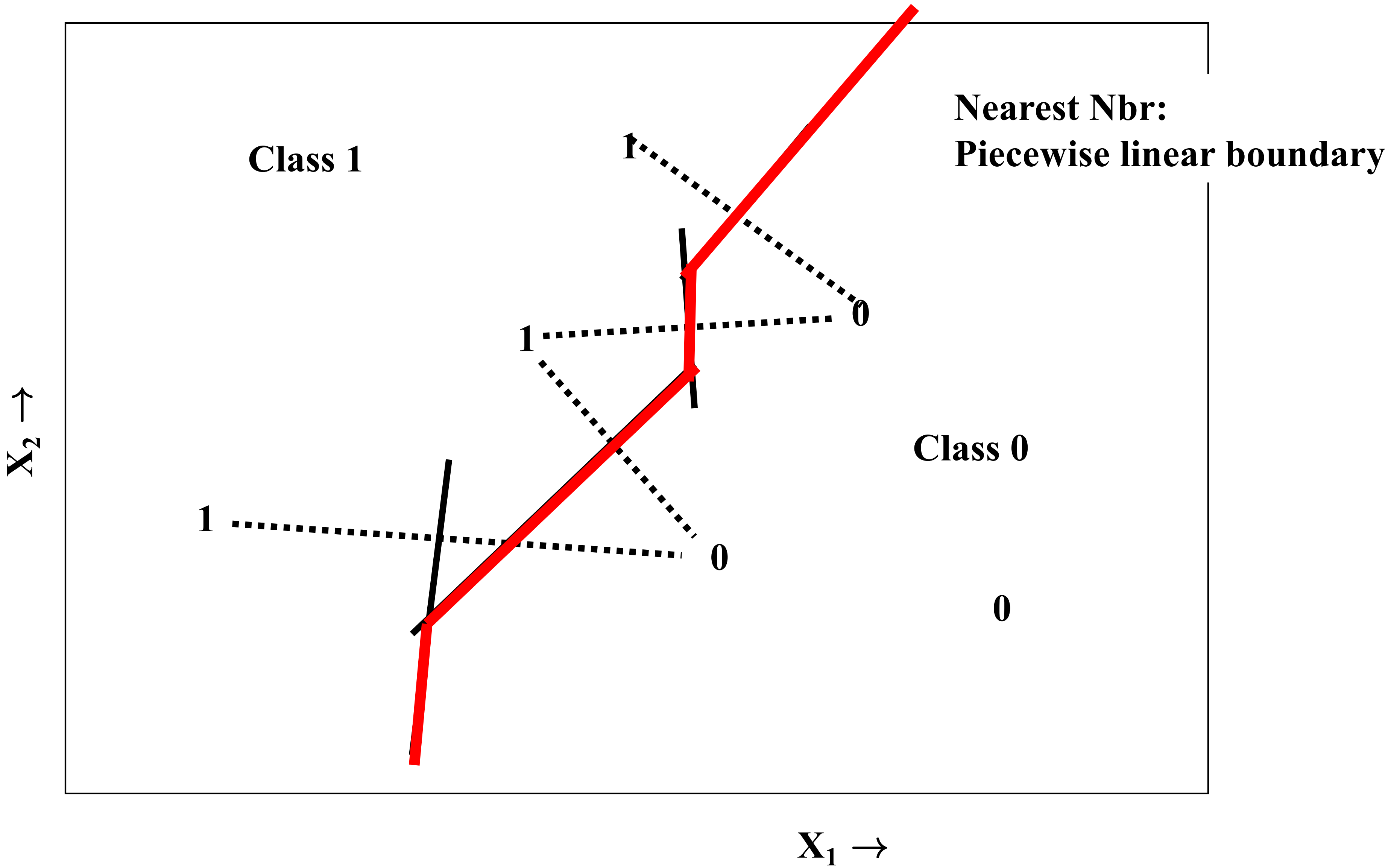
"Closest" training x?
Typically Euclidean distance:

