

Supervised Learning (Part II)

DS 6410 | Spring 2024

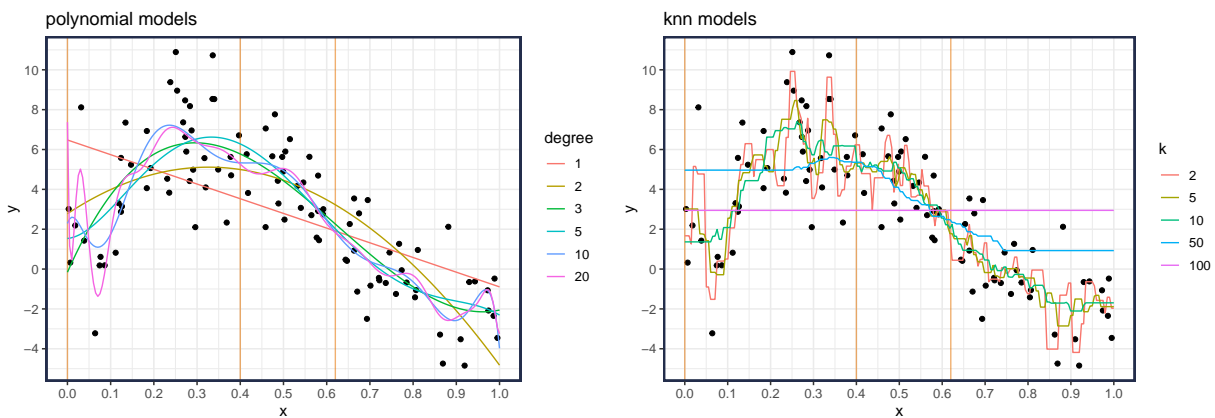
supervised_2.pdf

Contents

1	Training Data and Model Fits	2
2	Evaluate Simulated Test Data (or which model is best)	2
3	Ensemble Models	4
4	Bias-Variance Trade-off	6
4.1	Data Generating Functions	6
4.2	One Realization	6
4.3	A second realization	7
4.4	Bias, Variance, and Mean Squared Error (MSE)	8
4.5	Estimating the Bias, Variance, and Mean Squared Error (MSE)	9
4.6	What does it all mean	13
5	Appendix: R Code	16
5.1	Required R Packages	16
5.2	Training and Test Data	16
5.3	Evaluating Polynomial Models	17
5.4	Evaluating k nearest neighbor models	20
5.5	Comparison of best models	23

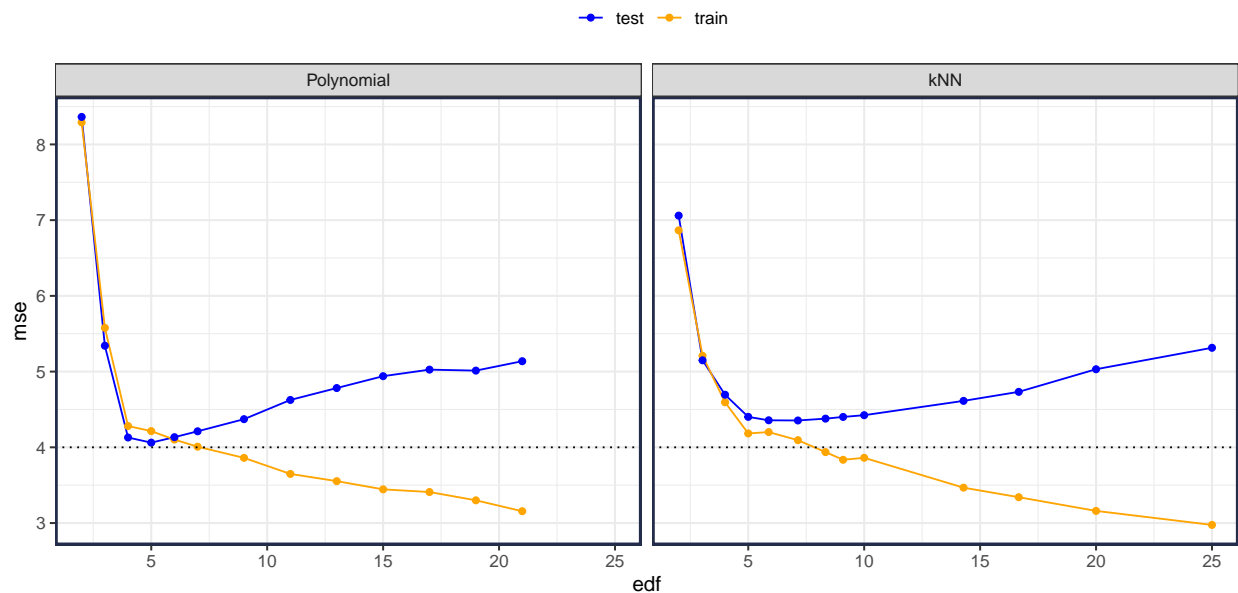
1 Training Data and Model Fits

Recall from last class that we considered several models from two model families (nearest neighbor and polynomial).



