

Announcement: Assignment 1 is out and due January the 26th.

Nearest Neighbor method:

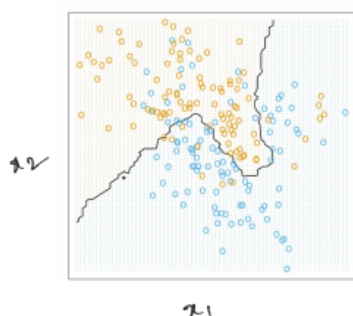
Use those predictions in the training set closest in input space to x to from \hat{y}

$$\hat{y} = \frac{1}{k} \sum_{x^{(i)} \in N_k(x)} y^{(i)}$$

$N_k(x)$ -neighborhood of x , closet k points $x^{(i)}$. What metric ? Euclidean distance.

$$\hat{y}(x) = \begin{cases} 0 & \text{if } \hat{y} \leq 0.5 \\ 1 & \text{if } \hat{y} > 0.5 \end{cases}$$

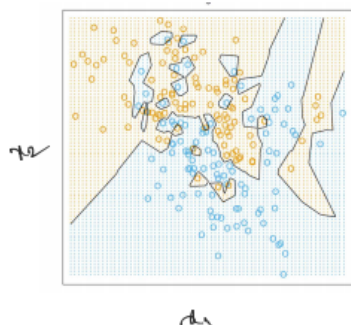
Assumption: This model assumes that the class distribution is locally smooth.



$k=15$

decision boundary is far more irregular
and responds to local clusters where
one class dominates.

\Rightarrow There are still some misclassifications.

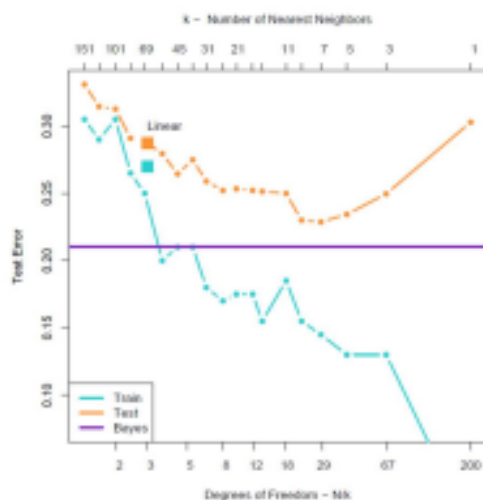


$k=1$

The decision boundary is even more
irregular than before!

\Rightarrow There are no misclassification.

K is hyper parameter. For $k = 1$, overfits the training data. We have to choose k based on a validation test.



Q: Are there any other hyper-parameteres for K-NN ?

A: Metric to compute NN.

Least squares VS Nearest neighbor :

- Decision boundary is very smooth.

- More stable

- assumes that the decision boundary is linear.
↳ strong assumption.

- high bias, low variance.

- Decision boundary is wiggly and depends on a handful of input points and their positions.

- less stable.

- does not have any such strong assumptions about the decision boundary.

- low bias, high variance.

$x \in \mathbb{R}^p$: real valued random input vector.

$y \in \mathbb{R}$: real valued random input variable.

$\Pr(x,y)$: joint distribution of x,y . **Goal:** find a function $f(x)$ for predicting y given values of x .

$L(y,f(x))$ = Loss function for penalizing errors in prediction.

$$L(y, f(x)) = (y - f(x))^2$$

$$EPE = \int \int (y - g(x))^2 Pr(x, y) dx dy$$

using Bayes: $f(x, y) = f(y | x) f(x)$

$$EPE = \int \int (y - g(x))^2 f(y | x) f(x) dx dy$$

$$EPE = \int f(x) \left(\int (y - g(x))^2 f(y | x) dy \right) dx$$

$$EPE = E_x \left(\int (y - g(x))^2 f(y | x) dy \right)$$

$$EPE = E_x E_{Y|X}([Y - g(X)]^2 | X)$$

it suffices to minimize EPE pointwise:

$$f^* = \underset{f}{\operatorname{argmin}} E_{Y|X}[(Y - f)^2 | X = x]$$

$$\frac{\partial}{\partial f} E_{Y|X}[(Y - f)^2 | X = x] = 0$$

$$\frac{\partial}{\partial f} E_{Y|X}(Y^2 | X = x) + f^2 - 2 E_{Y|X}(Y | X = x) f = 0$$

$$2f - 2 E_{Y|X}(Y | X = x) = 0$$

$$f^* = E_{Y|X}(Y | X = x)$$

↑
regression function.

the best prediction of Y at any point $X=x$ is the Conditional mean, when best is measured by average Squared error.

What is N.N. doing?

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

Two approximations to the regression function:

1. Expectation is approximated by averaging over sample data.
2. Conditioning at a point is relaxed to conditioning on some region "close" to the target point.