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

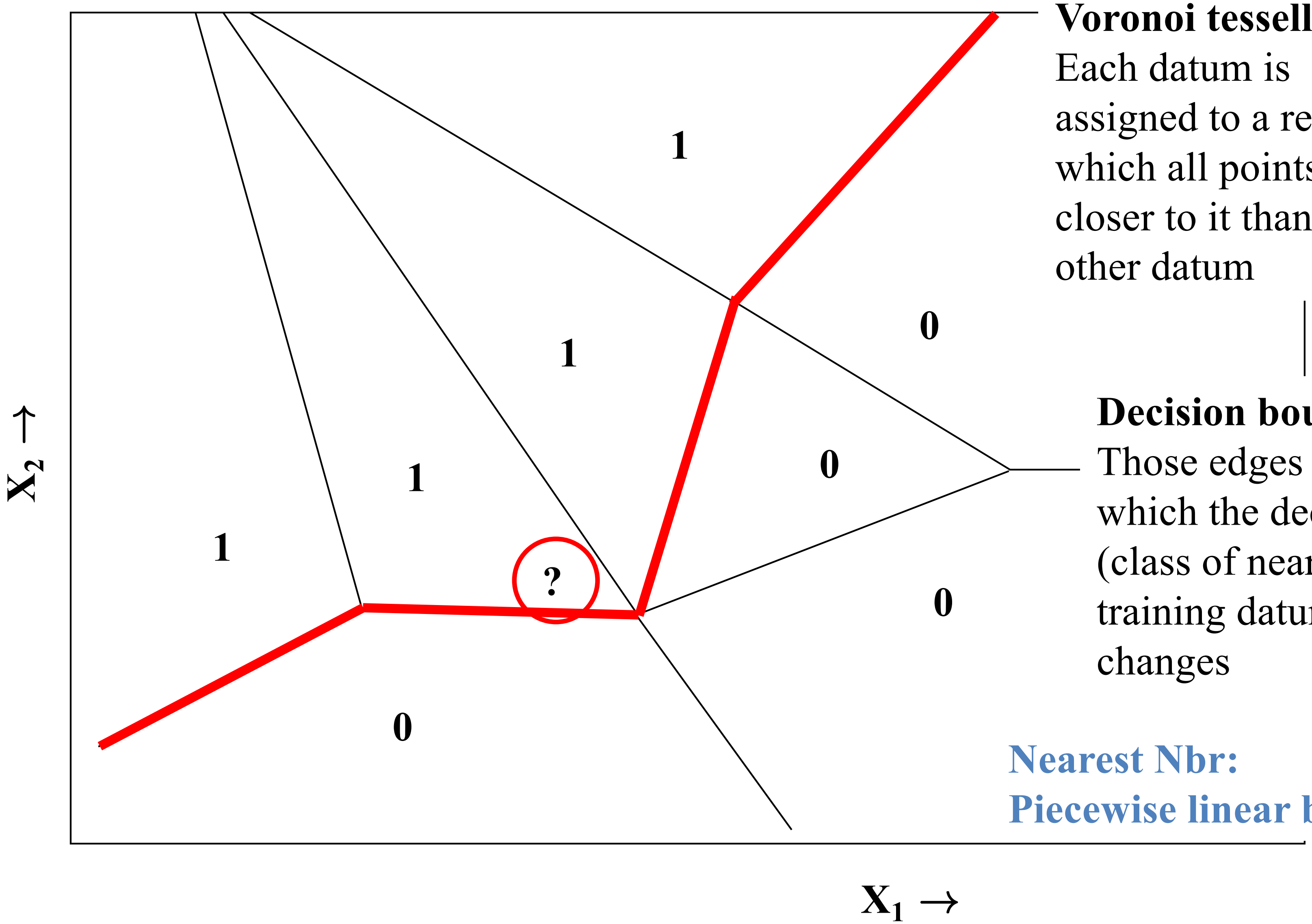
Nearest neighbor classifier



Nearest neighbor classifier



Nearest neighbor classifier

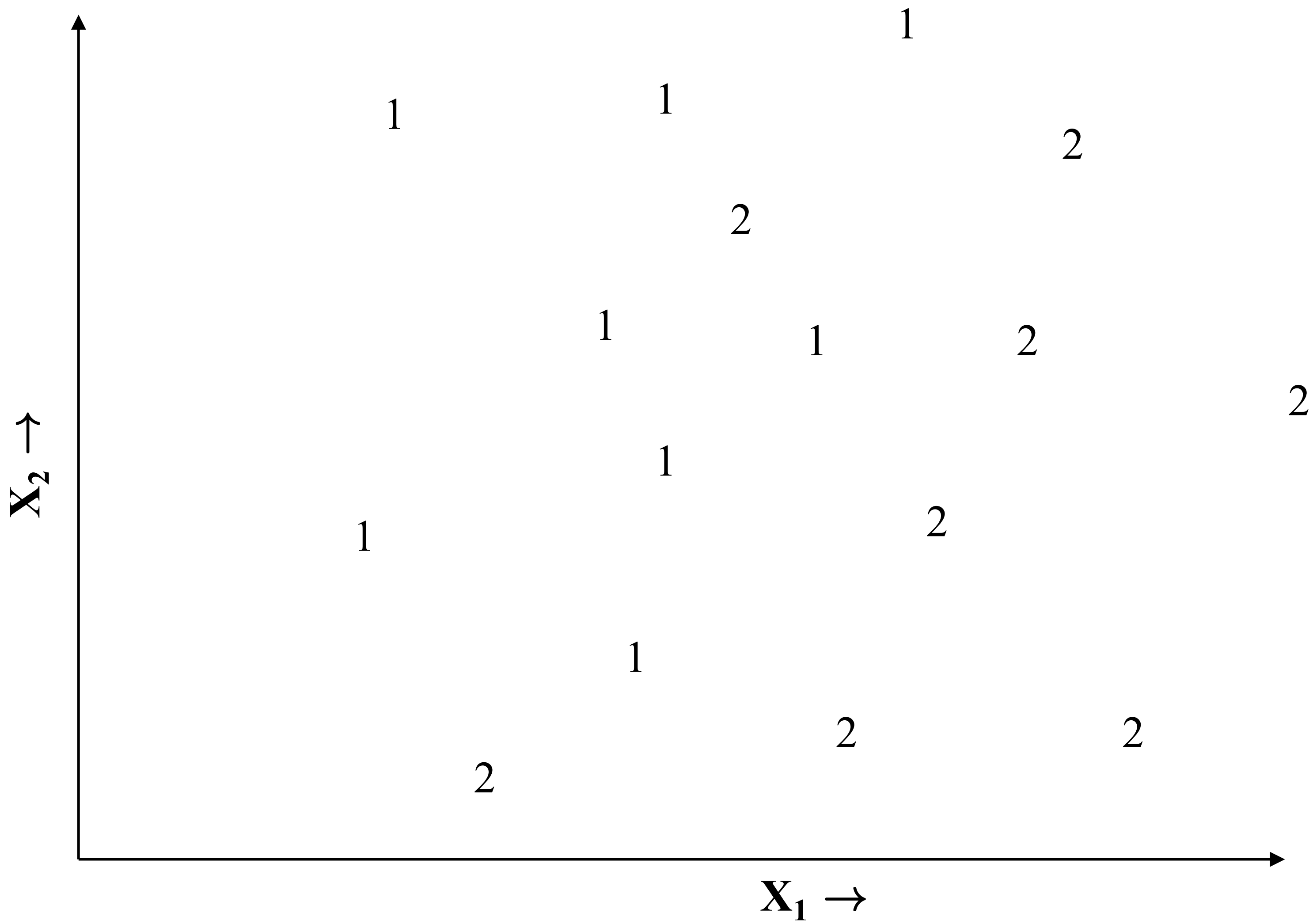


Voronoi tessellation: Each datum is assigned to a region, in which all points are closer to it than any other datum