2 Evaluate Simulated Test Data (or which model is best)

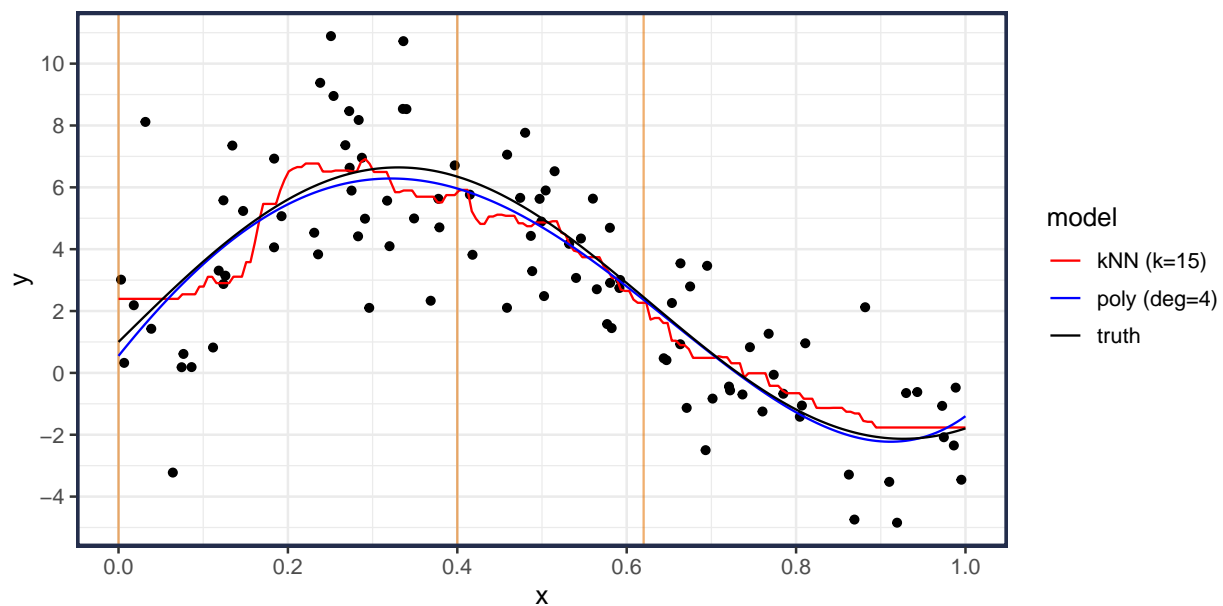
I simulated 50,000 test observations, evaluated the predictions from each model, and recorded the estimated MSE/Risk.



Polynomial				kNN			
degree	edf	mse_train	mse_test	k	edf	mse_train	mse_test
1	2	8.29	8.36	50	2.00	6.87	7.06
2	3	5.58	5.34	33	3.03	5.21	5.15
3	4	4.28	4.13	25	4.00	4.59	4.69
4	5	4.21	4.06	20	5.00	4.18	4.40
5	6	4.10	4.13	17	5.88	4.20	4.36
6	7	4.01	4.21	14	7.14	4.09	4.35
8	9	3.86	4.37	12	8.33	3.94	4.38
10	11	3.65	4.63	11	9.09	3.84	4.40
12	13	3.55	4.78	10	10.00	3.86	4.42
14	15	3.44	4.94	7	14.29	3.47	4.61
16	17	3.41	5.03	6	16.67	3.34	4.73
18	19	3.30	5.01	5	20.00	3.16	5.03
20	21	3.16	5.14	4	25.00	2.98	5.31

Observations:

- as the flexibility increases, both classes of models *overfit*.
 - overfit means model too complex
 - underfit means model is not complex enough
 - see discrepancy between training and test performance
- The polynomial with degree = 4 has the best test performance with an approximate MSE = 4.06.
- The optimal MSE = 4.
 - I only know this because I know how the data was generated



3 Ensemble Models

Last class you gave your votes for which model you thought was best:

model	edf	number of votes
polynomial (deg=2)	3.0	1
polynomial (deg=3)	4.0	1
nearest neighbor (k=20)	5.0	1
polynomial (deg=5)	6.0	1
nearest neighbor (k=15)	6.7	1
nearest neighbor (k=10)	10.0	1

- Can we use the collective *wisdom of the crowds* to help make a better prediction?
- An *ensemble model* is one that combines several models together.

