

# Supervised Learning (Part I)

DS 6030 | Fall 2023

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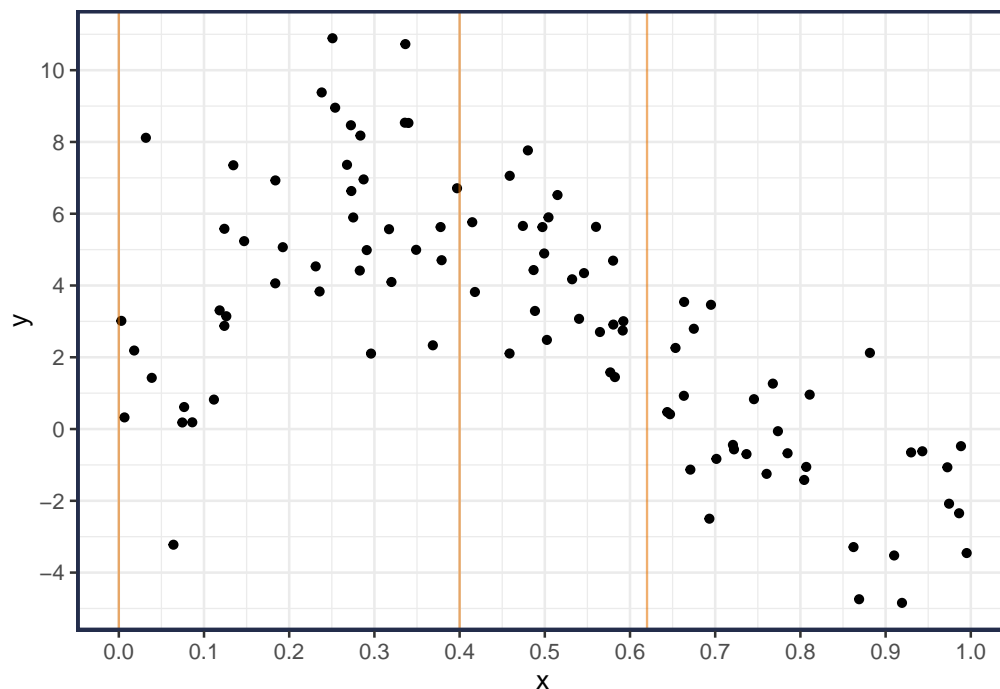
# 1 Supervised Learning Intro

## 1.1 Supervised Learning

- In *supervised learning*, each observation can be partitioned into two sets: the predictor variables and the outcome variable(s).
  - Predictor variables are sometimes called independent/feature variables
  - Outcome variables are sometimes called target/labels/response/dependent variables.
- 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 outcomes (i.e., no  $Y$ 's).

## 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

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

where  $x = [x_1, \dots, x_p]^T$  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. (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](#)

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

- where SSE is the *sum of squared errors* (also known as *residual sum of squares* (RSS))

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

- 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:

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

## 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 = tibble(x,y)      # create a data frame/tibble
m1 = lm(y~x, data=data_train) # fit simple OLS