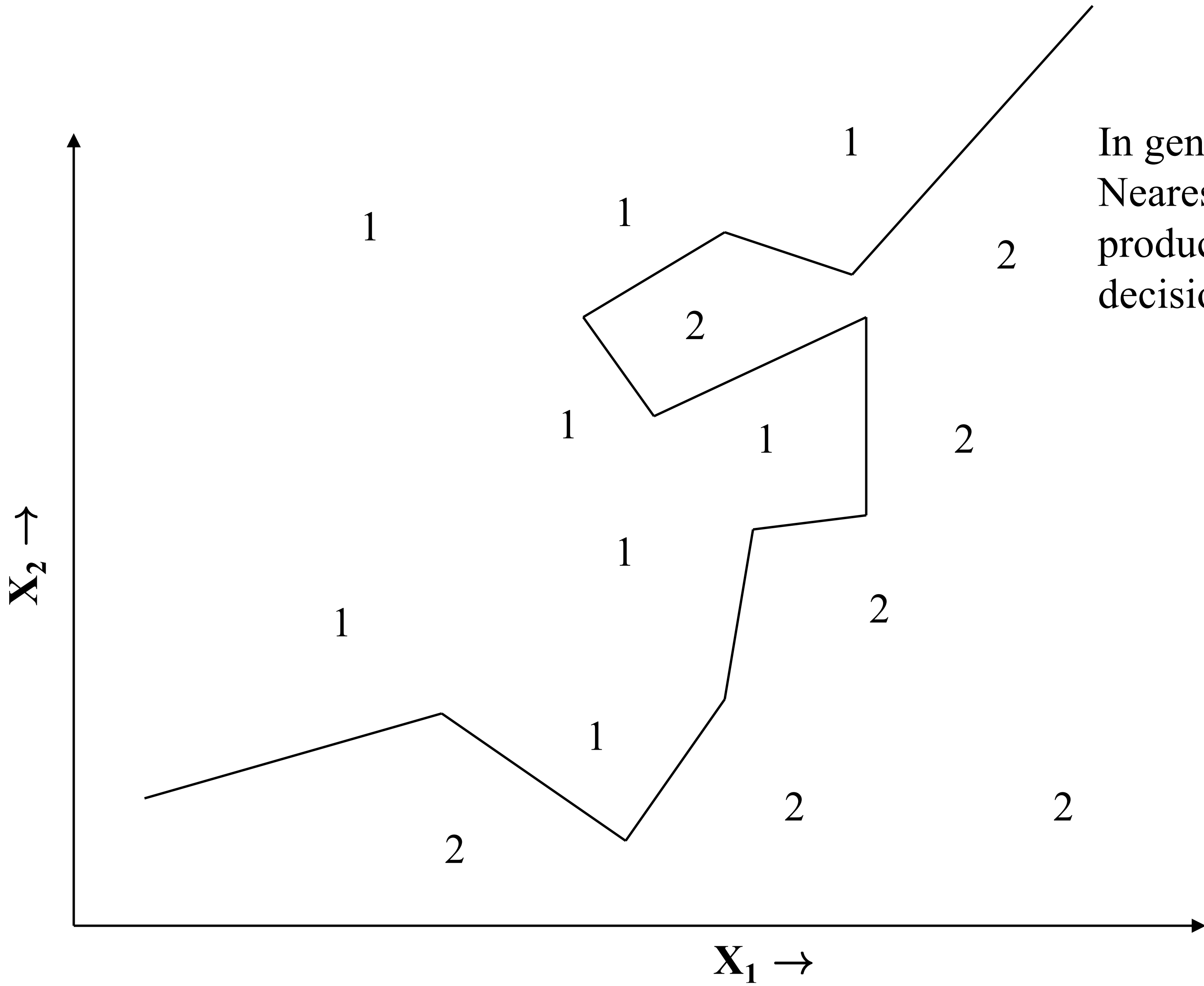
Decision boundary: Those edges across which the decision (class of nearest training datum) changes

Nearest Nbr: Piecewise linear boundary

More Data Points

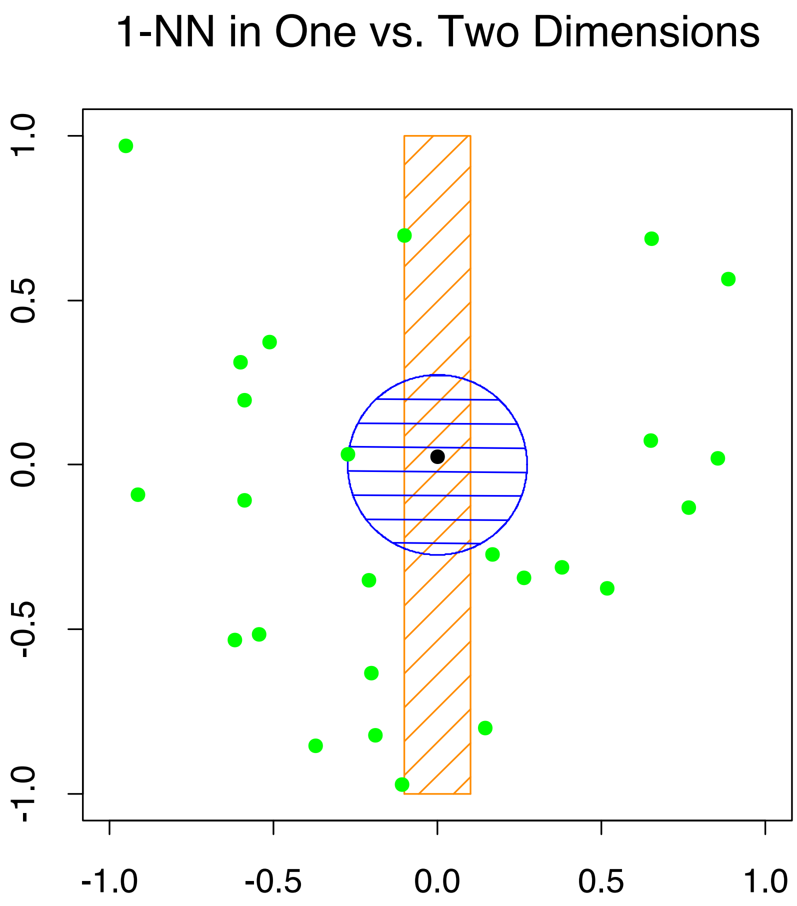


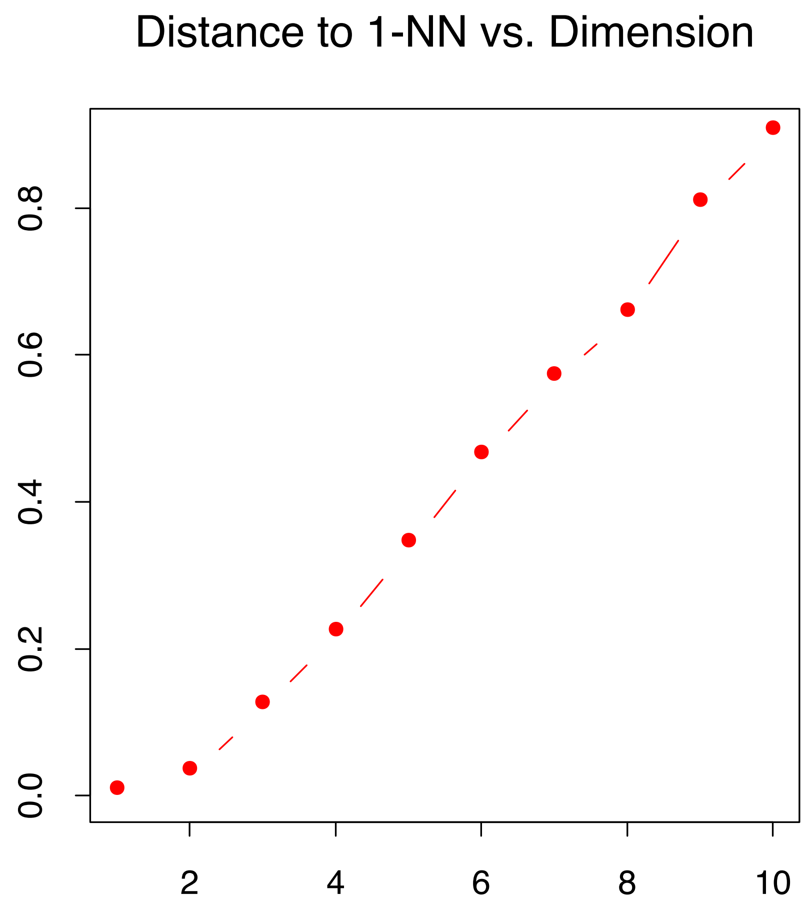
More Complex Decision Boundary



In general:
Nearest-neighbor classifier produces <u>piecewise linear</u> decision boundaries