The approach is to create a new ensemble model that is a weighted sum of the individual models

$$f_w(x) = \sum_{j=1}^p w_j f_j(x)$$

In our specific example, we had

$$\hat{f}_w(x) = \frac{1}{6} f_{\text{knn}}(x, k=10) + \frac{1}{6} f_{\text{knn}}(x, k=15) + \frac{1}{6} f_{\text{knn}}(x, k=20) + \dots + \frac{1}{6} f_{\text{poly}}(x, \text{deg}=5)$$

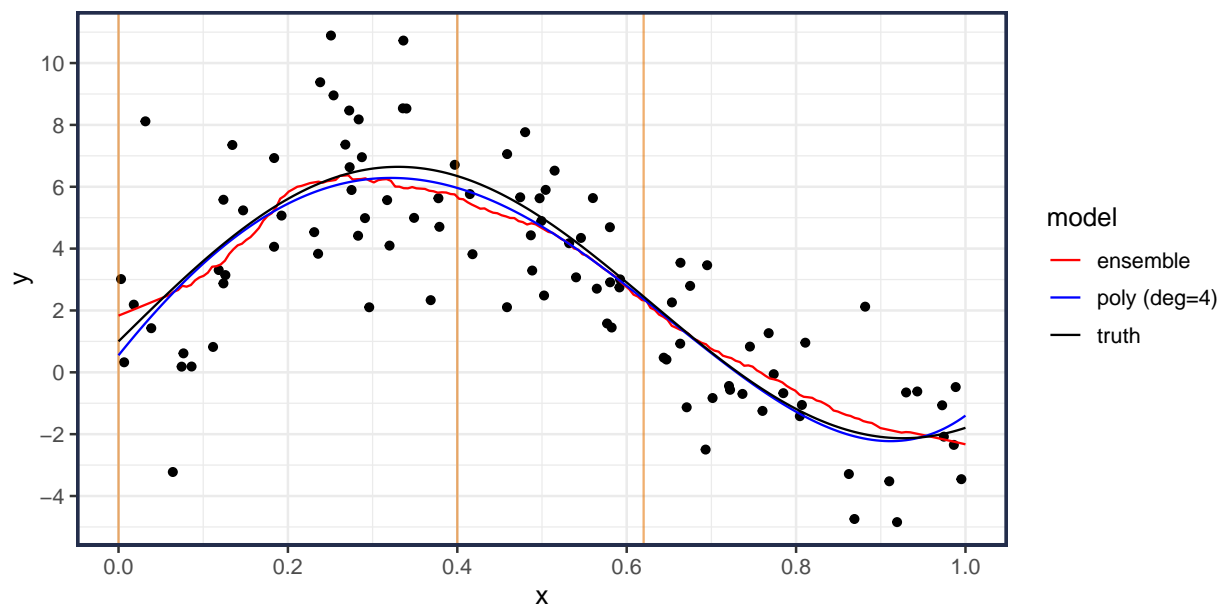
and the corresponding **test** performance is given by

$$R = \frac{1}{M} \sum_{j=1}^M (y_j - \hat{f}_w(x_j))^2$$

where M is the number of test observations.

This gives a **test** MSE of 4.19, which is better than most individual models

model	n	w	edf	mse
polynomial(deg=3)	1	0.17	4.00	4.13
polynomial(deg=5)	1	0.17	6.00	4.13
ensemble	NA	NA	NA	4.19
nearest neighbor(k=15)	1	0.17	6.67	4.37
nearest neighbor(k=20)	1	0.17	5.00	4.40
nearest neighbor(k=10)	1	0.17	10.00	4.42
polynomial(deg=2)	1	0.17	3.00	5.34



4 Bias-Variance Trade-off

This section explores the bias-variance trade-off for the examples we covered last class. This involves examining the theoretical properties of an estimator.

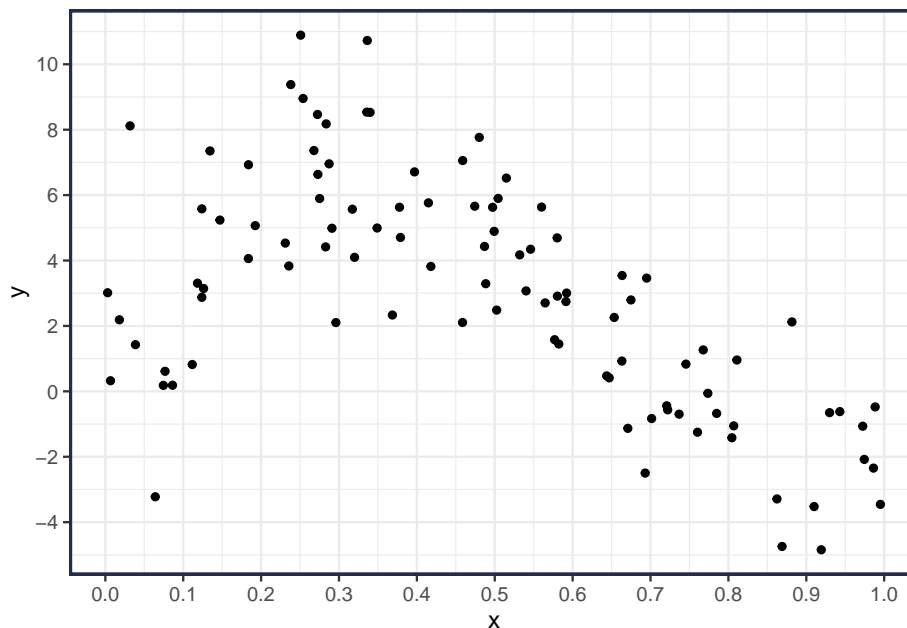
4.1 Data Generating Functions

Here we set the data generation functions. $X \sim U[0, 1]$ and $f(x) = 1 + 2x + 5 \sin(5x)$ and $y(x) = f(x) + \epsilon$, where $\epsilon \stackrel{\text{iid}}{\sim} N(0, 2)$.