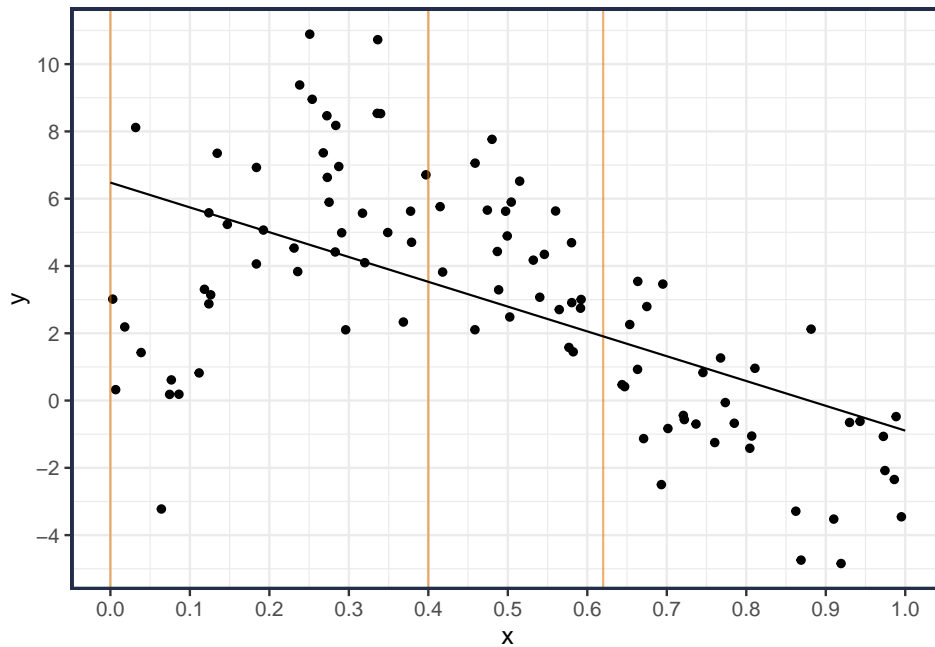
summary(m1)                   # summary of model
#>
#> Call:
#> lm(formula = y ~ x, data = data_train)
#>
#> Residuals:
#>      Min       1Q   Median       3Q      Max
#> -9.229 -1.635  0.019  1.940  6.728
#>
#> Coefficients:
#>              Estimate Std. Error t value Pr(>|t|)
#> (Intercept)    6.478      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
#>
#> 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.
#> # 3 more variables: deviance <dbl>, df.residual <int>, nobs <int>
```

- `lm()` uses the formula interface, which includes the intercept by default.
  - Some examples of using formulas as well as getting the underlying  $X$  (model/design matrix) can be found [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, xeval)         # vector of yhat's (predictions)
```



### 3.2.3 Questions

#### Your Turn #2

1. How did we do? If  $X_{\text{new}}$  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,  $\beta_0$  and  $\beta_1$ . Thus, the **model flexibility/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 flexibility 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 SSE loss function over the **training data**

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

#### 4.1.1 Matrix notation

- **Model**

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

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

#### Your Turn #3 : Matrix Notation

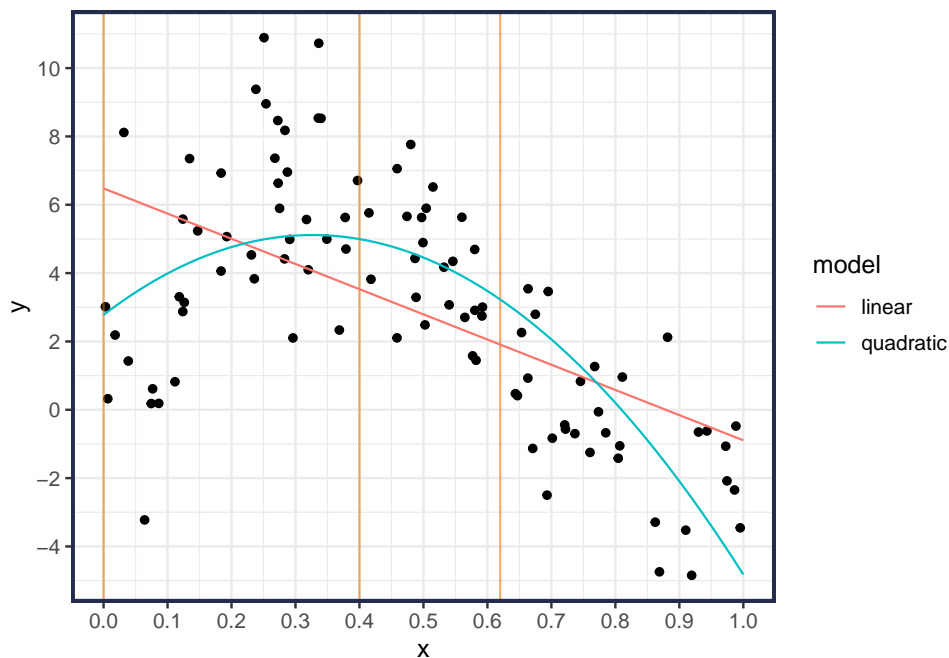
Solve for  $\hat{\beta}$  using matrix notation.

