

# Statistics 452: Statistical Learning and Prediction

## Chapter 3, Part 4: Linear Regression vs K-Nearest Neighbors

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# Parametric vs Non-Parametric

- ▶ Linear regression is parametric.
  - ▶ We assume a functional (parametrized) form for  $f$ , and then fitting  $f$  amounts to fitting parameters.
- ▶ Non-parametric regression does not assume a parametric form for  $f$ .
  - ▶ More flexible.
  - ▶ A simple example is  $K$ -nearest neighbors (KNN) regression.

# KNN Regression

- ▶ Define a neighborhood size  $K$ .
- ▶ For each  $x_i$ , take  $\hat{f}(x_i)$  to be the average of the  $y_j$ 's for  $x_j$ 's in the neighborhood of  $x_i$ .

# Example Neighborhood

```
Xdat <- advert[,c("TV", "radio")]  
dm <- as.matrix(dist(Xdat))  
dm[1:3, 1:3]
```

```
##           1           2           3  
## 1  0.0000 185.60606 213.05403  
## 2 185.6061  0.00000  28.08647  
## 3 213.0540  28.08647  0.00000
```

```
dd <- dm[,1] # distances from first x  
nbrThresh <- sort(dd)[9] # find 9th smallest distance  
nbrThresh
```

```
##           69  
## 12.62458
```

```
nn <- (dd <= nbrThresh)  
nn[1:3]
```

```
##           1           2           3  
## TRUE FALSE FALSE
```

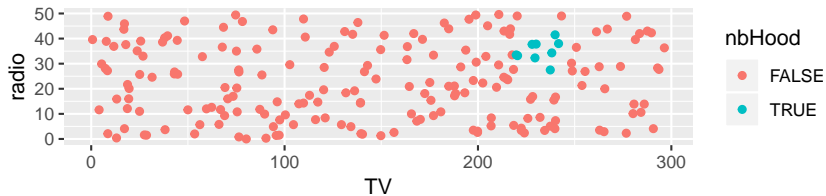
- Encapsulate computation in a function.

```
nbhd<-function(index,dat,K){  
  dd <- as.matrix(dist(dat))[,index]  
  nbrThresh <- sort(dd)[K]  
  return(factor(dd <= nbrThresh))  
}  
advert <- mutate(advert,nbHood = nbhd(1,Xdat,K=9))
```

```
advert[1,]
```

```
##      TV radio newspaper sales      cTV cRadio nbHood  
## 1 230.1  37.8      69.2  22.1 83.0575 14.536   TRUE
```

```
ggplot(advert,aes(x=TV,y=radio,color=nbHood)) + geom_point()
```



## KNN Prediction for First City

```
advert[1,]
```

```
##          TV radio newspaper sales      cTV cRadio nbHood  
## 1 230.1  37.8          69.2  22.1 83.0575 14.536   TRUE
```

```
with(advert, mean(sales[nbHood==TRUE]))
```

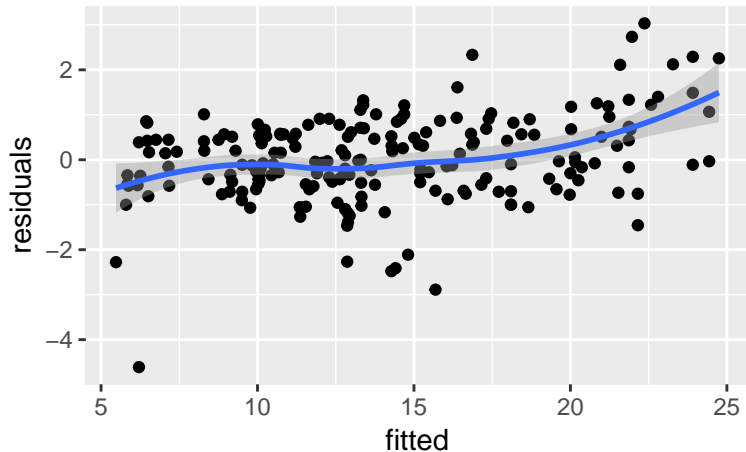
```
## [1] 20.84444
```

## KNN Predictions for Advertising Data

```
n <- nrow(advert)
K <- 9
KNNpred <- rep(NA,n)
for(i in 1:n) {
  advert <- mutate(advert,nbHood=nbhd(i,Xdat,K))
  KNNpred[i] <- with(advert,mean(sales[nbHood==TRUE]))
}
```