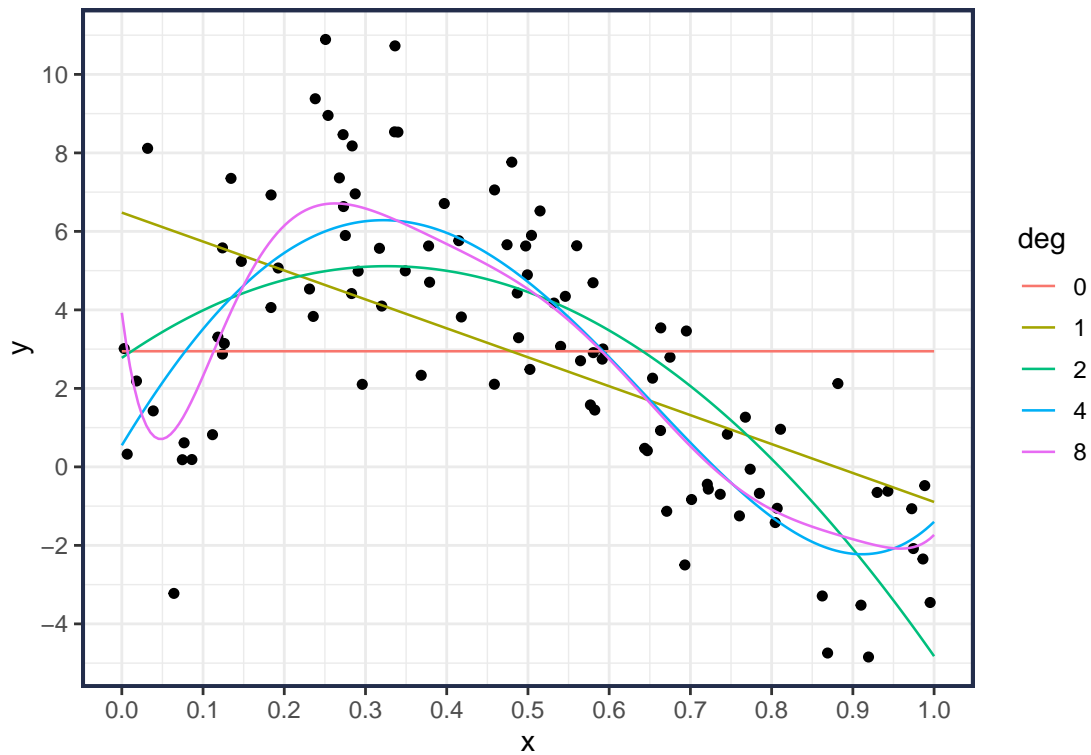
```
#- Simulation functions
sim_x <- function(n) runif(n) # U[0,1]
f <- function(x) 1 + 2*x + 5*sin(5*x) # true mean function
sim_y <- function(x, sd){ # generate Y|X from N{f(x),sd}
  n = length(x)
  f(x) + rnorm(n, sd=sd)
}
#- Simulation settings
n = 100 # number of obs
sd = 2 # stdev for error
```

4.2 One Realization

Last class, we explored one realization from this system.

