Supervised Learning (Part I)

SYS 6018 | Spring 2021

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Contents

1 Supervised Learning Intro **2**
1.1 Required R Packages . . . 2
1.2 Supervised Learning . . . 2

2 Example Data **2**

3 Linear Models **3**
3.1 Simple Linear Regression . . . 3
3.2 OLS Linear Models in **R** . . . 4

4 Polynomial inputs **7**
4.1 Estimation . . . 7
4.2 Performance Comparison (on Training Data) . . . 9

5 k-nearest neighbor models **11**
5.1 knn in action . . . 12

6 Predictive Model Comparison (or how to choose the best model) **15**
6.1 Predictive Model Evaluation . . . 15
6.2 Statistical Decision Theory . . . 15
6.3 Choose the best *predictive* model . . . 17

1 Supervised Learning Intro

1.1 Required R Packages

We will be using the R packages of:

- `FNN` for k nearest neighbor models
- `tidyverse` for data manipulation and visualization
- `broom` for tidying model output

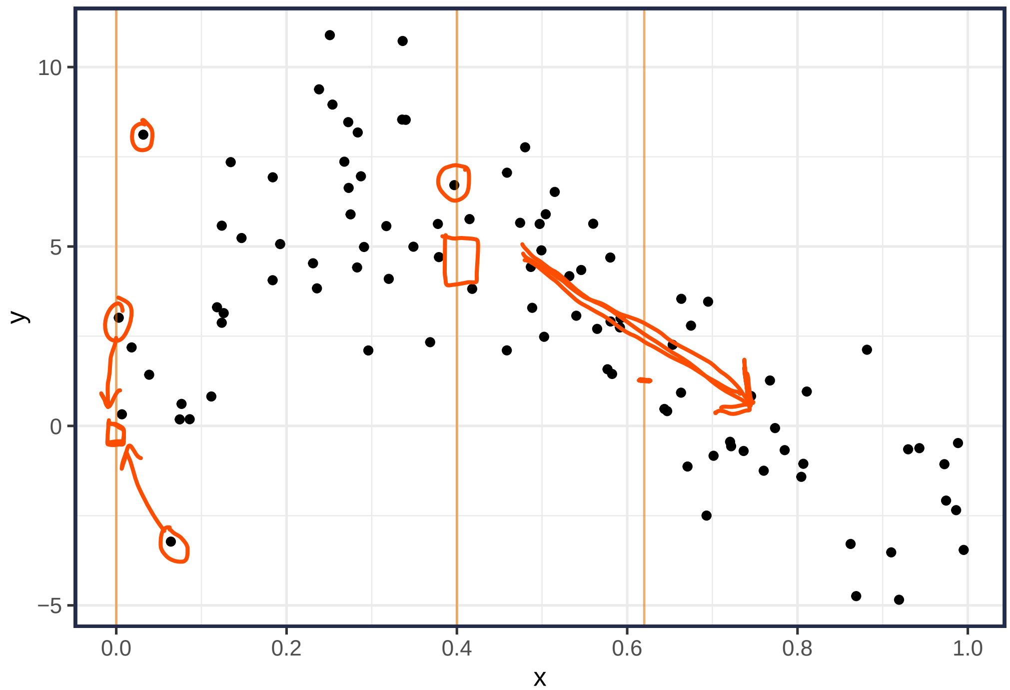
```
library(FNN)
library(broom)
library(tidyverse)
```

1.2 Supervised Learning

- In *supervised learning*, each observation can be partitioned into two sets: the predictor/independent/feature variables and the target/labels/response/dependent variable(s).
- Usually the predictor variables are represented by X and the response variables represented by Y
- The goal in supervised learning is to find the patterns and relationships between the predictors, X, and the response, Y.
  - Usually the goal is to *predict* the value of Y given X.
- Later in the course we will explore the *unsupervised learning* topics of association analysis, network analysis, density estimation, clustering, and anomaly detection which do not have any labels or target states.

2 Example Data

Consider some data $D = \{(X_i, Y_i)\}_{i=1}^{n}$ with $Y_i \in \mathbb{R}$, $X_i \in [0, 1]$ and $n = 100$.



Your Turn #1

The goal is to predict new Y values if we are given the X's.

- If $x = .40$, predict Y.
- If $x = 0$, predict Y.
- If $x = .62$, predict Y.
- How should we build a *model* that will automatically predict Y for any given X?

