06 - Supervised Learning

SYS 4582/6018 | Spring 2019

06-supervised.pdf

Contents

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

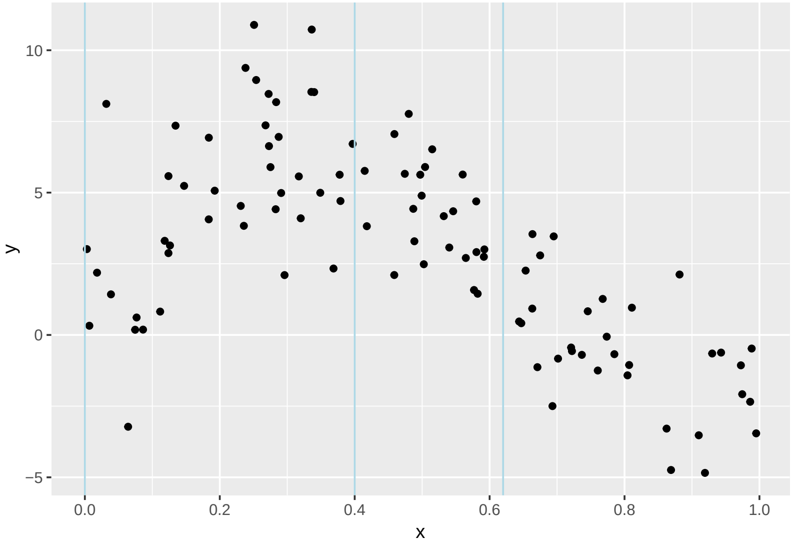
```
library(FNN)
library(tidyverse)
```

1.2 Supervised Learning

- Up to this point, the data we used to for association analysis, network analysis, density estimation, clustering, and anomaly detection did not have any labels or target states we were trying to predict.
  - These are all examples of *unsupervised 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.

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?

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

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

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

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

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

- where RSS is the *residual sum of squares*

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

- The solutions are

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

- Definitions:

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

3.2 OLS Linear Models in R

3.2.1 Estimation with `lm()`

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

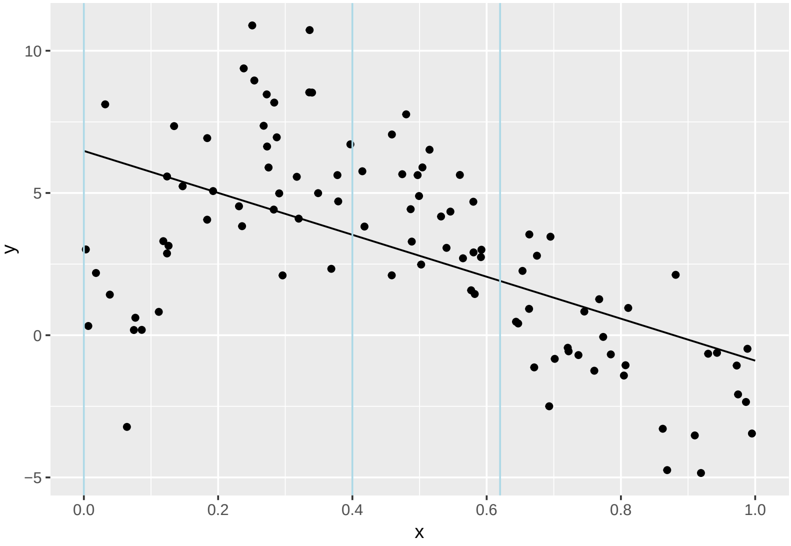
```
data.train = data.frame(x,y)
m1 = lm(y~x, data=data.train) # fit simple OLS
summary(m1)                   # summary of model
#>
#> Call:
#> lm(formula = y ~ x, data = data.train)
#>
#> Residuals:
#>    Min     1Q Median     3Q    Max
#> -9.229 -1.635  0.019  1.940  6.728
#>
#> Coefficients:
#>             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
#>
#> 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
```

- `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 = data.frame(x = xseq)          # make into a data.frame 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 $f(x;\beta) = \beta_0 + \beta_1 x + \beta_2 x^2$