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

### 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, xeval)
```



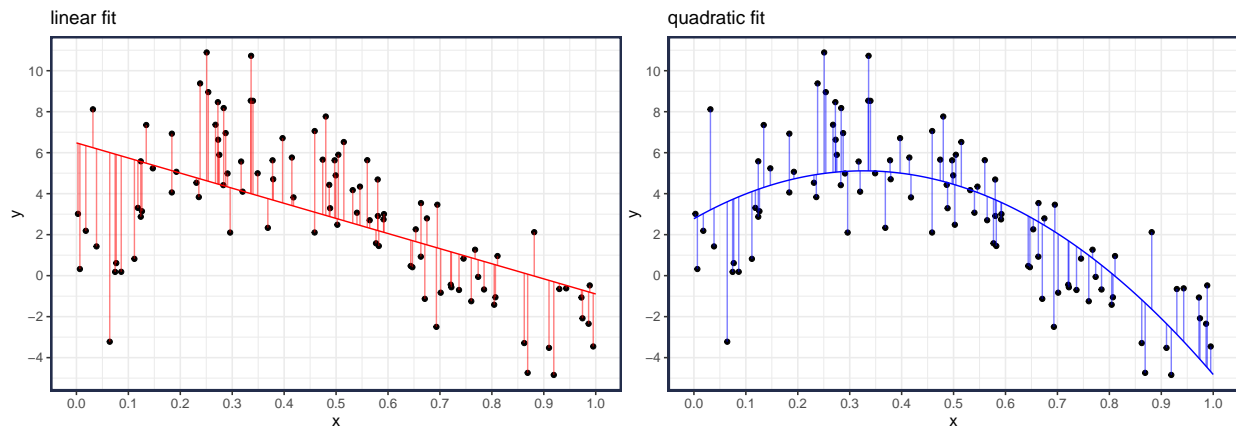
#### Your Turn #4

1. How did we do? If  $X_{\text{new}}$  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/flexibility* of the quadratic model?

## 4.2 Performance Comparison (on Training Data)

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

degree	MSE	npars
1	8.29	2
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.

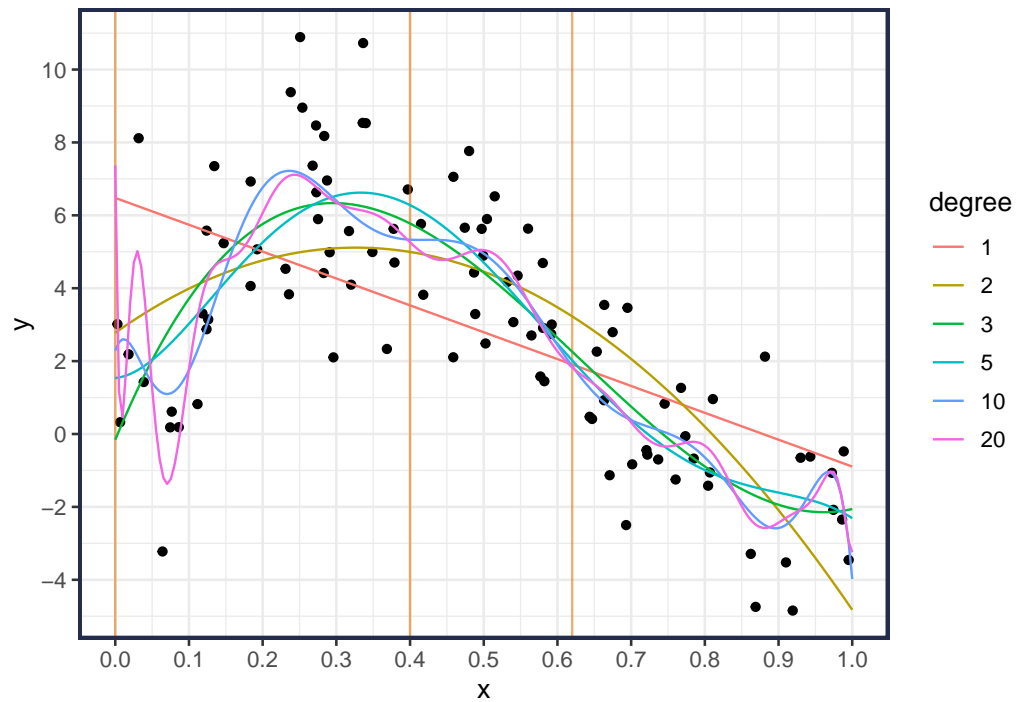
- Polynomial of degree  $d$

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

degree	MSE	npars
