Overview of Supervised Learning I

Statistical Data Mining I

Rachael Hageman Blair

Modeling Assumptions of this class

1. Many statistical learning methods are relevant and useful in a wide-range of academic and non-academic disciplines beyond biostatistics.
2. Statistical learning should not be viewed as a series of black boxes.
3. While it is important to know what job is performed by the black box, it is not necessary to create the black box.
4. It is presumed that the student is interested in applying data-mining methods to real-world problems.

Our Goal: Practical yet rigorous.

Two Simple Approaches to Prediction

	Linear Model	K-nearest neighbors
Structural Assumptions	High	Low
Stability	Stable	Can be Unstable
Accuracy	Can be inaccurate	Accurate

Q: Why are we looking at these two simple methods?

Two Simple Approaches to Prediction

	Linear Model	K-nearest neighbors
Structural Assumptions	High	Low
Stability	Stable	Can be Unstable
Accuracy	Can be inaccurate	Accurate

Q: Why are we looking at these two simple methods?

A: Other more sophisticated methods are extensions of these!

Linear Model and Least Squares

Linear Model: $\hat{Y} = \hat{\beta}_0 + \sum_{j=1}^{p} X_j \hat{\beta}_j$

Matrix-vector form: $\hat{Y} = X^T \hat{\beta}$

How do we fit a Linear Model to a set of training data?
Least Squares – find the $\hat{\beta}$ (parameters) that minimize the RSS.

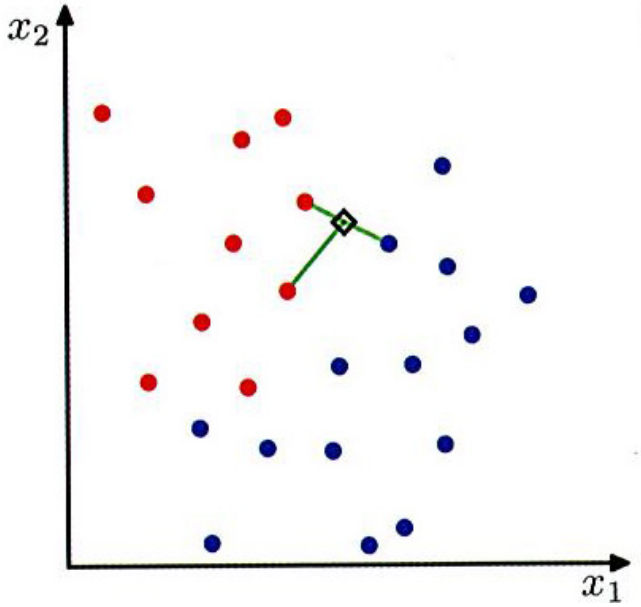
$$RSS(\beta) = \sum_{i=1}^{N} (y_i - x_i^T \beta)^2$$

$$= (y - X\beta)^T (y - X\beta)$$

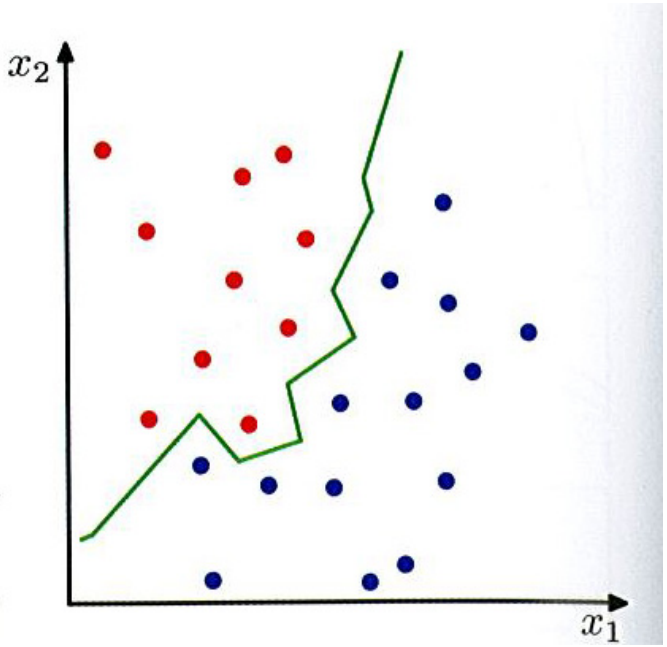
Solution: The normal equations: $\hat{\beta} = (X^T X)^{-1} X^T y$

When X is full rank, and well conditioned.