Note 1: For large training sample size N , the points in the neighborhood are likely to be close to x .

Note 2: As ' k ' gets larger, the average will get more stable

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Under mild regularity conditions on $Pr(X,Y)$, one can show that

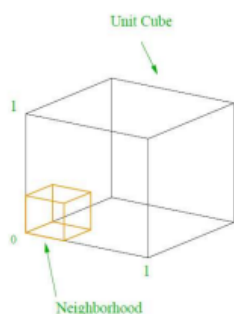
$$\text{as } n, k \rightarrow \infty \text{ such that } k/n \rightarrow 0,$$

$$\hat{f}(x) \rightarrow E(Y|X=x)$$

Looks like we have an universal function approximator!?

No. As the number of features increases, in high dimensions, we need very large samples.

Local methods in high dimensions: Consider inputs uniformly distributed in a p-dimensional hypercube.

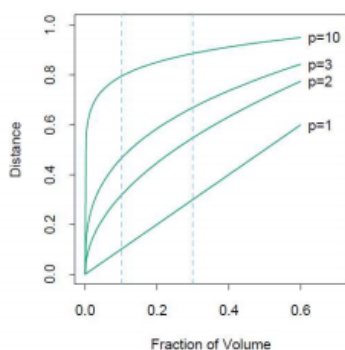


Consider a hypercubical neighborhood about a target point to capture a fraction 'r' of the observations.

↳ this corresponds to a fraction 'r' of the unit volume.

$r =$

The expected edge length $e_p(r) = r^{\frac{1}{p}} e_{10}(0.01) = 0.63, e_{0.1} = 0.83$.
To capture 1 or 10 percent of data, to from a local range, cover 63 or 83 of the range of the input variable. \Rightarrow such neighborhood are no longer local. If you reduce "r", with fewer observations, variance will be high.



This is known as "Curse of Dimensionality" (Bellman, 1961).

Warning: Our intuitions breaks down in higher dimensions.

What is Linear regression doing ?

$$\hat{f}(x) = x^T w$$

This is a model based approach. We are specifying a model for the regression fn.

$$w = [E(xx^T)]^{-1} E(XY)$$

Assumptions:

1. Least squares \rightarrow approximated by a globally linear fn.
2. K-NN \rightarrow assumes $f(n)$ is well approximated by a locally constant function.
These assumptions \Rightarrow inductive bias of the algorithm

Additive models:

$$f(x) = \sum_{j=1}^p f_j(x_j)$$

This retains the additivity of the linear model but each coordinate function f_j is arbitrary. Q: What happens if we replace L_2 loss with L_1 ?

A: $\hat{f}(x) = \text{median}(y|X = x)$

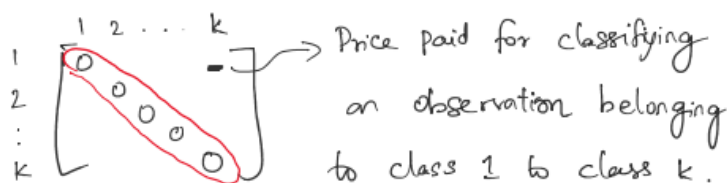
Classification: Output is categorical variable G.

some paradigms work here, we need a different loss function for penalizing prediction error.

G: set of possible classes.

\hat{G} : prediction.

loss fn: $k \times k$ matrix where $k = \text{Card}(G)$



$L(k, l)$ - price for classifying an observation belonging to class k to class l .

$$EPE = E[L(G, \hat{G}(x))]$$

Expectation is with respect to $\Pr(G, x)$.

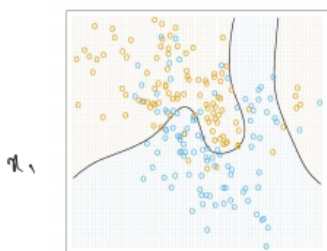
$$= E_x \sum_{k=1}^K L(G, \hat{G}(x)) \Pr(G, x)$$

Again, it suffices to minimize EPE pointwise:

$$\hat{G}(x) = \underset{g \in G}{\text{argmin}} \sum_{k=1}^K L(G_k, g) \Pr(G_k, |X = x)$$

For 0-1 loss:

$$\begin{aligned} \hat{G}(x) &= \underset{g \in G}{\text{argmin}} (1 - \Pr(g|X = x)) \\ &= \underset{g \in G}{\text{argmax}} \Pr(g|X = x) \end{aligned}$$



The optimal Bayes decision boundary.

The error rate of the Bayes classifier is called the Bayes rate.

K-NN directly approximate this solution
Majority voting in neighborhood.

1. conditional probability at a point is related to conditional probability within a neighborhood of a point.
2. Probabilities are estimated by training sample proportions.