3 Linear Models

- Linear models refer to a class of models where the output (predicted value) is a linear combination (weighted sum) of the input variables

model

$$f(x; \beta) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$$

parameters

vector

^ = estimated

where $x = [x_1, \ldots, x_p]^\mathsf{T}$ is a vector of features/variables/attributes and $\boxed{\hat{Y}|x = f(x; \hat{\beta})}$ is the predicted response at $X = x$

- the coefficients (or weights), $\hat{\beta}$ are often selected by minimizing the squared residuals of the *training data* (may also be described as *ordinary least squares*)
  - But, there are other, and better, ways to estimate the parameters in linear regression that we will discuss later in the course. (e.g., Lasso, Ridge, Robust)

3.1 Simple Linear Regression

- single predictor variable $x \in \mathbb{R}$

- $f(x;\beta) = \beta_0 + \beta_1 x$
- Use *training data*: $D_{\text{train}} = \{(x_i, y_i)\}_{i=1}^n$
- OLS uses the weights/coefficients that minimize the RSS loss function over the training data

$$\boxed{\hat{\beta} = \arg\min_{\beta} \text{RSS}(\beta)}$$

- where RSS is the *residual sum of squares*

$$\begin{aligned}
\text{RSS}(\beta) &= \sum_i^n (y_i - f(x_i, \beta))^2 \\
&= \sum_i^n (y_i - \beta_0 - \beta_1 x_i)^2 \\
&\boxed{= \sum_i^n \hat{\epsilon}_i^2} \qquad \text{where } \hat{\epsilon}_i = y_i - \hat{y}_i \text{ is the residual}
\end{aligned}$$

All training data

- The solutions are

$$\begin{cases}
\hat{\beta}_0 = \bar{y} - \beta_1 \bar{x} \\
\hat{\beta}_1 = \dfrac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}
\end{cases}$$

- Definitions:

$$\begin{aligned}
\text{MSE}(\beta) &= \frac{1}{n}\text{RSS}(\beta) \\
&= \frac{1}{n}\sum_{i=1}^n (y_i - f(x_i;\beta))^2
\end{aligned}$$

Root MSE $\quad \text{RMSE} = \sqrt{\text{MSE}} = \sqrt{\text{RSS}}/\sqrt{n}$

3.2 OLS Linear Models in R

3.2.1 Estimation with `lm()`

In **R**, the function `lm()` fits an OLS linear model

```
data_train = tibble(x,y)        # create a data frame/tibble
m1 = lm(y~x, data=data_train)  # fit simple OLS
summary(m1)                      # summary of model
#>
#> Call:
#> lm(formula = y ~ x, data = data_train)
#>
#> Residuals:
#>    Min     1Q Median     3Q    Max
#> -9.229 -1.635  0.019  1.940  6.728
#>
#> Coefficients:
#>             Estimate Std. Error t value Pr(>|t|)
#> (Intercept)    6.478      0.584   11.09  < 2e-16 ***
#> x             -7.372      1.058   -6.97  3.7e-10 ***
#> ---
#> Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

$\hat{\beta}$

model metrics

new functions

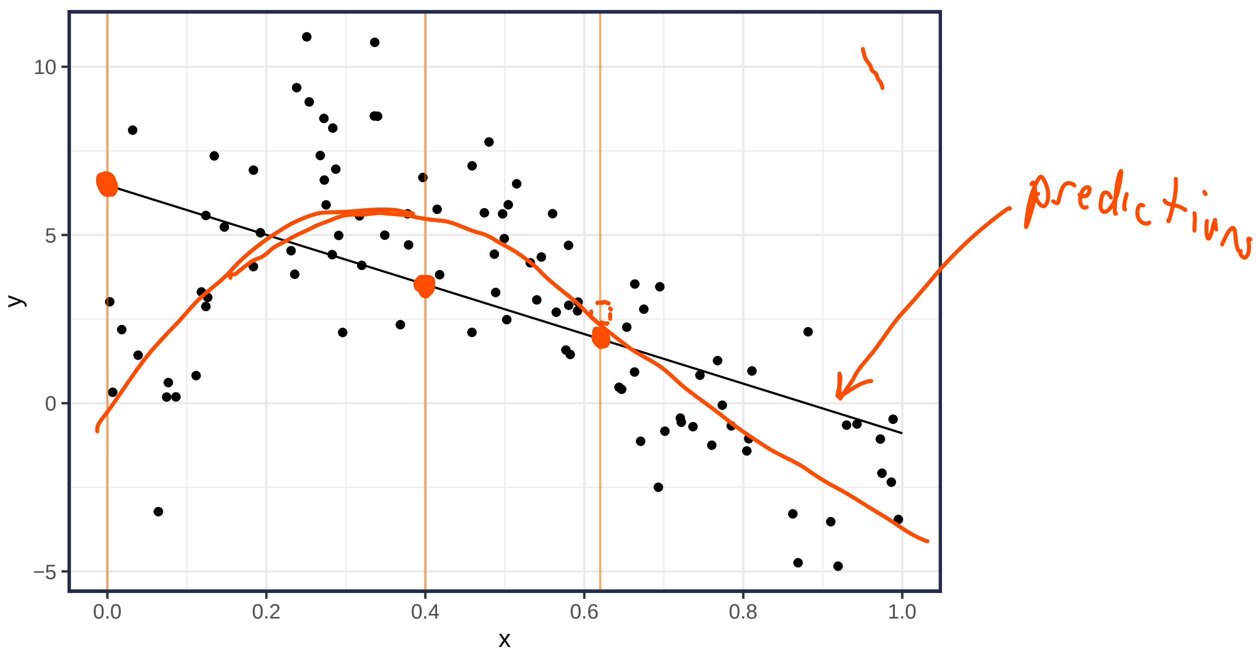
```
#>
#> Residual standard error: 2.91 on 98 degrees of freedom
#> Multiple R-squared:  0.331,  Adjusted R-squared:  0.325
#> F-statistic: 48.6 on 1 and 98 DF,  p-value: 3.69e-10
broom::tidy(m1)                 # model coefficients (as a data frame)
#> # A tibble: 2 x 5
#>   term        estimate std.error statistic  p.value
#>   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
#> 1 (Intercept)     6.48     0.584      11.1  5.39e-19
#> 2 x              -7.37     1.06       -6.97 3.69e-10
broom::glance(m1)               # model properties
#> # A tibble: 1 x 12
#>   r.squared adj.r.squared sigma statistic  p.value    df logLik   AIC   BIC
#>       <dbl>         <dbl> <dbl>     <dbl>    <dbl> <dbl>  <dbl> <dbl> <dbl>
#> 1     0.331         0.325  2.91      48.6 3.69e-10     1  -248.  501.  509.
#> # ... with 3 more variables: deviance <dbl>, df.residual <int>, nobs <int>
```

- `lm()` uses the `formula` interface, which includes the intercept by default. Some examples here.

3.2.2 Prediction with `predict()`

The function `predict()` is used to get the predicted values.