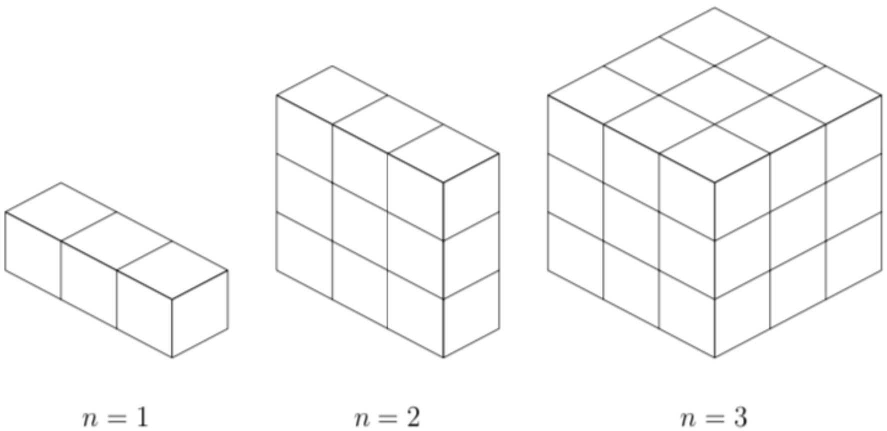
Issue: Neighbor Distance & Dimension





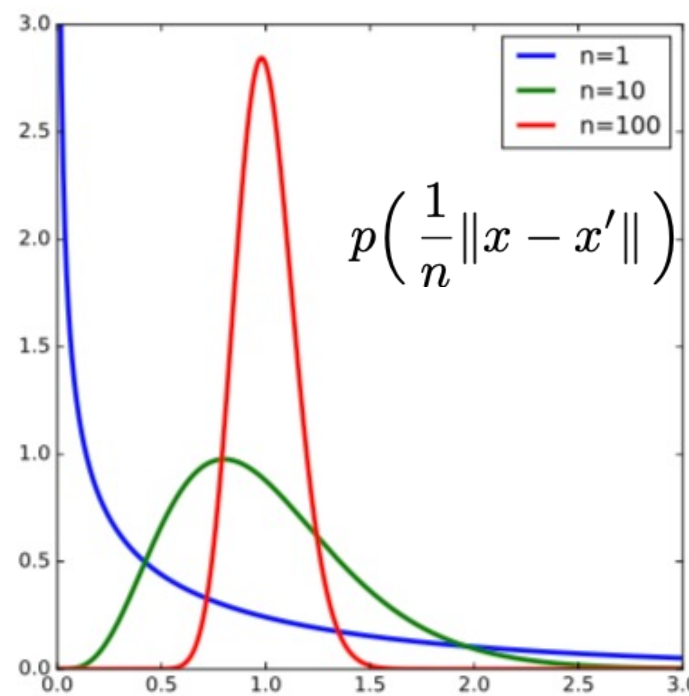
For m=1000 data in unit hypercube

The "Curse of Dimensionality"



- Function is "smooth"?
  - Want a training example that is close by (epsilon)
  - How many data do we need?

- How far away are the other data points?
  - In higher dimension, "almost all" data are equally far away!



Machine Learning

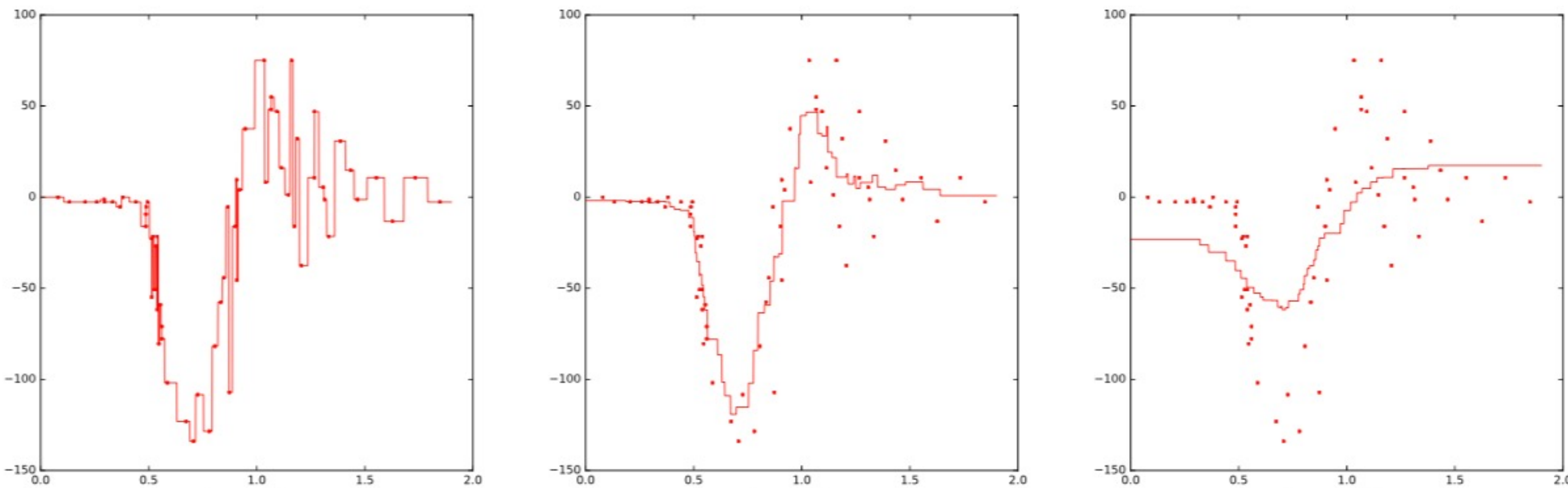
Complexity and Overfitting

Nearest Neighbors

K-Nearest Neighbors

K-Nearest Neighbor (kNN) Predictor

- Find the k-nearest neighbors to x in the data
  - i.e., rank the feature vectors according to Euclidean distance
  - select the k vectors which are have smallest distance to x
- Regression
  - Ranking gives k closest examples and their target values “y”
  - Usually just average the y-values of the k closest training examples
  - Larger k = average over a larger area for prediction