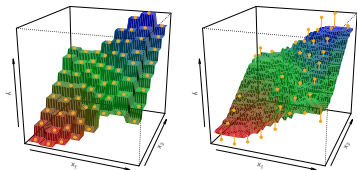


```
mutate(advert,fitted = KNNpred, residuals=sales-KNNpred) %>%  
  ggplot(aes(x=fitted,y=residuals)) + geom_point() +  
  geom_smooth()
```



## Example from Text

- Plots of  $\hat{f}(X)$  using KNN on 64 observations with  $K = 1$  (left panel) and  $K = 9$  (right panel).



- For  $K = 1$  the KNN interpolates and for  $K = 9$  it smooths.
  - Which is best? The one that gives the best test set error rates
  - We will discuss methods for estimating the test set error rate, but for now we simply break the advertising data into a training and test set.

## Test Set Predictions from KNN

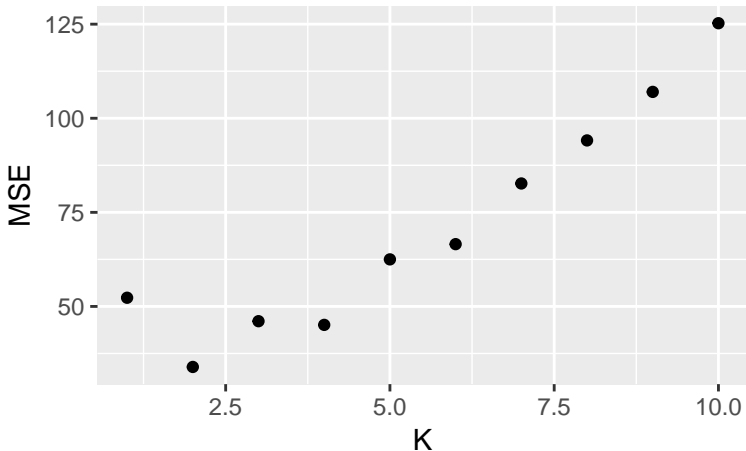
- For a prediction point  $x_0$ , find the neighborhood  $\mathcal{N}_0$  of the  $K$  closest points in the training set, and take

$$\hat{f}(x_0) = \frac{1}{K} \sum_{x_i \in \mathcal{N}_0} y_i$$

# KNN on Advertising Data

```
library(caret) # install.packages("caret") if not already done
Y <- advert$sales
trainset <- (1:(.8*n))
trainX <- Xdat[trainset,]
trainY <- Y[trainset]
testset <- ((.8*n+1):n)
testX <- Xdat[testset,]
testY <- Y[testset]
maxK <- 10
testMSE <- rep(NA,maxK)
for(k in 1:maxK) {
  fit <- knnreg(trainX, trainY, k)
  testMSE[k] <- sum((testY - predict(fit, testX))^2)
}
```

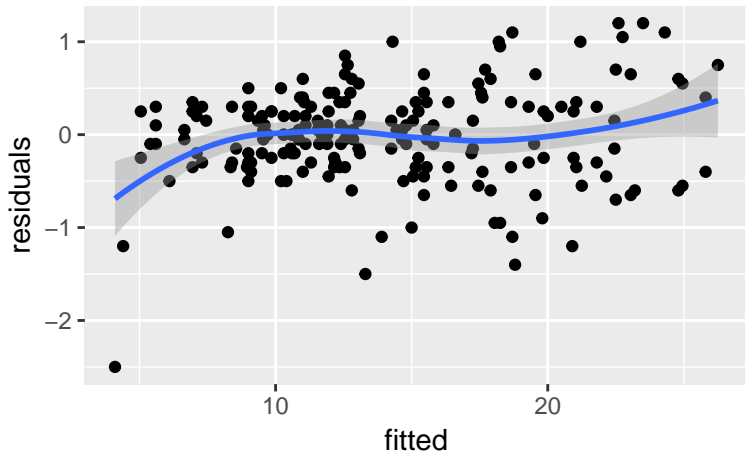
```
data.frame(MSE = testMSE, K=1:maxK) %>%  
  ggplot(aes(x=K,y=MSE)) + geom_point()
```



- ▶ According to the current test set,  $K = 2$  gives the best test set MSE.