```
xseq = seq(0, 1, length=200)          # sequence of equally spaced values from 0 to 1
xeval = tibble(x = xseq)              # make into a tibble object
yhat1 = predict(m1, newdata=xeval)    # vector of yhat's (predictions)
```



3.2.3 Questions

Your Turn #2

1. How did we do? If X_{new} is close to 0, or close to 0.4, or close to $.62$?
2. How to make it better?

4 Polynomial inputs

- In the *simple* linear regression model, we had 2 parameters that we needed to estimation, β_0 and β_1. Thus, the model complexity is minimal.
  - The only thing simpler is an intercept only model.
- But the data appears to have a more *complex* structure than linear.
- A *parametric approach* to add complexity is to incorporate *polynomial terms* into the model.
  - A quadratic model is $f(x;\beta) = \beta_0 + \beta_1 x + \beta_2 x^2$

Int slope quadratic

non-linear: $\hat{Y} = \hat{\beta}_0 e^{\hat{\beta}_1}$

4.1 Estimation

- OLS uses the weights/coefficients that minimize the RSS loss function over the training data

$$
\begin{aligned}
\hat{\beta} &= \arg\min_{\beta} \ \mathrm{RSS}(\beta) \qquad \text{Note: } \beta \text{ in this problem is a } \textit{vector} \\
&= \arg\min_{\beta} \ \sum_{i=1}^{n} (y_i - f(x_i;\beta))^2 \quad \text{• vector} \\
&= \arg\min_{\beta} \ \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i - \beta_2 x_i^2)^2
\end{aligned}
$$

4.1.1 Matrix notation

- **Model**

$$f(\mathbf{x};\beta) = \mathbf{x}^{\mathsf{T}}\beta$$

Intercept

$$\mathbf{x} = \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix} \qquad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

Your Turn #3 : Matrix Notation

Solve for $\hat{\beta}$ using matrix notation.

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} \qquad X = \begin{bmatrix} 1 & X_1 & X_1^2 \\ 1 & X_2 & X_2^2 \\ \vdots & \vdots & \vdots \\ 1 & X_n & X_n^2 \end{bmatrix} \qquad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}$$

$RSS(\beta) = (Y - X\beta)^T (Y - X\beta) \approx \sum_{i=1}^{n} (Y_i - X_i\beta)^2$

solve for β: $\frac{\partial RSS(\beta)}{\partial \beta} = 2X^T(Y - X\beta) = 0$

solve for β

$\Rightarrow X^T Y = X^T X \beta$

$(X^TX)^{-1}$ both sides

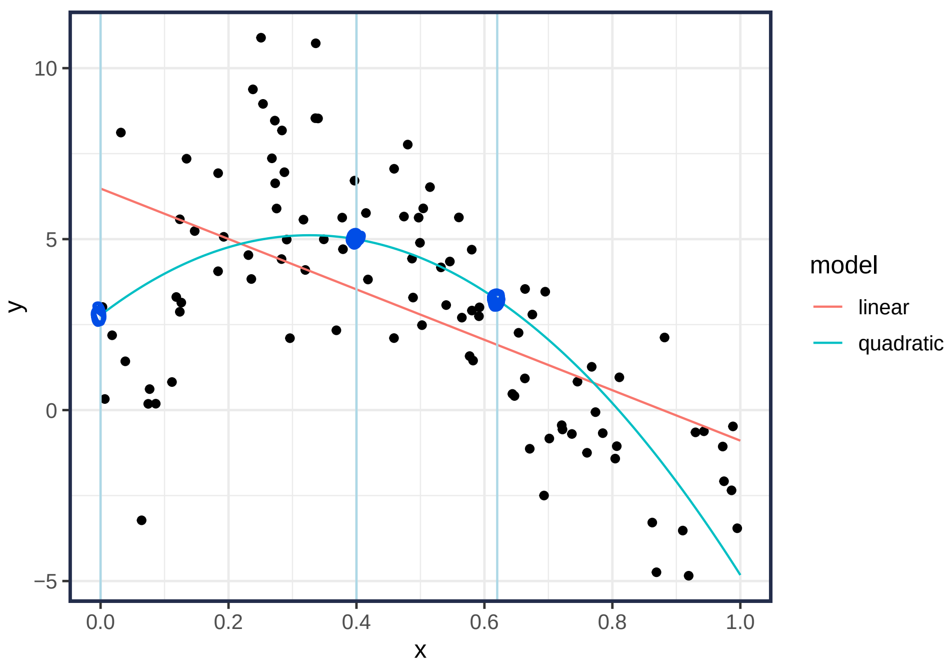
$\boxed{(X^TX)^{-1} X^T Y = \hat{\beta}}$

4.1.2 R implementation

In **R**, the function `poly()` is a convenient way to get polynomial terms

poly( )