Nearest-neighbor methods

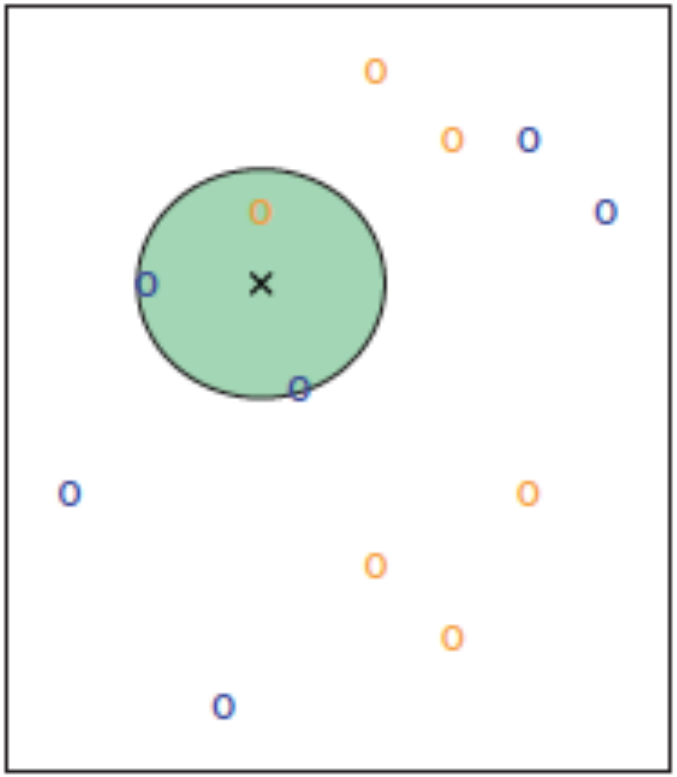


A new point arrives, it is classified according to the majority class membership of its K closest neighbors.

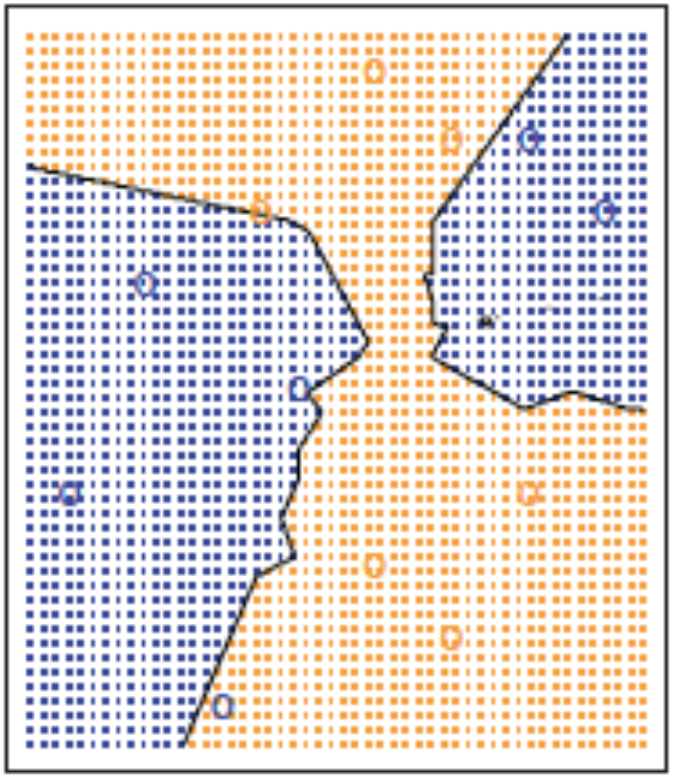


When K=1, the decision boundary is a hyper-plane that form perpendicular bisectors for pairs of points from different classes.