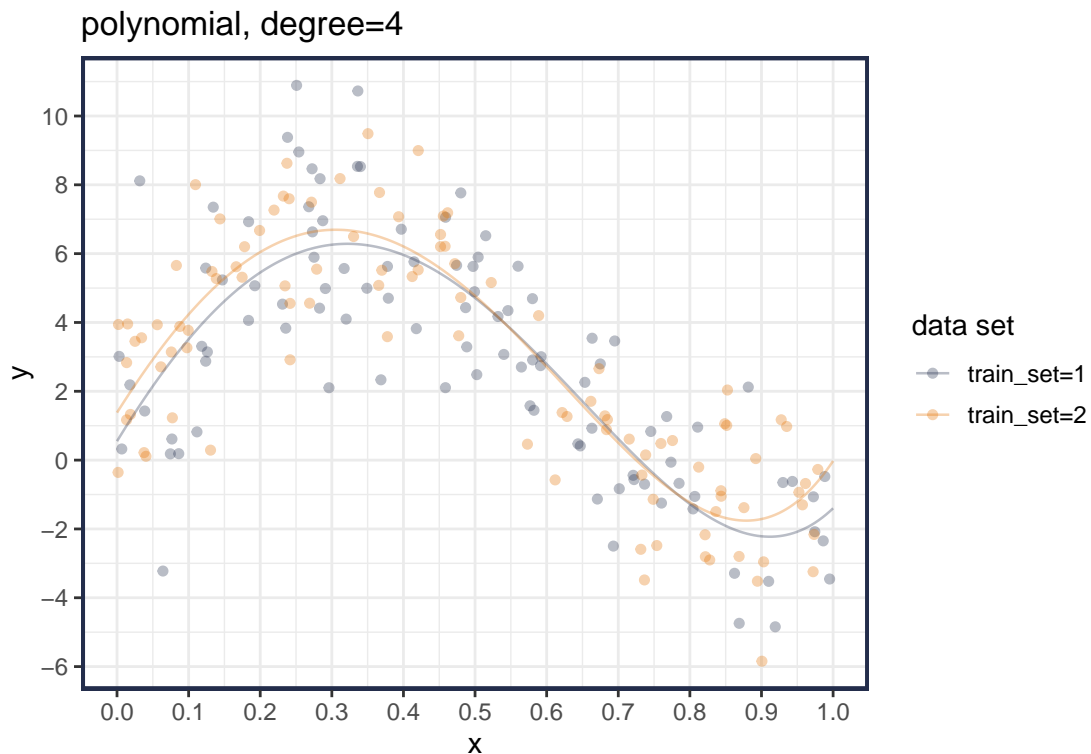


And then fit several polynomial regression models. Recall by polynomial regression I mean using a predictor function $\hat{y}(x) = f(x, d) = \sum_{j=0}^d x^j \beta_j$, where $d \in \{0, 1, \dots\}$ is the degree.



4.3 A second realization

Suppose we drew another training set (using same distributions and sample size n):



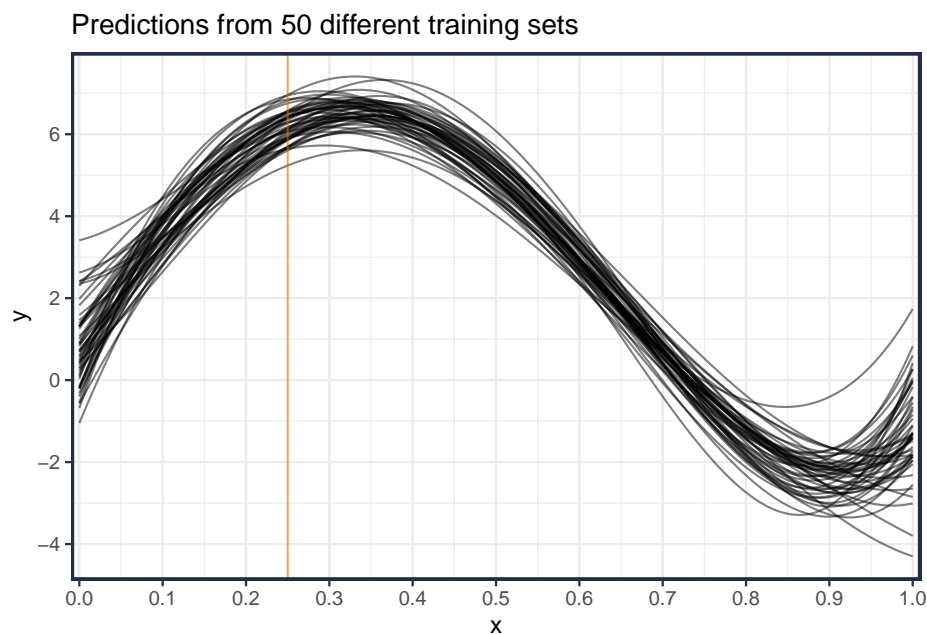
- We get another fitted curve using the new training data.
- While the two curves are visually similar, they are not identical.
- If we took more training samples, we would get more fitted curves
- What we want to study in this section is the likelihood that we will happen to get a *good* fit given a single training data set.

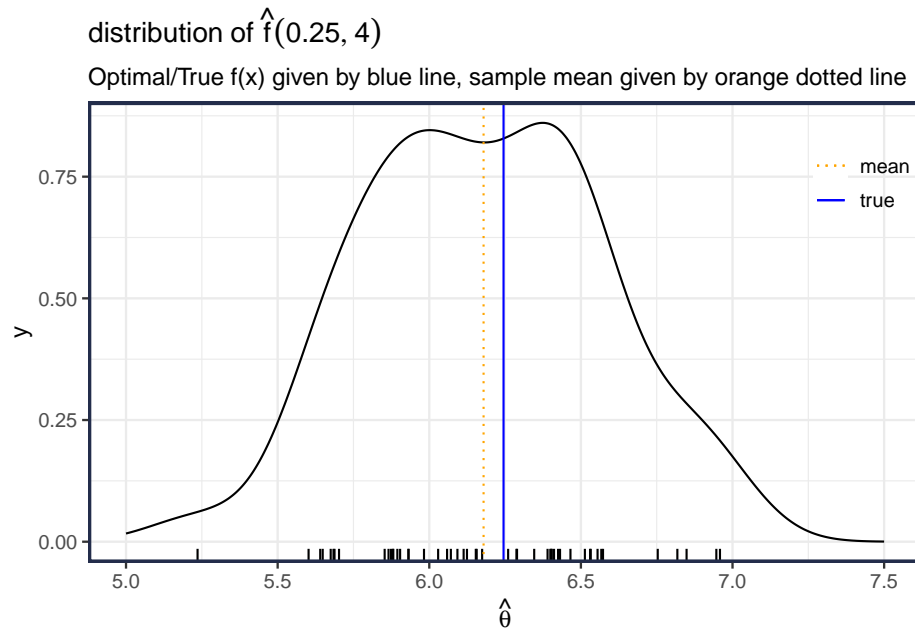
4.4 Bias, Variance, and Mean Squared Error (MSE)