1	8.29	2
2	5.58	3
3	4.28	4
5	4.10	6
10	3.65	11
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 MSE, but the fitted curve would be more “complex” and may not be as good for new data.

## 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

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

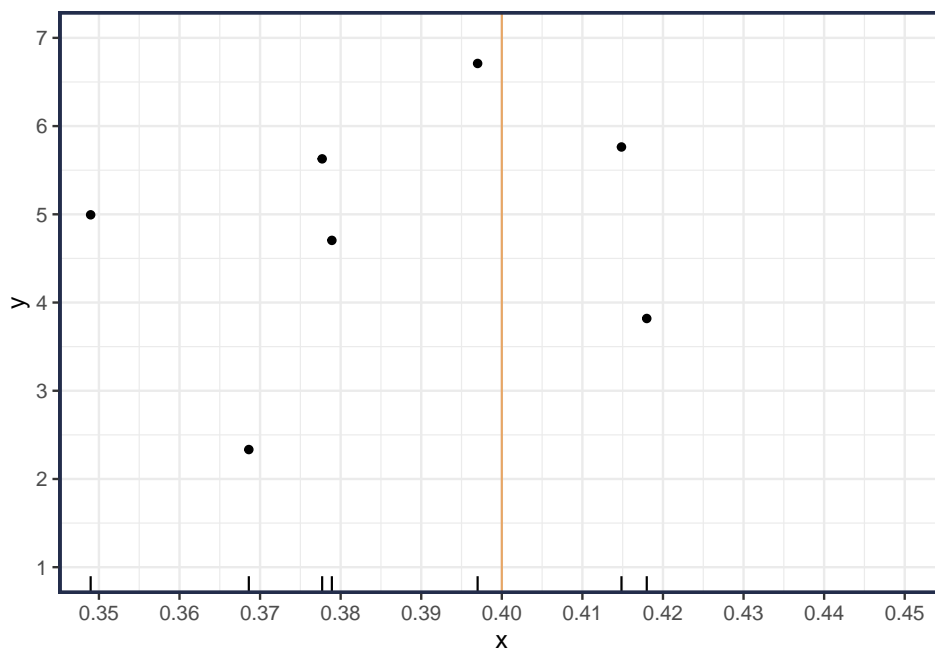
- $N_k(x)$  are the set of  $k$  nearest neighbors to  $x$
- only the  $k$  closest  $y$ 's are used to generate a prediction
- it is a *simple mean* of the  $k$  nearest observations

### Your Turn #5

What is the estimate  $f_{\text{knn}}(x; k = n)$ ?

#### 5.0.1 Example

Let's zoom in on the region around  $x = 0.4$