Nearest-neighbor methods

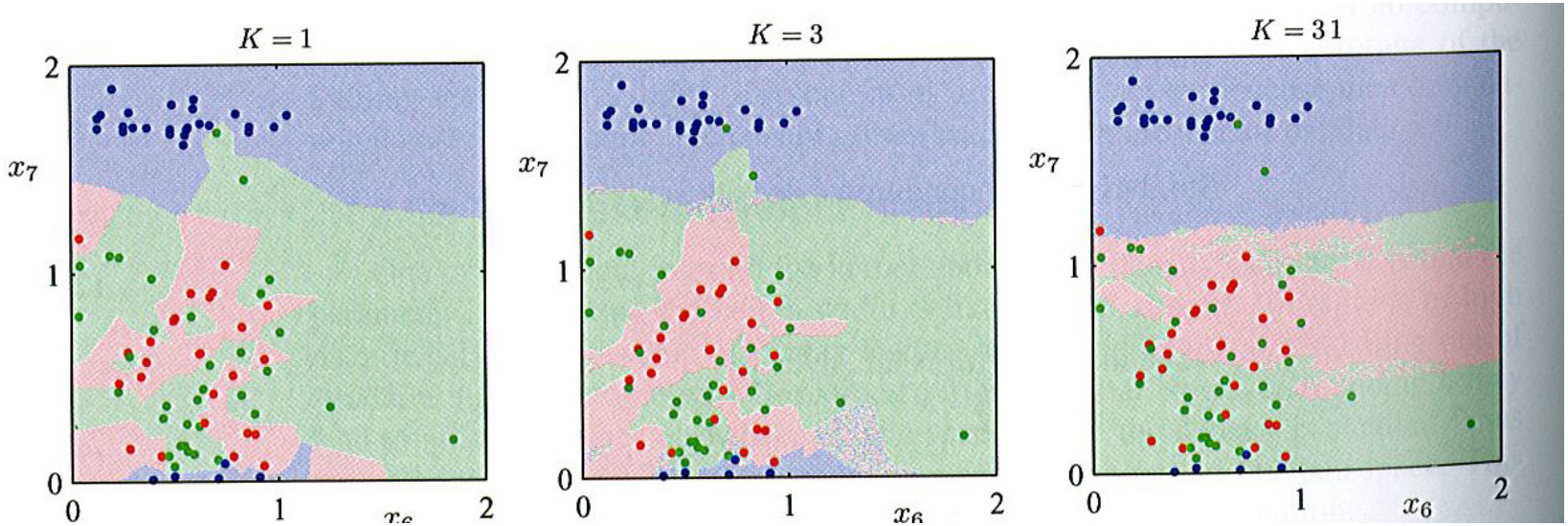


A new point arrives, it is classified according to the majority class membership of its K closest neighbors.



Simulation of a “grid” of test points.

Nearest-neighbor methods



K - pertains to the fit. The k- nearest neighbor fit for $\hat{Y}(x)$ is defined as follows:

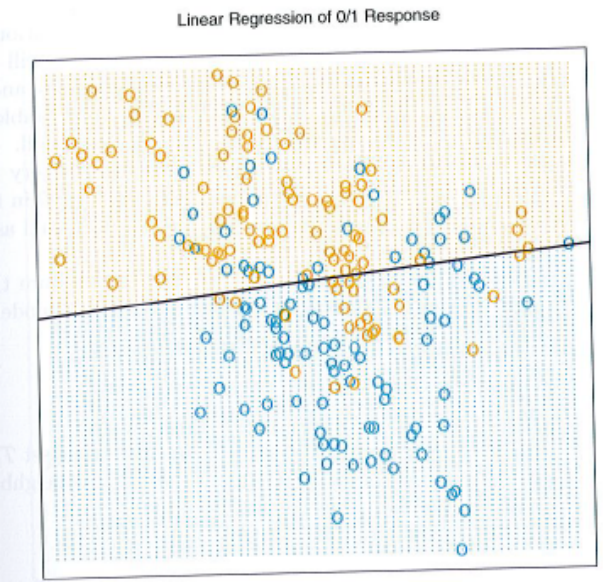
$$\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$$

Neighborhood of x defined by the k closes points x_i.