- The statistical properties of an estimator can help us understand its potential performance
- Let $D = [(X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n)]$ be *training data*
- Let $\hat{\theta} = \hat{\theta}(D)$ be the estimated value *calculated from the training data* D
 - E.g. $\theta = f(x)$, $\hat{\theta} = \hat{f}(x | D)$
 - $\hat{\theta}$ is a *random variable* because we are treating the data as random; it has a distribution.

4.4.1 Distribution of $\hat{\theta}$

- Consider the distribution of $\hat{\theta} = \hat{f}_{\text{poly}}(0.25, d = 4)$.
 - This is the distribution of the fit at $x = 0.25$ from a polynomial (of degree 4) using different *training sets*
- I generated 50 different training data sets (each with $n = 100$), fit a polynomial (deg=4) model to each data set, and recorded the estimate at $x = 0.25$.





4.4.2 Some properties of an estimator

- **Bias** of an estimator is defined as $E_D[\hat{\theta}] - \theta$
- **Variance** of an estimator is defined as $V_D[\hat{\theta}] = E_D[\hat{\theta}^2] - E_D[\hat{\theta}]^2$
- **MSE** of an estimator is defined as $MSE(\hat{\theta}) = E_D[(\hat{\theta} - \theta)^2]$

$$\begin{aligned}
 MSE(\hat{\theta}) &= E_D[(\hat{\theta} - \theta)^2] \\
 &= V_D[\hat{\theta} - \theta] + E_D[\hat{\theta} - \theta]^2 \\
 &= V_D[\hat{\theta}] + E_D[\hat{\theta} - \theta]^2
 \end{aligned}$$

- Estimators are often evaluated based on MSE, being unbiased, and/or having minimum variance (out of all unbiased estimators)
- These properties are based on the *distribution of an estimate*.
 - Once we observe the training data, the resulting estimate may be great or horrible.
 - However these theoretical properties provide insight into what we can expect and how much confidence we can have in the estimates.

4.5 Estimating the Bias, Variance, and Mean Squared Error (MSE)

- Last class, we examined the Risk (e.g., MSE) *conditioning on the training data* (See Section 6.2.1)
- Now we will relax this and bring in the uncertainty in the training data D

Under a squared error loss function $L(Y, f(X)) = (Y - f(X))^2$, the *overall Risk* (or Risk before we see

any training data) at a particular $X = x$ is

$$\begin{aligned}\text{MSE}_x(f) &= \mathbb{E}_{D|Y|X}[(Y - \hat{f}_D(x))^2 | X = x] \\ &= \mathbb{V}[Y | X = x] + \mathbb{V}[\hat{f}_D(x) | X = x] + \left(\mathbb{E}[\hat{f}_D(x) | X = x] - f(x)\right)^2 \\ &= \text{irreducible error} + \text{model variance} + \text{model squared bias}\end{aligned}$$

where D is the training data, f is the true model, and $\hat{f}_D(x)$ is the prediction at $X = x$ estimated from the training data D .