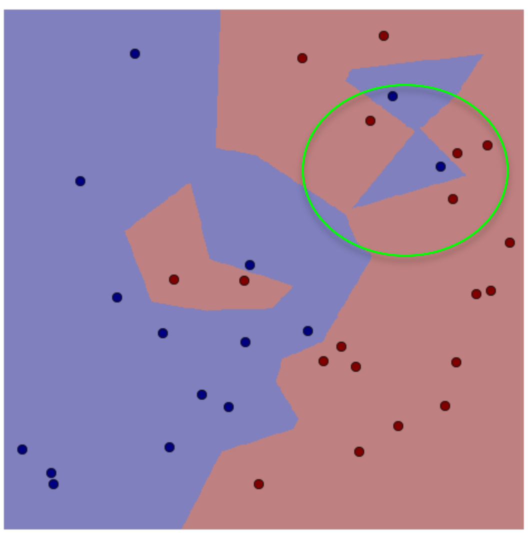


$k = 1$ $k = 5$ $k = 25$

K-Nearest Neighbor (kNN) Predictor

- Find the k-nearest neighbors to x̲ in the data
  - i.e., rank the feature vectors according to Euclidean distance
  - select the k vectors which are have smallest distance to x̲

- 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”)
  - Note: for two-class problems, if k is odd (k=1, 3, 5, …) there will never be any “ties”; otherwise, just use (any) tie-breaking rule

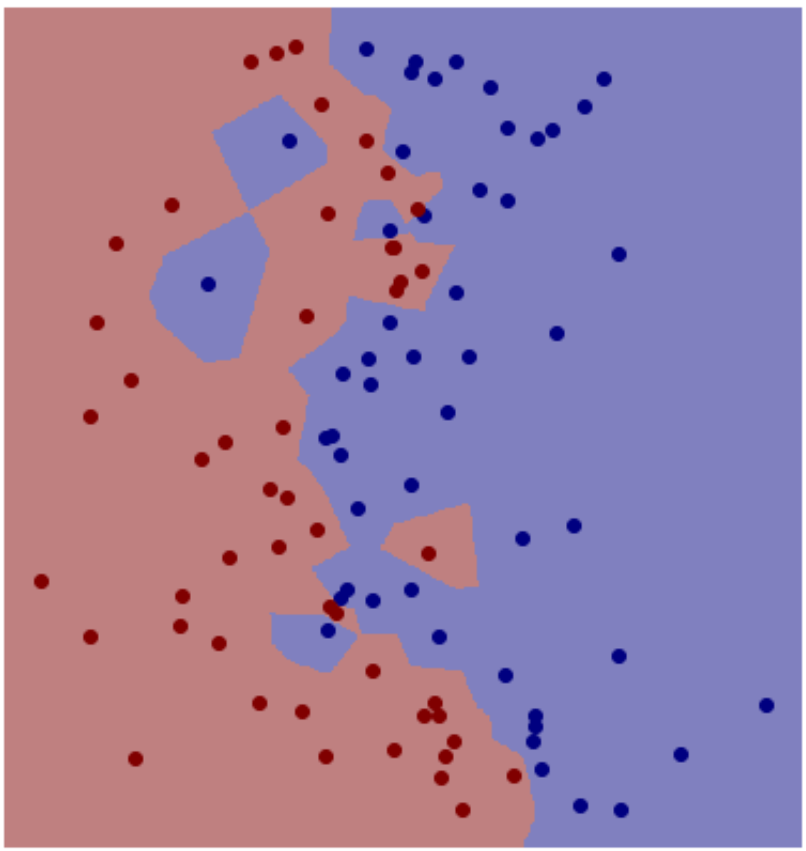


Predict blue?
Or just noise?