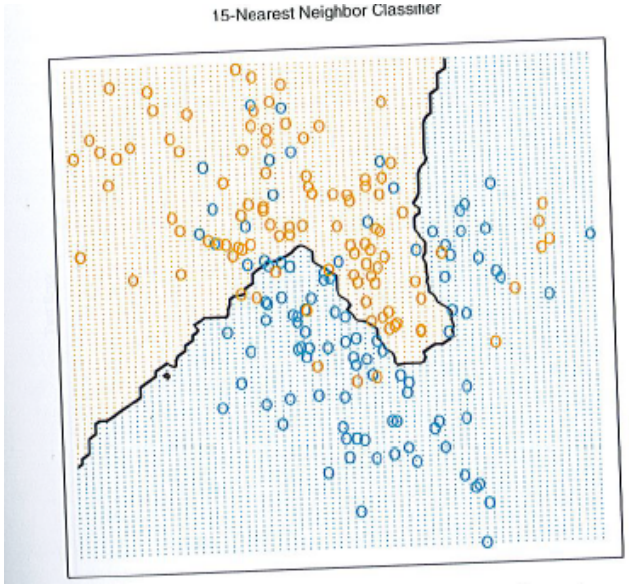
Small K - many small regions.
Larger K - fewer large regions.

Which is best…. ?

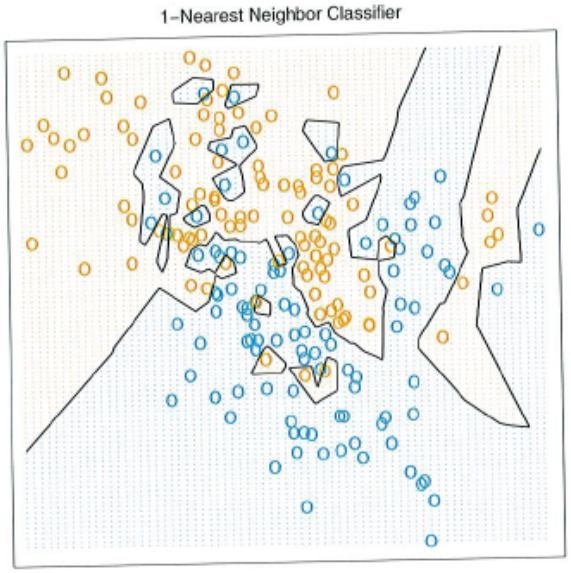
Linear Regression



Nearest Neighbor (k=15)

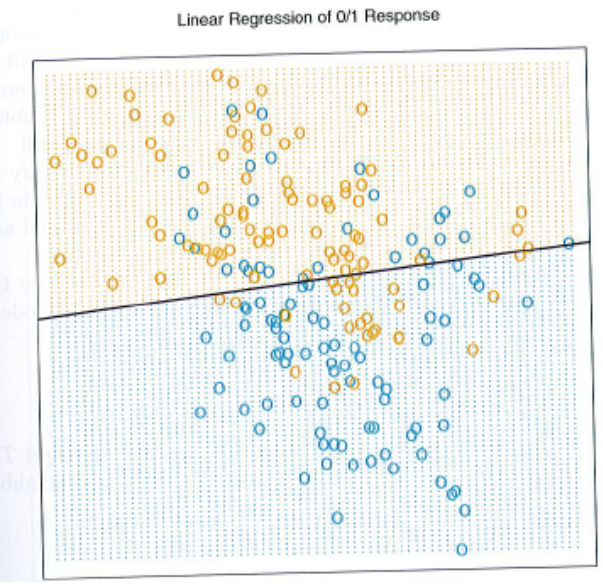


Nearest Neighbor (k=1)