4.1 Estimation

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

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

4.1.1 Matrix notation

- **Model**

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

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

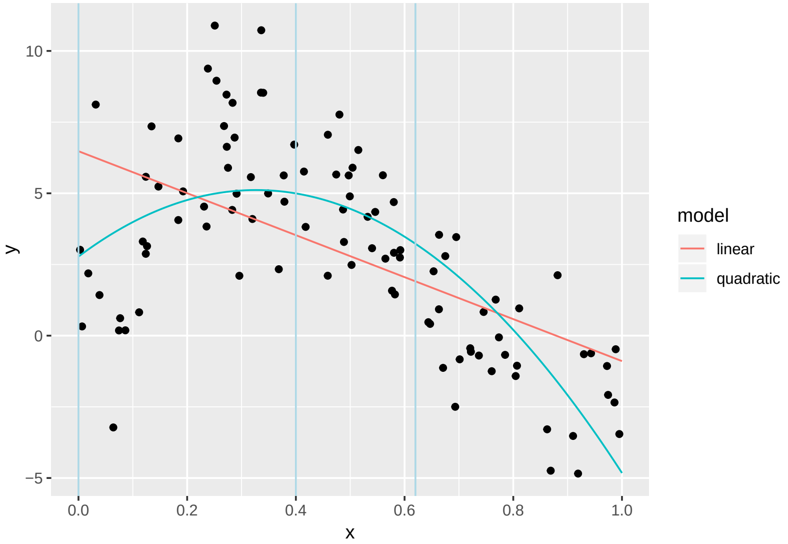
Your Turn #3 : Matrix Notation

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

4.1.2 R implementation

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

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



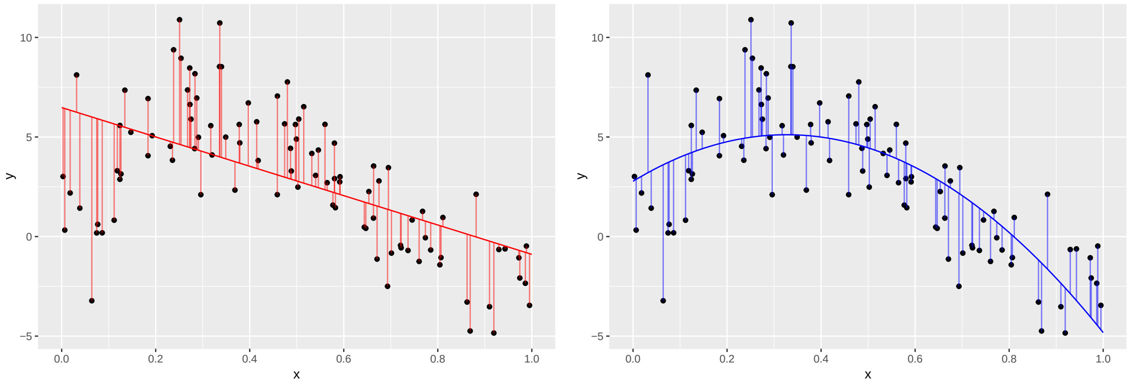
Your Turn #4

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*?
3. What is the *complexity* of the quadratic model?

4.2 Performance Comparison (on Training Data)

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

degree	RSS	npars
1	829.1	2
2	557.8	3



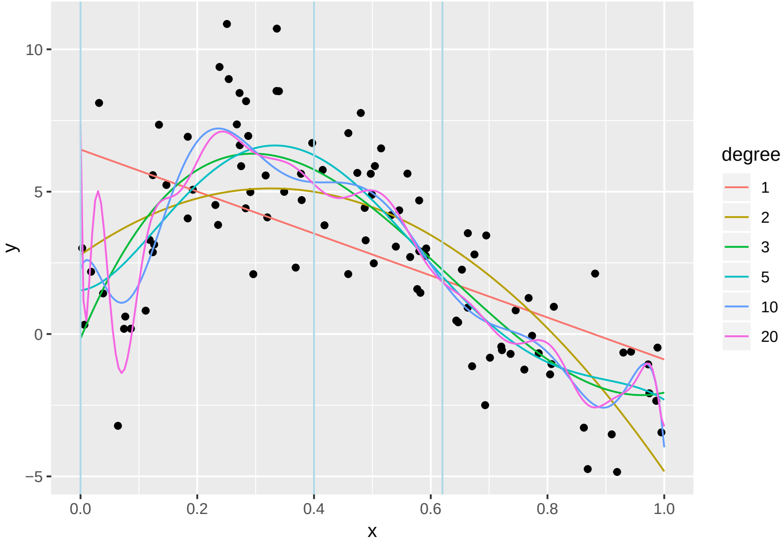
As my kids always reason, “if a little is good, than a lot must be better”. So why not try more complex models by increasing the polynomial degree.