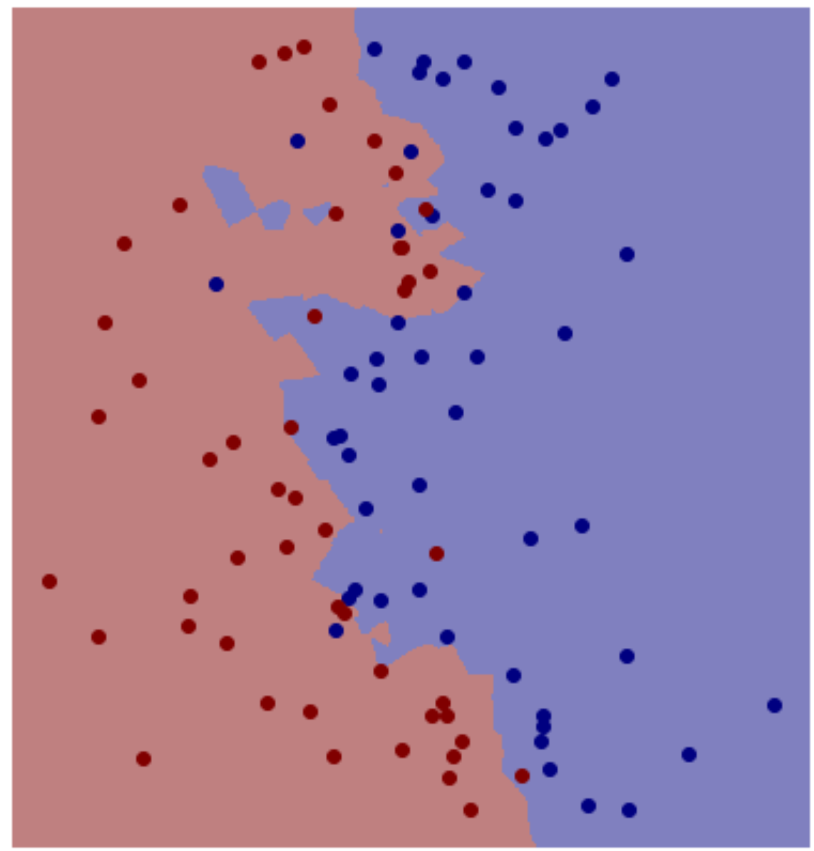
kNN Decision Boundary

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

K = 1



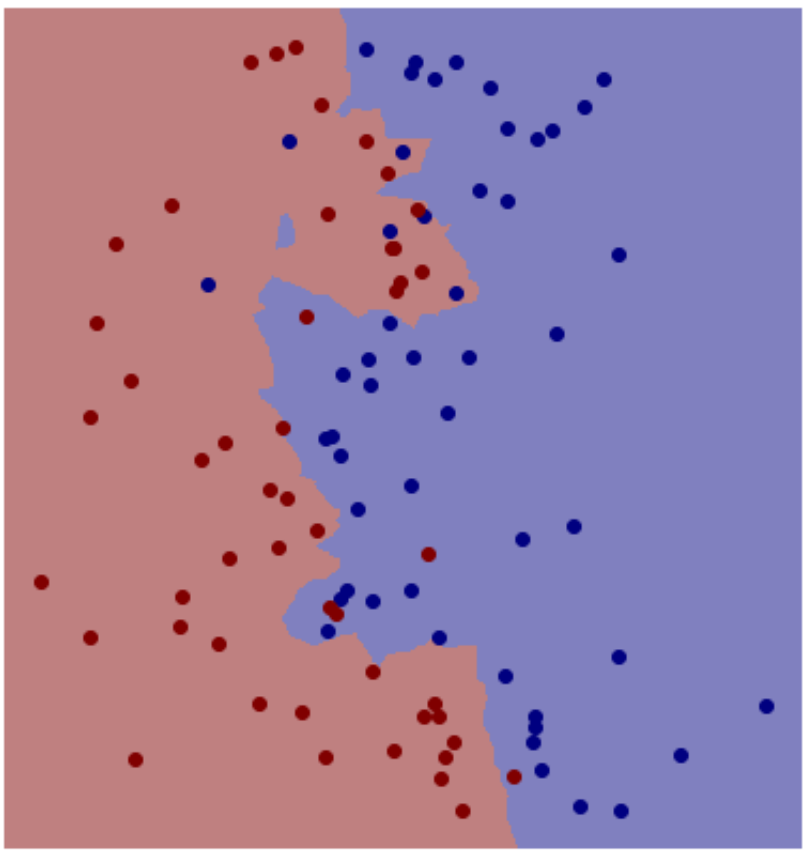
K = 3



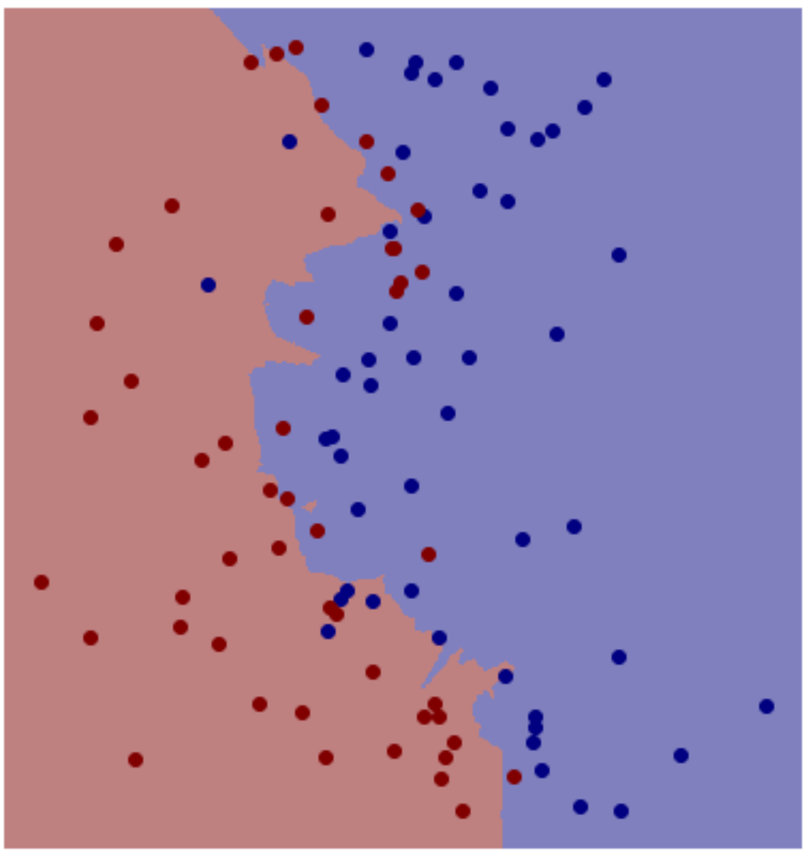
kNN Decision Boundary

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