```
m2 = lm(y~poly(x, degree=2), data=data_train)
yhat2 = predict(m2, newdata=xeval)
```



Your Turn #4

1. How did we do? If X_{new} is close to 0, or close to 0.4, or close to .62?
2. But does the quadratic model fit better *overall*? Yes!
3. What is the *complexity* of the quadratic model?

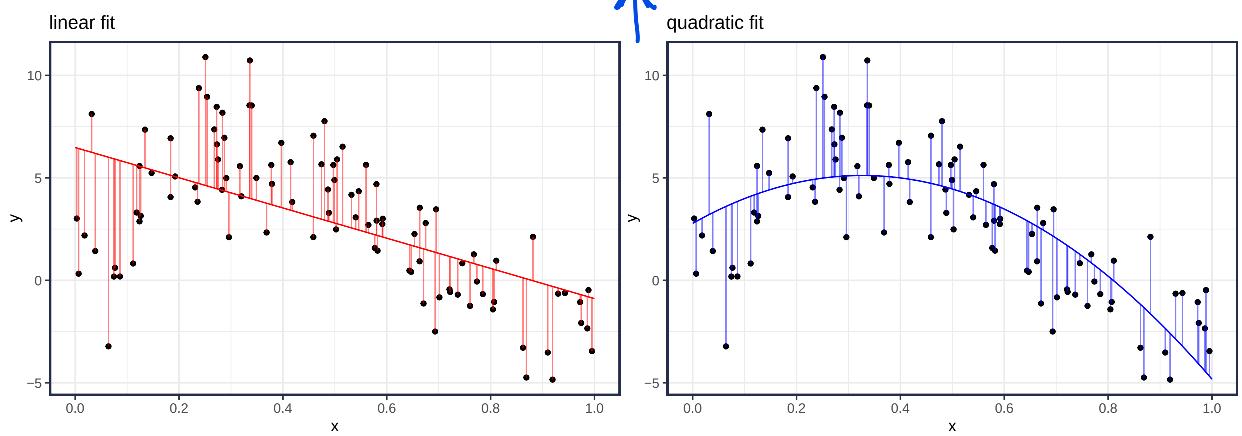
estimated parameters (edf effective degrees freedom)

$= 3$

4.2 Performance Comparison (on Training Data)

Comparing the two models (according to MSE), the quadratic model does much better!

	degree	MSE	npars = complexity
linear	1	8.29	2
quadratic	2	5.58	3



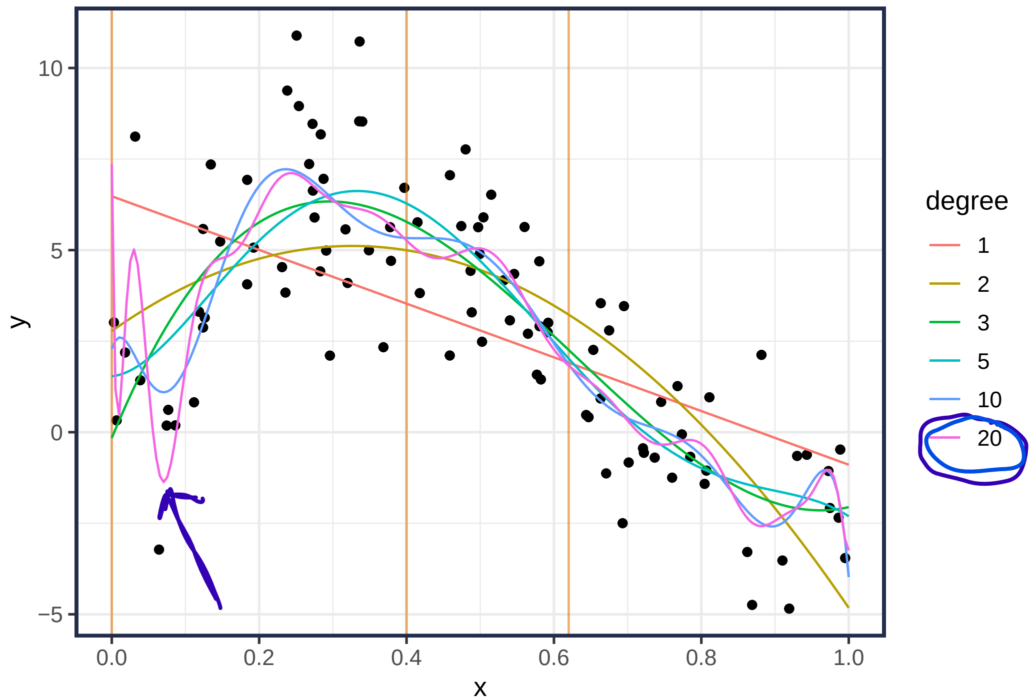
As my kids always reason, "if a little is good, than a lot must be better". So why not try more complex models by increasing the polynomial degree.

- Polynomial of degree d

$$f_{\text{poly}}(x; \beta, d) = \beta_0 + \sum_{j=1}^{d} \beta_j x^j$$

	degree	MSE	npars
	1	8.29	2
	2	5.58	3
cubic	3	4.28	4
	5	4.10	6
	10	3.65	11
20 degree polynomial	20	3.16	21

And its always good to observe the plot



- For `degree=20`, the behavior at the end points are a bit erratic.