- Polynomial of degree d

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

degree	RSS	npars
1	829.1	2
2	557.8	3
3	428.1	4
5	410.2	6
10	364.9	11
20	315.6	21

And its always good to observe the plot



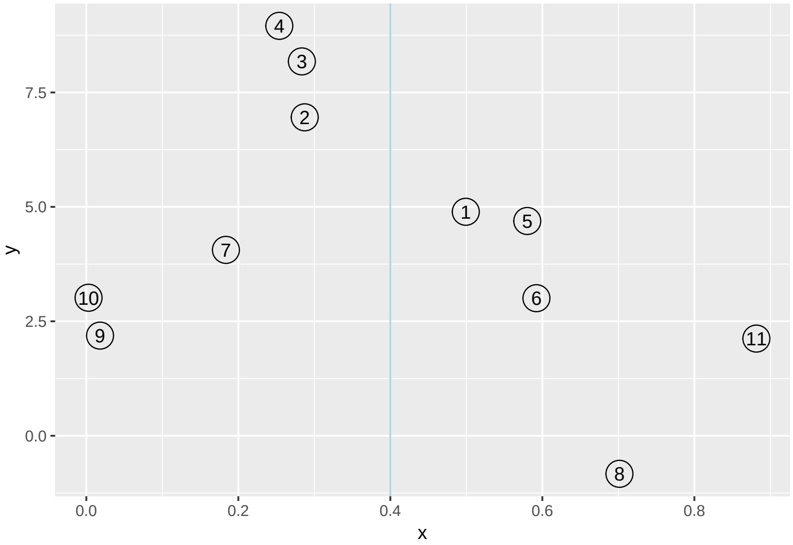
- For `degree=20`, the behavior at the end points are a bit erratic.
- Using a higher degree would further reduce the RSS, but the fitted curve would be less "smooth"

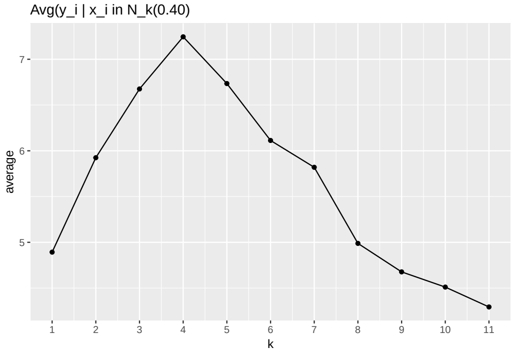
5 k-nearest neighbor models

- 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.
- The model is simple to describe

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

  - $N_k(x)$ 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
  - What is the estimate if $k = n$?
- Consider the following example where we wish to estimate $Y \mid X = 0.40$





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

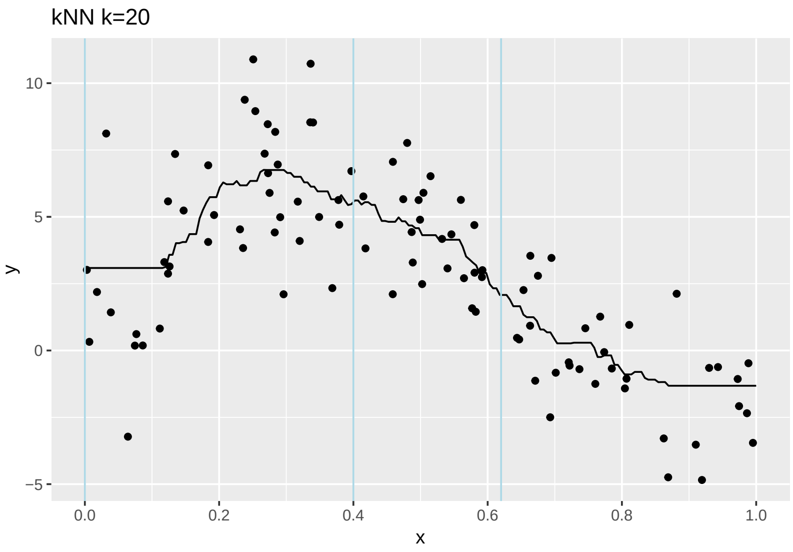
- One drawback of knn methods is that all the training data must be stored in order to make predictions
- Another drawback comes from the *curse of dimensionality* when the distance to neighbors grows exponentially