K = 5



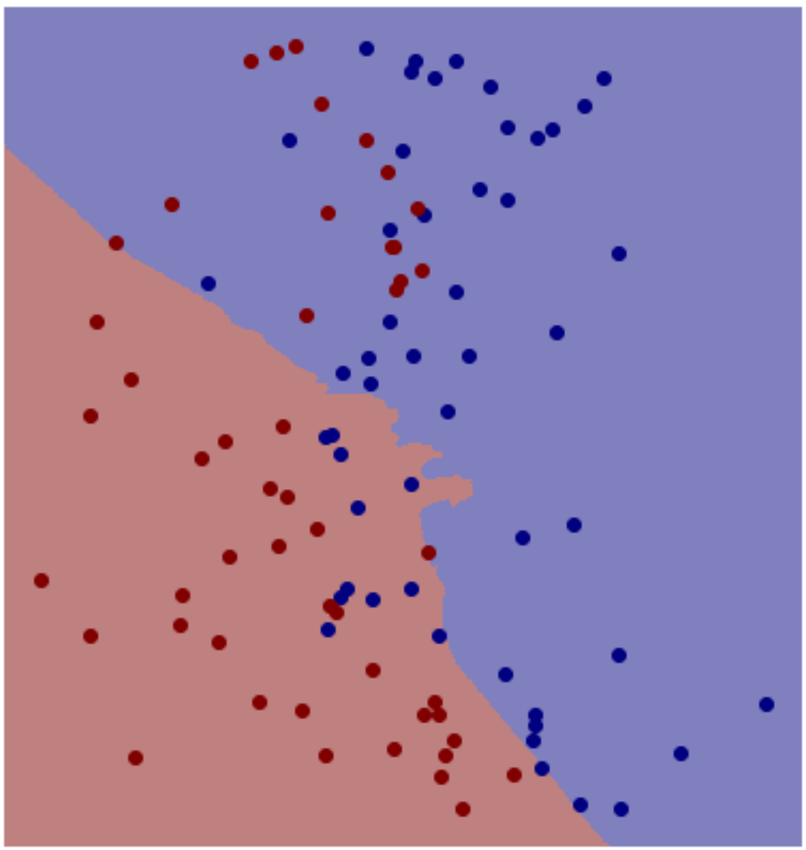
K = 20



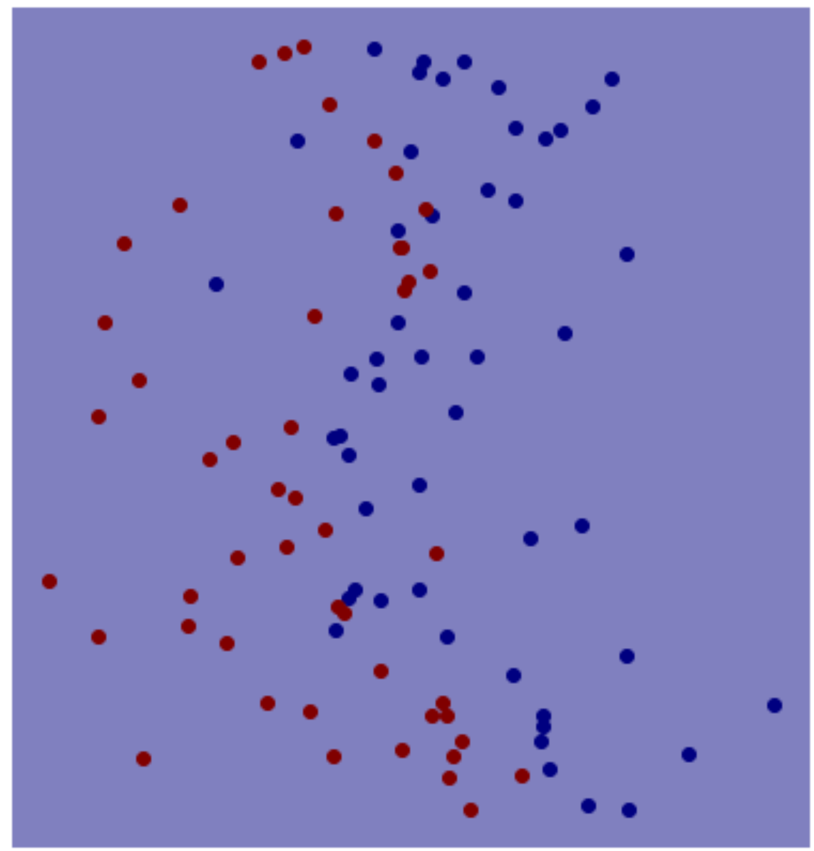
kNN Decision Boundary

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

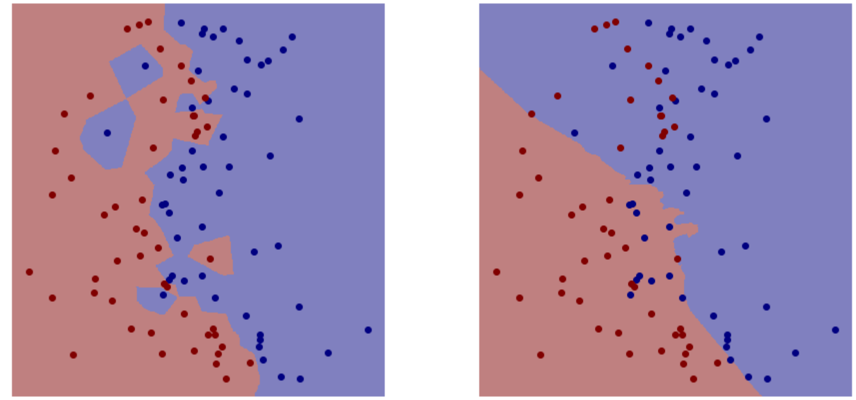
K = 70

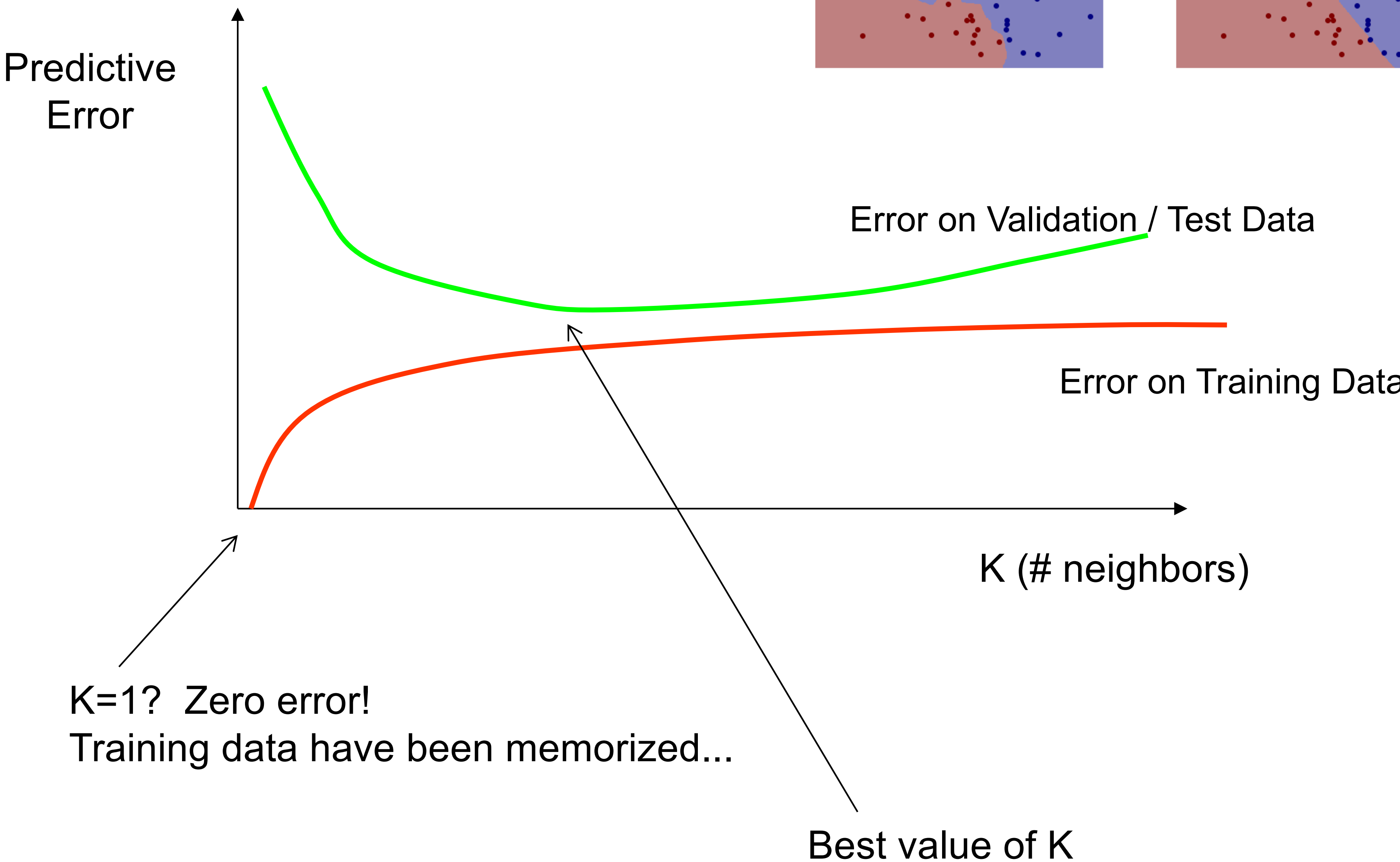


K = 100 (=m)