## KNN with $K = 2$ on Advertising Data

```
K <- 2
for(i in 1:n) {
  advert <- mutate(advert, nbHood=nbhd(i, Xdat, K))
  KNNpred[i] <- with(advert, mean(sales[nbHood==TRUE]))
}
mutate(advert, fitted=KNNpred, residuals=sales-KNNpred) %>%
  ggplot(aes(x=fitted, y=residuals)) + geom_point() + geom_smooth()
```

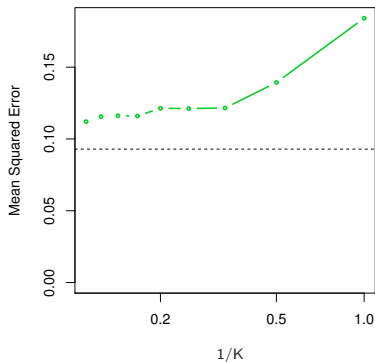
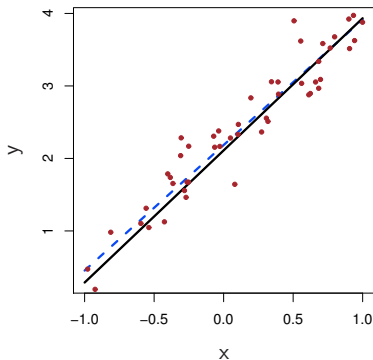


# Comparison of KNN to Linear Regression

- ▶ The text compares KNN to linear regression (with main effects) under different relationships (linear or non-linear) and different numbers of predictors  $p$ .

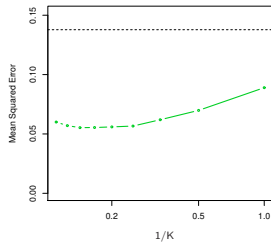
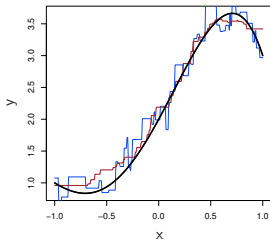
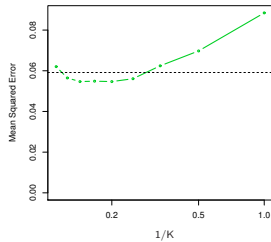
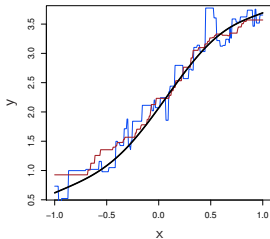
## Linear $f$ , $p = 1$ .

- ▶ When the true  $f$  is linear, linear regression MSE (dotted line) is slightly better than KNN MSE (green).



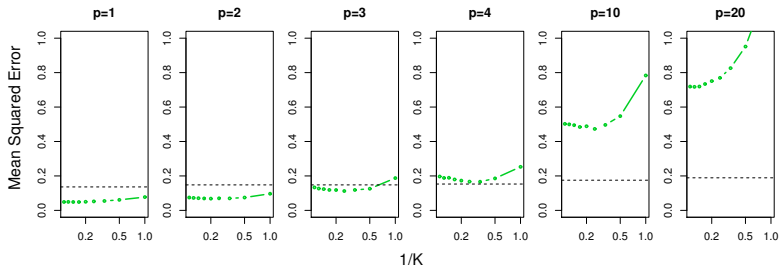


# Non-Linear $f$ , $p = 1$



## Non-Linear $f$ , Varying $p$

- ▶ KNN is better for small  $p$  but worse for large  $p$



- ▶ When  $p = 20$ , for example, the “nearest” neighbors are not very near, and so do a poor job of predicting  $f$ .
  - ▶ This phenomenon is known as the “curse of dimensionality”.