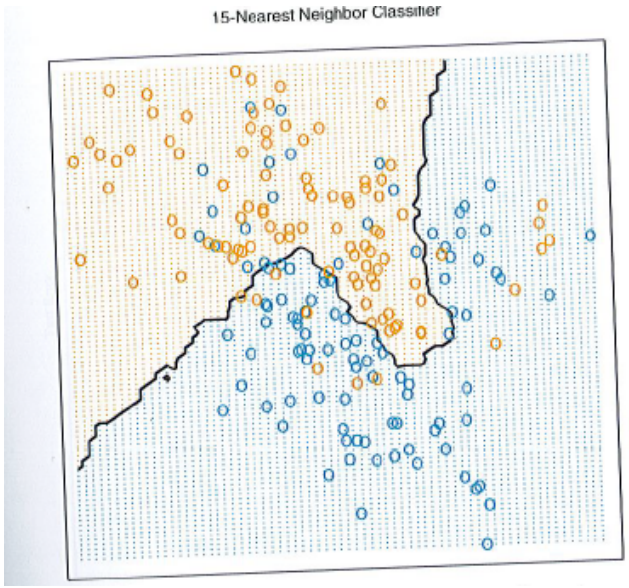


Which is best…. ?

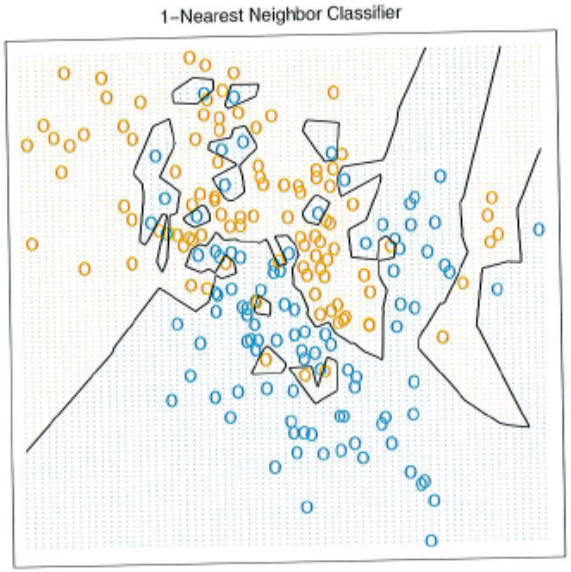
Linear Regression



Nearest Neighbor (k=15)



Nearest Neighbor (k=1)

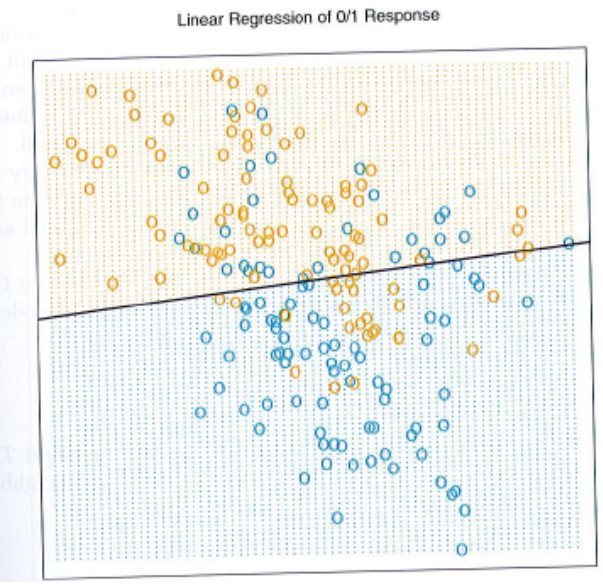


Scenario 1: The training data in each class were generated from bivariate Gaussian distributions with uncorrelated components and different means.