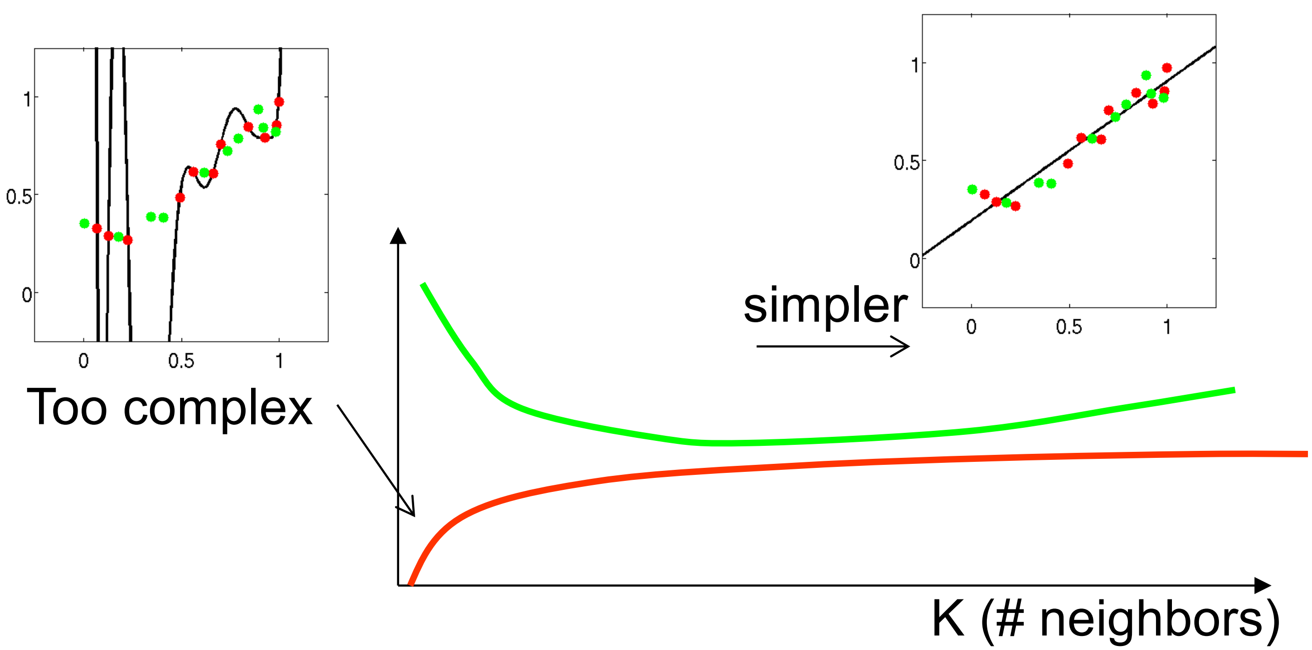
Error rates and K





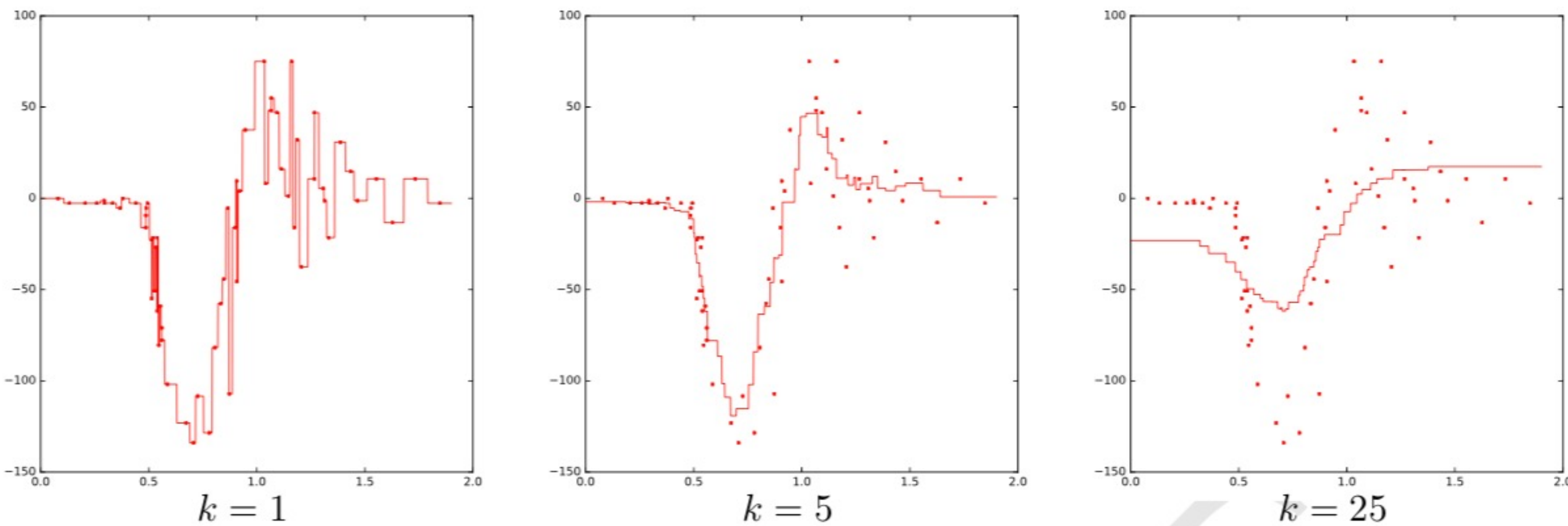
Complexity & Overfitting

- 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.



Regression example

- Similar behavior for regression predictions:



  - K (& data density) defines a local area to average over
  - K too small: follow "noise" in the data
  - K too big: smooth over too large an area

K-Nearest Neighbor (kNN) Classifier

- Theoretical Considerations
  - as k increases
    - we are averaging over more neighbors
    - the effective decision boundary is more “smooth”
  - as m 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 $d(x, x') = \sqrt{\sum_i w_i (x_i - x'_i)^2}$
    - e.g., some features may be more important; others may be irrelevant
  - Fast search techniques (indexing) to find k-nearest points in d-space
  - Weighted average / voting based on distance

Digit & Hand Gesture Recognition

Athitsos et al., CVPR 2004 & PAMI 2008

Tricks to build efficient & accurate nearest-neighbor classifiers:

- **Gather large training sets (possibly by generating synthetic data)**
- **Engineer clever distance functions that are invariant to aspects of the data unrelated to the class label**
- **Use algorithms to find (approximate) nearest neighbors in sub-linear time (locality sensitive hashing, class-sensitive embeddings, KD-trees, etc.)**

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