Note

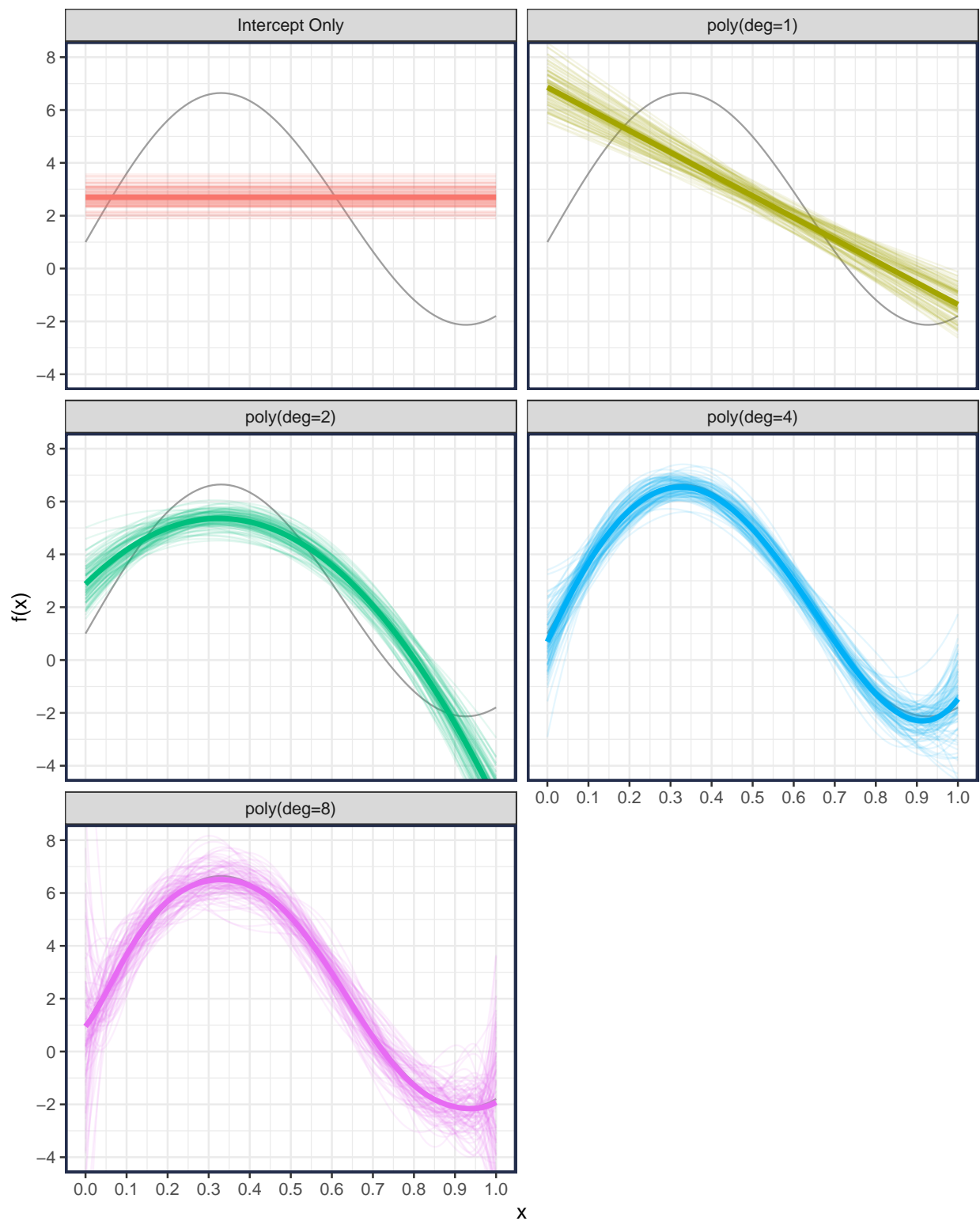
$$\begin{aligned}\text{MSE}_x(f) &= \mathbb{E}_{D|Y|X}[(Y - \hat{f}_D(x))^2 | X = x] \\ &= \mathbb{E}_{D|Y|X}[(Y - f(x) + f(x) - \hat{f}_D(x))^2 | X = x] \\ &= \mathbb{E}_{D|Y|X}[(Y - f(x))^2] + \mathbb{E}_{D|Y|X}[(f(x) - \hat{f}_D(x))^2] + \mathbb{E}_{D|Y|X}[2(Y - f(x))(f(x) - \hat{f}_D(x))] \\ &= \mathbb{V}[Y | X = x] + \mathbb{E}_{D|Y|X}[(f(x) - \hat{f}_D(x))^2] + 0 \\ &= \mathbb{V}[Y | X = x] + \mathbb{V}_{D|Y|X}(\hat{f}_D(x)) + \mathbb{E}_{D|Y|X}(f(x) - \hat{f}_D(x))^2\end{aligned}$$

- We can estimate the model variance and bias with simulation
 - Generate new data $D_m = \{(Y_i, X_i)\}_{i=1}^n$ for simulations $m = 1, 2, \dots, M$ (use the same sample size n)
 - Fit the models with data D_m getting $\hat{f}_{D_m}(\cdot)$
 - Now we can estimate the items of interest:

$$\begin{aligned}\mathbb{E}[\hat{f}_D(x)] &\approx \bar{f}(x) = \frac{1}{M} \sum_{m=1}^M \hat{f}_{D_m}(x) \\ \mathbb{V}[\hat{f}_D(x)] &\approx s_f^2(x) = \frac{1}{M-1} \sum_{m=1}^M (\hat{f}_{D_m}(x) - \bar{f}(x))^2\end{aligned}$$