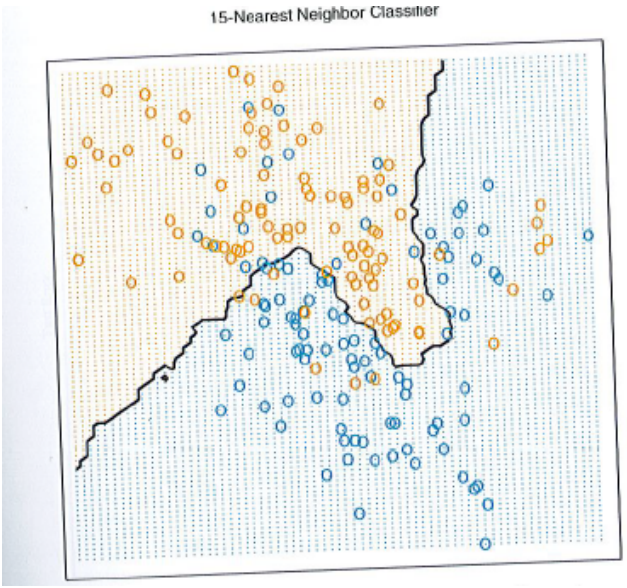
Scenario 2: The training data in each class came from a mixture of 10 low variance Gaussian distributions with individual means themselves distributed as Gaussian.

Which is best…. ?

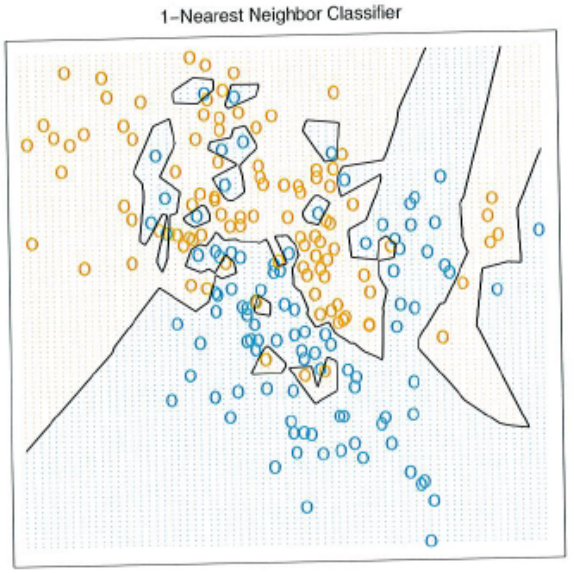
Linear Regression



Nearest Neighbor (k=15)



Nearest Neighbor (k=1)



LINEAR REGRESSION

Scenario 1: The training data in each class were generated from bivariate Gaussian distributions with uncorrelated components and different means.

Scenario 2: The training data in each class came from a mixture of 10 low variance Gaussian distributions with individual means themselves distributed as Gaussian.

K-Nearest Neighbors

Statistical Decision Theory

The Setup: Let $X \in \mathbf{R}^p$ denote a real valued random input vector and $Y \in \mathbf{R}$ be a real valued random output variable, with a joint distribution $P(X,Y)$.

The Objective: We want a function, for predicting the output for given values of the input. We can use **squared error loss** to penalize errors in prediction: $L(Y, f(x)) = (Y - f(x))^2$.

Statistical Decision Theory

Let $X_1, X_2, \ldots, X_p$ denote a set of predictors that contain relevant Information for the risk of disease Y.

Natural to use $X_1, X_2, \ldots, X_p$ to predict Y.

Rephrase as functional approximation:

$$Y = f(X) + \varepsilon$$

"black box"

Statistical Decision Theory

How do we choose f(x)?

$$f(x) = E(Y \mid X = x)$$

Best predictor when dealing with squared error loss.

Nearest neighbors tries to do this using training data:

$$\hat{f}(x) = Ave(y_i \mid x_i \in N_k(x))$$

Neighborhood containing the k points In Training Data that are closest to x.

Least squares also averages over the training data:

$$f(x) \approx x^T \beta$$

$$\beta = \left[E\left(XX^T\right)\right]^{-1} E(XY)$$

Local Methods in High Dimensions

Curse of Dimensionality… where the wheels come off!