- Using a higher degree would further reduce the RSS, but the fitted curve would be less "smooth"

5 k-nearest neighbor models

- The k-NN method is a non-parametric *local* method, meaning that to make a prediction $\hat{y}|x$, it only uses the training data in the *vicinity* of x.
  - contrast with OLS linear regression, which uses all X's to get prediction.

$\hat{\beta} = \underbrace{(X^TX)^{-1}X^Ty}_{\text{all data}}$

- The model is simple to describe

$$\boxed{\begin{aligned} f_{\text{knn}}(x;k) &= \frac{1}{k} \sum_{i:x_i \in N_k(x)} y_i \\ &= \text{Avg}(y_i \mid x_i \in N_k(x)) \end{aligned}}$$

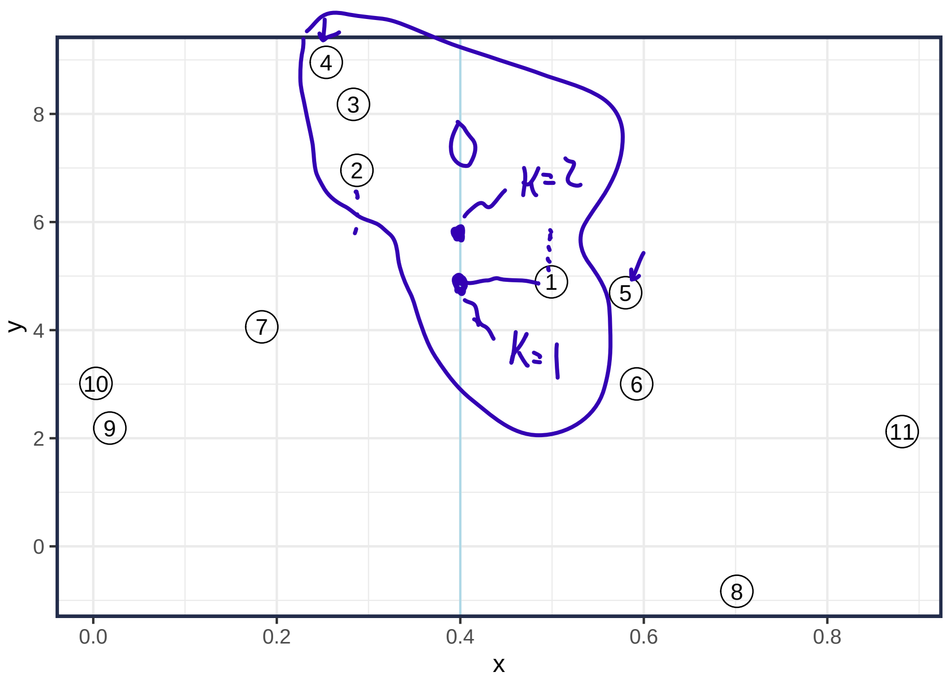
  - $N_k(x)$ are the set of k nearest neighbors
  - only the k closest y's are used to generate a prediction
  - it is a *simple mean* of the k nearest observations

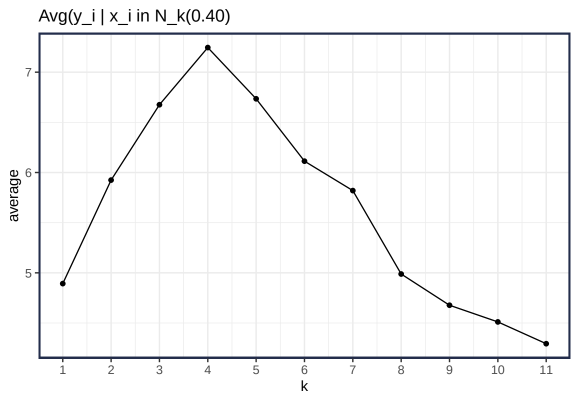
Your Turn #5

What is the estimate $f_{\text{knn}}(x;k)$ if $k = n$? $\bar{y}$ or Intercept-only model

5.0.1 Example

Consider the following example where we wish to estimate $Y \mid X = 0.40$





Distance

x	y	k	D	$\hat{f}_{\text{knn}}(x;k)$
0.50	4.89	1	0.10	4.89