x	y	k	D	$\hat{f}_{\text{knn}}(x; k)$
0.397	6.710	1	0.003	6.710
0.415	5.763	2	0.015	6.237
0.418	3.819	3	0.018	5.431
0.379	4.705	4	0.021	5.249
0.378	5.628	5	0.022	5.325
0.369	2.333	6	0.031	4.826
0.349	4.994	7	0.051	4.850

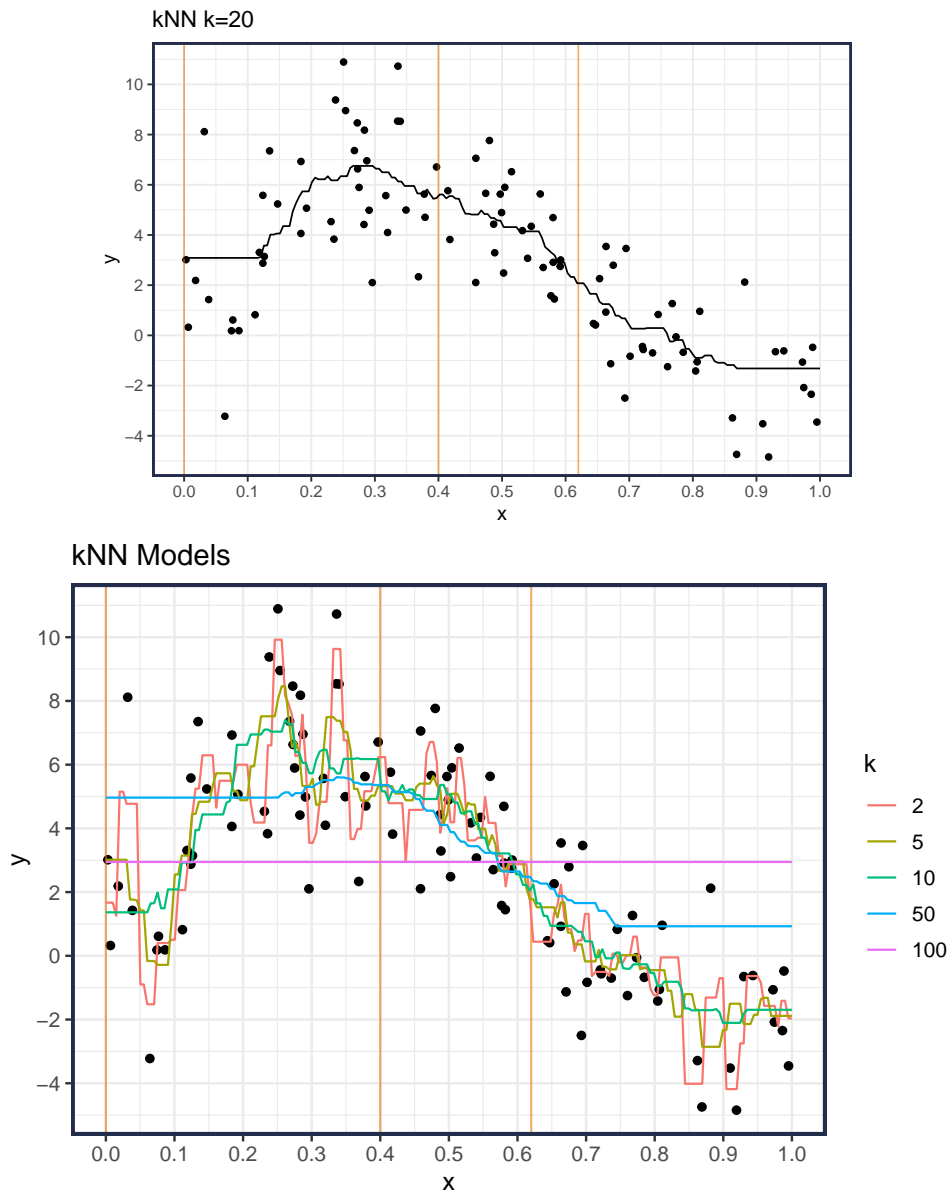
### 5.0.2 Notes about knn

- 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)
- The *flexibility* 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 *flexibility/complexity*. It is approximately the number of parameters that are estimated in the model (to allow comparison with parametric models)

## 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