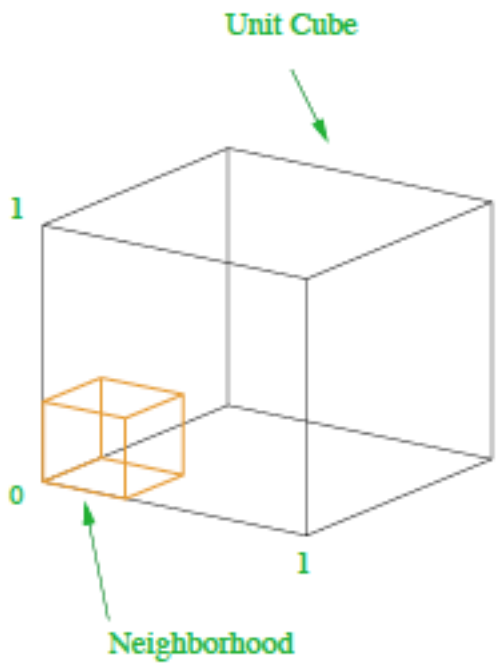
A contrived example:
Consider a p-dimensional hypercube on the range [0,1].

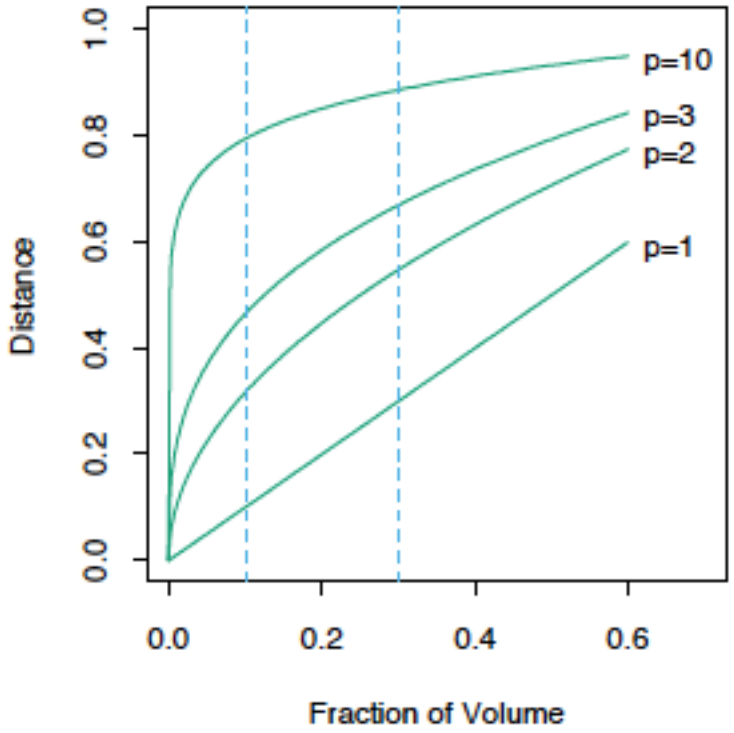
The expected edge length for an "r" fraction of observations (unit volume): $e_p(r) = r^{1/p}$.