0.29	6.96	2	0.11	5.92
0.28	8.18	3	0.12	6.68
0.25	8.95	4	0.15	7.25
0.58	4.69	5	0.18	6.73
0.59	3.00	6	0.19	6.11
0.18	4.06	7	0.22	5.82
0.70	-0.83	8	0.30	4.99
0.02	2.19	9	0.38	4.68
0.00	3.01	10	0.40	4.51
0.88	2.12	11	0.48	4.29

5.0.2 Notes about knn

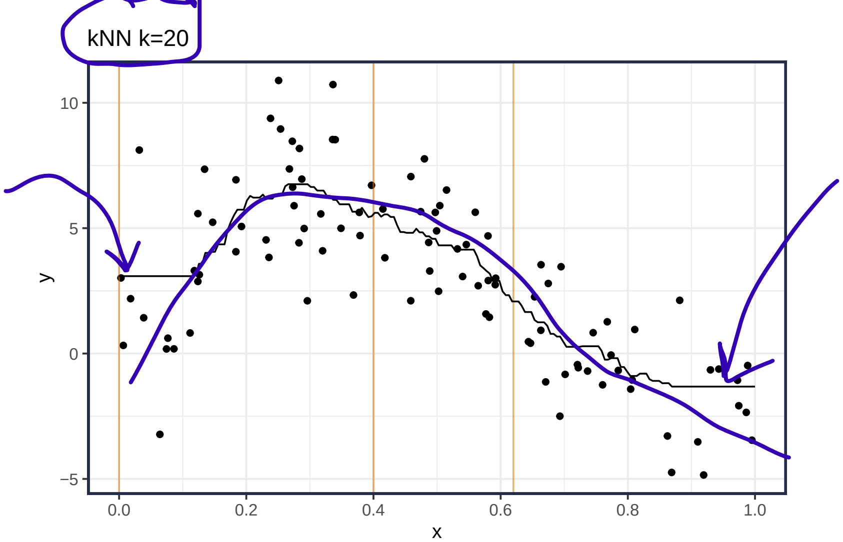
- A suitable *distance* measure (e.g. Euclidean) must be chosen.
  - And predictors are often *scaled* (same sd or range) so one variable doesn't dominate the distance calculation
- Because the distance to neighbors grows exponentially with increased dimensionality/features, the *curse of dimensionality* is often referenced with respect to knn.
  - This means that in high dimensions most *neighbors* are not very close and the method becomes less *local*
- One computational drawback of knn methods is that all the training data must be stored in order to make predictions.
  - For large training data, may need to sample (or use prototypes)

5.1 knn in action

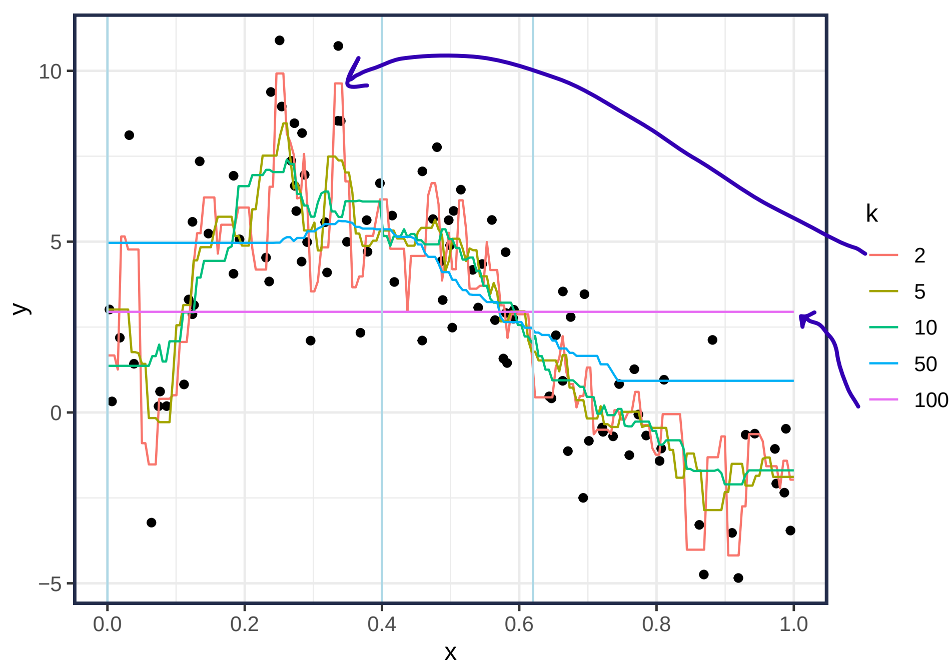
In **R**, the function `knn.reg()` from the `FNN` package will fit a knn regression model. Here is a $k = 20$ nearest neighbor model