```
library(FNN) # library() loads the package. Access to knn.reg()
knn.20 = knn.reg(select(data_train, x), test=xeval, y=data_train$y, k=20)
```



### 5.1.1 Performance of the knn models (on training data)

k	MSE	edf
100	12.40	1
50	6.87	2
20	4.18	5
10	3.86	10
5	3.16	20
2	1.84	50

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

### 6.1 Predictive Model Evaluation

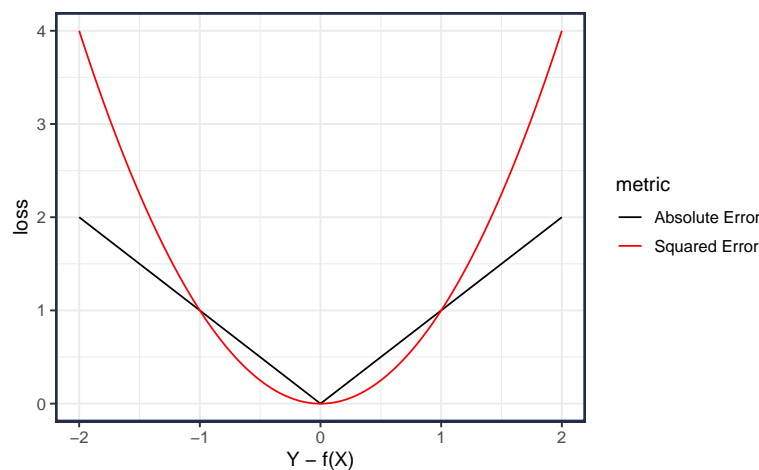
Our goal is prediction, so we should evaluate the models on their *predictive performance*.

- 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*  $D_{\text{test}} = \{(X_j, Y_j)\}_{j=1}^J$ 
  - 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 *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)**

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

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

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

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  $Y$ .

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

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

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

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

### Your Turn #6

What is the optimal prediction at  $X = x$  under the squared error loss?

- I.e., find  $f^*(x)$ .

## 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  $f^*(x) = E[Y \mid X = x]$ .
  - And the minimum Risk/MSE is  $R_x(f^*) = V[Y \mid X = x]$

- **Summary:** Under *squared error loss* the Risk (at input  $x$ ) is

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

### 6.2.2 kNN and Polynomial Regression

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

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

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 expected error from *test data* (out-of-sample), or data that was not used to estimate  $\hat{f}$

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

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*?

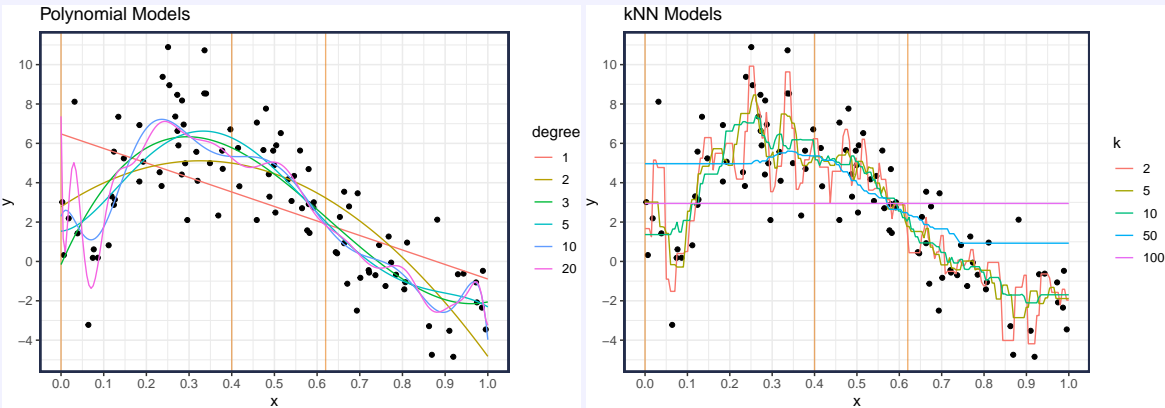
$$\begin{aligned}
 \hat{R}_n(f) &= \frac{1}{n} \sum_{i=1}^n L(y_i, f(x_i)) \\
 &= \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 \quad \text{for squared error loss}
 \end{aligned}$$

## 6.3 Choose the best *predictive* model

### Your Turn #7

Which model will you choose?

You can access the survey from [Canvas/Quizzes/Surveys/Best Predictive Model](#).



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