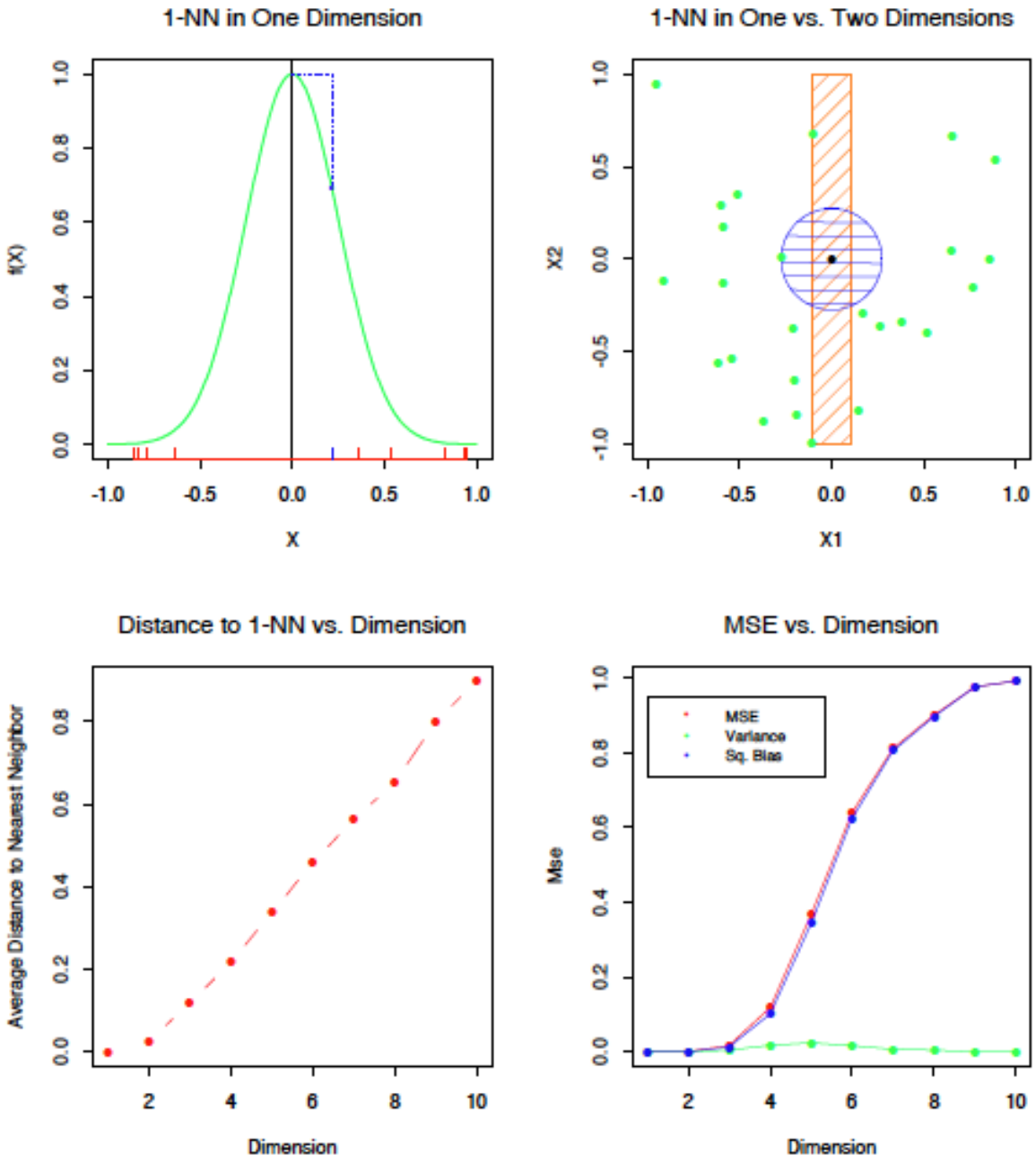
In 10 dimensions ….
If you want to capture 1% of the data, $e_p(.01) = .01^{1/10} = .63$.
If you want to capture 10% of the data, $e_p(.1) = .1^{1/10} = .80$.

Suppose 1000 data points generated in a p-dimensional hypercube on the range [0,1].

Local Methods in High Dimensions






1-NN in One Dimension
f(X)
X
1-NN in One vs. Two Dimensions
X2
X1
Distance to 1-NN vs. Dimension
Average Distance to Nearest Neighbor
Dimension
MSE vs. Dimension
MSE
Variance
Sq. Bias
Mse
Dimension

Local Methods in High Dimensions

- The complexity of functions grows of many variables grows exponentially with the number of dimensions.

- In order to estimate with accuracy with local models, we need massive coverage (lots of training samples).

The relationship between X and Y

Back to our goal ….
We want to estimate $\hat{f}(x)$

Our example was contrived to illustrated a point.

The reality: We don't know $f(x)$.

- (X,Y) may not even have a deterministic relationship.
- Unmeasured variables may contribute to Y (e.g, measurement error, technical effects, latent variables).