```
# install.packages("FNN")       # to install FNN package
library(FNN)                    # library() loads the package. Access to knn.reg()

#- fit a k=20 knn regression
knn.20 = knn.reg(select(data_train, x), test=xeval, y=data_train$y, k=20)
```



- The *complexity* of a knn model increases as k decreases.
- The least complex model, which is a constant, occurs when $k = n$
- The most complex model when $k = 1$
- The effective degrees of freedom or *edf* for a knn model is n/k
  - this is a measure of the model *complexity*. It is approximately the number of parameters that are estimated in the model (to allow comparison with parametric models)



5.1.1 Performance of the knn models (on training data)

k	MSE	edf
100	12.40	1
50	6.87	2
10	3.86	10

k	MSE	edf
5	3.16	20
2	1.84	50
1	0	100

more complex

training data performance

6 Predictive Model Comparison (or how to choose the best model)

6.1 Predictive Model Evaluation

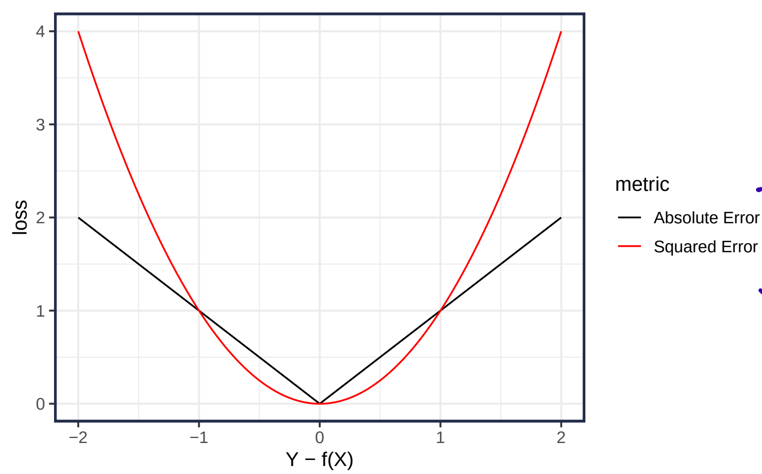
Our goal is prediction, so we should evaluate the models on their *predictive performance*.

- We need to use hold-out data (i.e., data not used to fit the model) to evaluate how well our models do in prediction
- Call these data *test data* $\boxed{D_{\text{test}}} = \{(X_j, Y_j)\}_{j=1}^{J}$
  - Note: assume that the test data comes from the same distribution as the training data
  - Or $P_{\text{test}}(X, Y) = P_{\text{train}}(X, Y)$
  - **both** Y and X from same distribution
- Later in the course we will cover ways to do this when we only have training data (e.g., cross-validation)
- but for today, we have an unlimited amount of *test data* at our disposal (since we know how the data were generated)

6.2 Statistical Decision Theory

- In a prediction context, we want a *point estimate* for the value of an unobserved r.v. $Y \in \mathbb{R}$ given an input feature $X \in \mathbb{R}$.
- Let $f(X)$ be the prediction of Y given X.
- Define a $\boxed{\textit{loss function } L(Y, f(X))}$ that indicates how bad it is if we estimate the value Y by $f(X)$
  - E.g. Y is the number of customers complaints in a call center and X is the day of week
  - If we guess $f(X) = 500$, but there are really $Y = 2000$, how bad would that be?
- A common loss function is *squared error*

$$L(Y, f(X)) = (Y - f(X))^2$$



- The best model is the one that minimizes the *expected loss* or Risk or Expected Prediction Error (EPE)

$$\text{Risk} = \text{EPE} = \text{E}[\text{loss}]$$

- For *squared error*, the *risk* for using the model f is:

$$\begin{aligned} R(f) &= E_{XY}[L(Y, f(X))] \\ &= E_{XY}[(Y - f(X))^2] \end{aligned}$$

with respect X, Y distribution

where the expectation is w.r.t. the *test values* of X, Y.

- Note under squared error loss, the risk is also known as the *mean squared error* (MSE)

- To simplify a bit, let's examine the risk of model f at a given fixed input $X = x$. This removes the uncertainty in X, so we only have uncertainty coming from Y.