5.1 knn in action

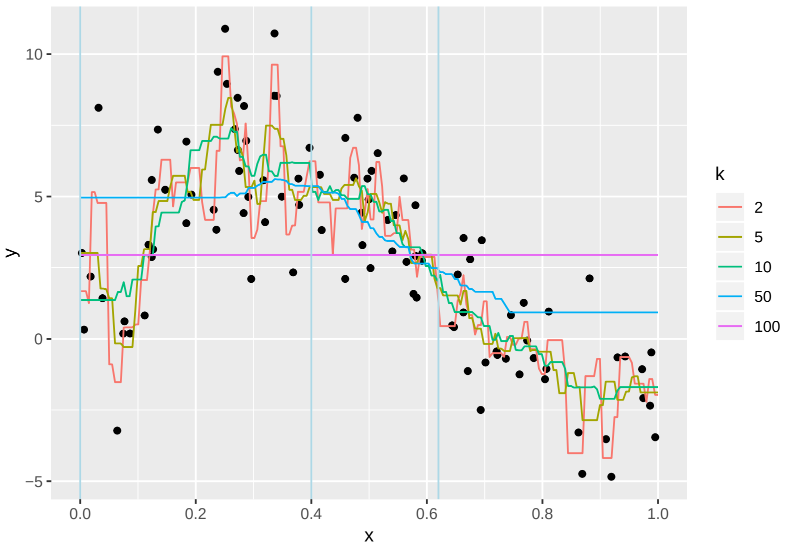
In R , the function `knn.reg()` from the `FNN` package will fit a knn regression model. Here is a $k = 20$ nearest neighbor model

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

#- fit a k=20 knn regression
knn.20 = knn.reg(data.frame(x), test=xeval, y=y, k=20)
```



- The *complexity* of a knn model increases as k decreases.
- The least 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 about how many parameters are estimated in the model (to allow comparison with parametric models)



5.1.1 Performance of the knn models (on training data)

k	RSS	edf
100	1240.2	1
50	686.5	2
10	386.1	10
5	316.0	20
2	183.9	50

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

6.1 Predictive Model Evaluation

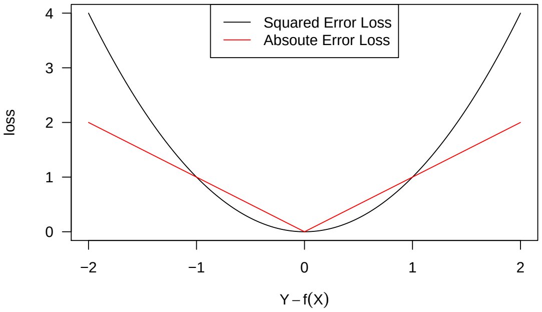
Our goal is prediction, so we should evaluate the models on their *predictive performance*.

- So we need to use new data (i.e., data not used to fit the model) to evaluate how well our models do in prediction
- Call these data *test data* $D_{\text{test}} = \{(X_j, Y_j)\}_{j=1}^{J}$
  - 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 about 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 *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 predictor is the one that minimizes the *expected loss* or Risk or Expected Prediction Error (EPE)

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

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

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

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 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

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

Your Turn #5

What is the optimal prediction at $X = x$, $f^*(x)$?

- **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 $R_x(f^*) = \mathrm{V}[Y|X = x]$
- Under *squared error loss* the Risk is

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

6.2.1 kNN and Polynomial Regression

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

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

  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

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

6.2.2 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)

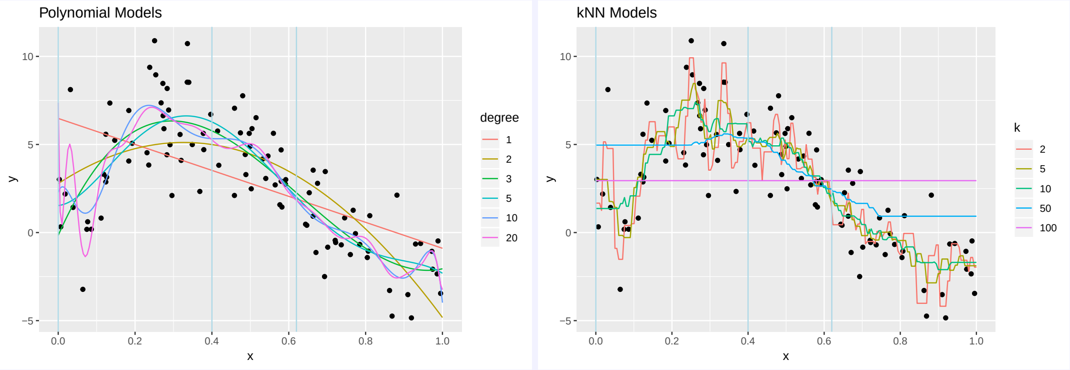
- But is it a bad idea to choose the best model according to *empirical risk* or *training error*?

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

6.3 Choose the best *predictive* model

Your Turn #6

Which model will you choose?



Polynomial

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kNN

k	RSS	edf
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