$$\begin{aligned} R_x(f) &= E[L(Y, f(x)) \mid X = x] \\ &= \mathrm{E}[(Y - f(x))^2 \mid X = x] \qquad \text{for squared error loss} \end{aligned}$$

where the expectation is taken with respect to $Y|X = x$

- The best prediction $f^*(x)$, given $X = x$, is the value that minimizes the risk

$$\boxed{\begin{aligned} f^*(x) &= \arg\min_c R_x(c) \\ &= \arg\min_c \mathrm{E}[(Y - c)^2 \mid X = x] \end{aligned}}$$

Your Turn #6

What is the optimal prediction at $X = x$ under the squared error loss?
- I.e., find $f^*(x)$.

Conditional expectation

$f^*(x) = \arg\min_c E[(Y-c)^2 \mid X=x]$

Recall : $V(\theta) = E[\theta^2] - (E[\theta])^2$

$\Rightarrow E[\theta^2] = V(\theta) + (E[\theta])^2$

If $\theta = Y - c$:

$E[(Y-c)^2] = V(Y-c) + (E[Y-c])^2$

$= V(Y) + (E[Y] - c)^2$ since c is constant

Add contition on $X=x$:

$E[(Y-c)^2 \mid X=x] = V[Y \mid X=x] + (E[Y \mid X=x] - c)^2$

This is minimized if $c = E[Y \mid X=x] \longrightarrow c^* = E[Y \mid X=x]$

6.2.1 Squared Error Loss Functions

- **Conclusion:** If quality of prediction is measured by squared error, then the best predictor is the (conditional) expected value $f^*(x) = \mathrm{E}[Y|X = x]$.
  - And the minimum Risk/MSE is $R_x(f^*) = \mathrm{V}[Y|X = x]$

- **Summary:** Under *squared error loss* the Risk is

$$\begin{aligned}
R_x(f) &= \mathrm{E}_Y[L(Y, f(X)) \mid X = x] \\
&= \mathrm{E}_Y[(Y - f(x))^2 \mid X = x] \\
&= \mathrm{V}[Y \mid X = x] + (E_Y[Y \mid X = x] - f(x))^2 \\
&= \text{Irreducible Variance} + \text{squared error}
\end{aligned}$$

6.2.2 kNN and Polynomial Regression

- The kNN model estimates the conditional expectation by using the data in a *local region* around x

$$\hat{f}_{\text{knn}}(x; k) = \mathrm{Ave(y_i \mid x_i \in N_k(x))}$$

  This assumes that the true $f(x)$ can be well approximated by a *locally constant* function

- Polynomial (linear) regression, on the other hand, assumes that the true $f(x)$ is well approximated by a *globally polynomial* function

$$\hat{f}_{\text{poly}}(x; d) = \beta_0 + \sum_{j=1}^{d} \beta_j x^j$$

6.2.3 Empirical Risk

- The actual Risk/EPE is based on the error from *test data* (out-of-sample), or data that was not used to estimate $\hat{f}$

$$\begin{aligned}
R(f) &= E_{XY}[L(Y, f(X))] \\
&= E_{XY}[(Y - f(X))^2] \qquad \text{for squared error loss}
\end{aligned}$$

  where X, Y are from $\Pr(X, Y)$ (i.e., test data)

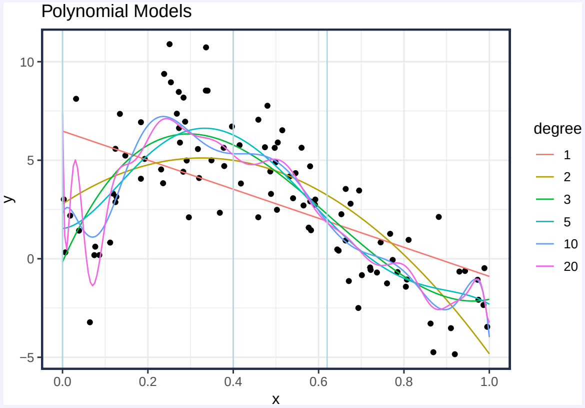
- But is it a bad idea to choose the best model according to *empirical risk* or *training error*?

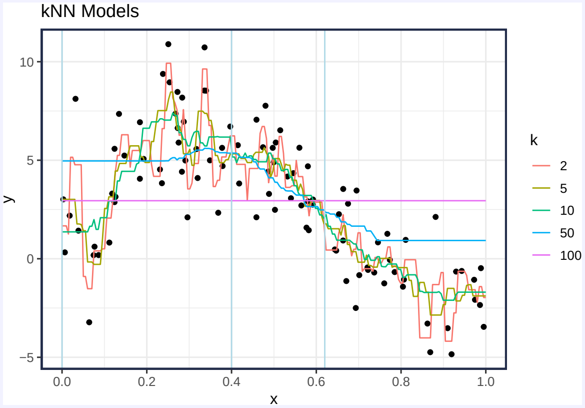
$$\begin{aligned}
R_n(f) &= \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i)) \\
&= \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 \qquad \text{for squared error loss}
\end{aligned}$$

6.3 Choose the best *predictive* model

Your Turn #7

Which model will you choose?
Enter your answer here: https://pollev.com/michaelporte865





Polynomial

degree	MSE	npars
1	8.29	2
2	5.58	3
3	4.28	4
5	4.10	6
10	3.65	11
20	3.16	21

kNN

k	MSE	edf
50	6.87	2.00
30	5.06	3.33
20	4.18	5.00
15	4.13	6.67
10	3.86	10.00
5	3.16	20.00