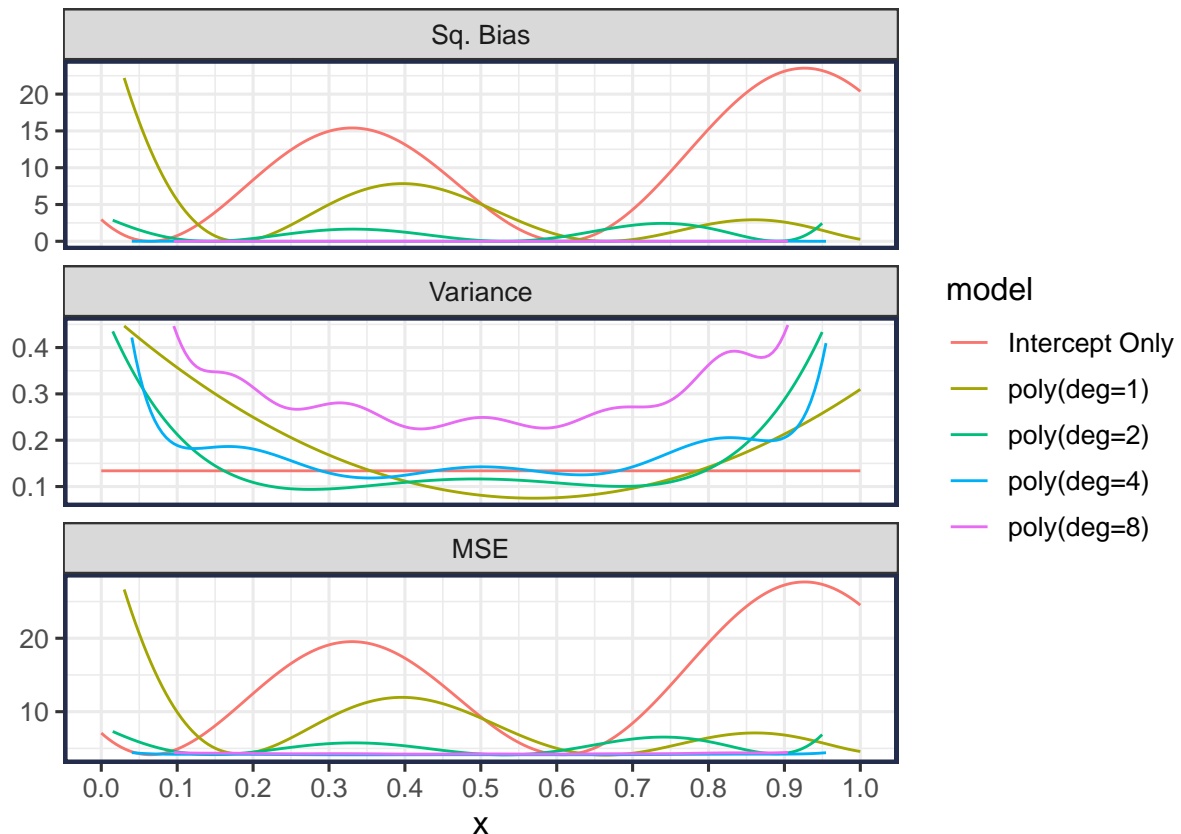
4.5.1 Simulation

I ran 2000 simulations to generate $\{\hat{f}_m(x, \text{deg} = d) : d \in \{0, 1, 2, 4, 8\}, m \in \{1, 2, \dots, 2000\}\}$.



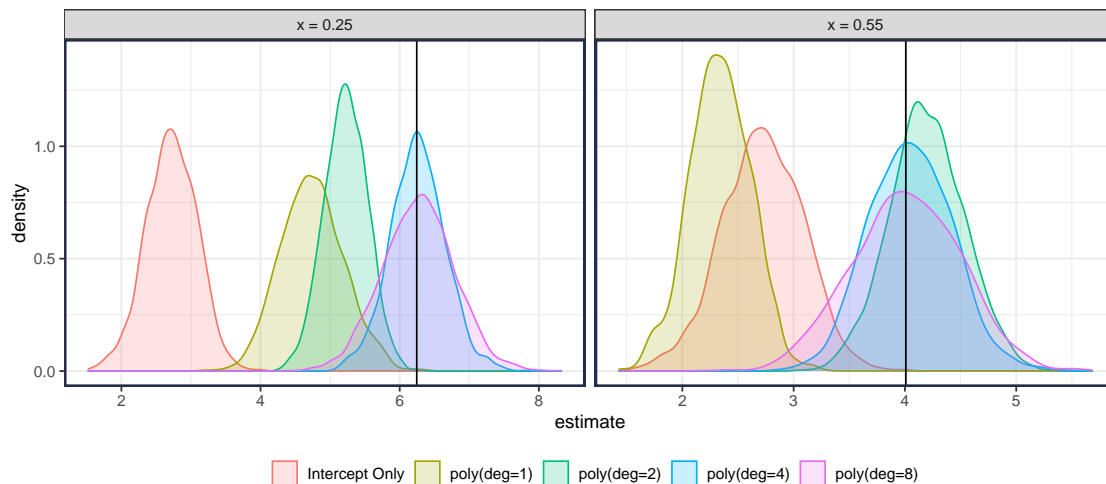
4.5.2 Observations

- This shows the bias and variance of each model.
- You can see that as the flexibility (e.g., degree) of the model increases, the bias decreases but the variance (especially at the edges) increases.
 - The **bias** is the difference between the true regression function (dark gray line) and the model mean (dark colored line).
 - The **variation** is seen in the width of the transparent curves, one for each simulation.



4.5.3 Bias, Variance, and MSE at a single input

- Notice that model variance and model bias vary over x .
- To help see what is going on, we now look at the distributions at $x = 0.25$ and $x = 0.55$.



4.5.4 Integrated MSE

The above analysis examines the $\text{MSE}_x(f)$ over a set of x 's. However, in a real setting, the overall test error will be based on *all* of the actual test X values. So we are usually more interested in the *integrated* MSE:

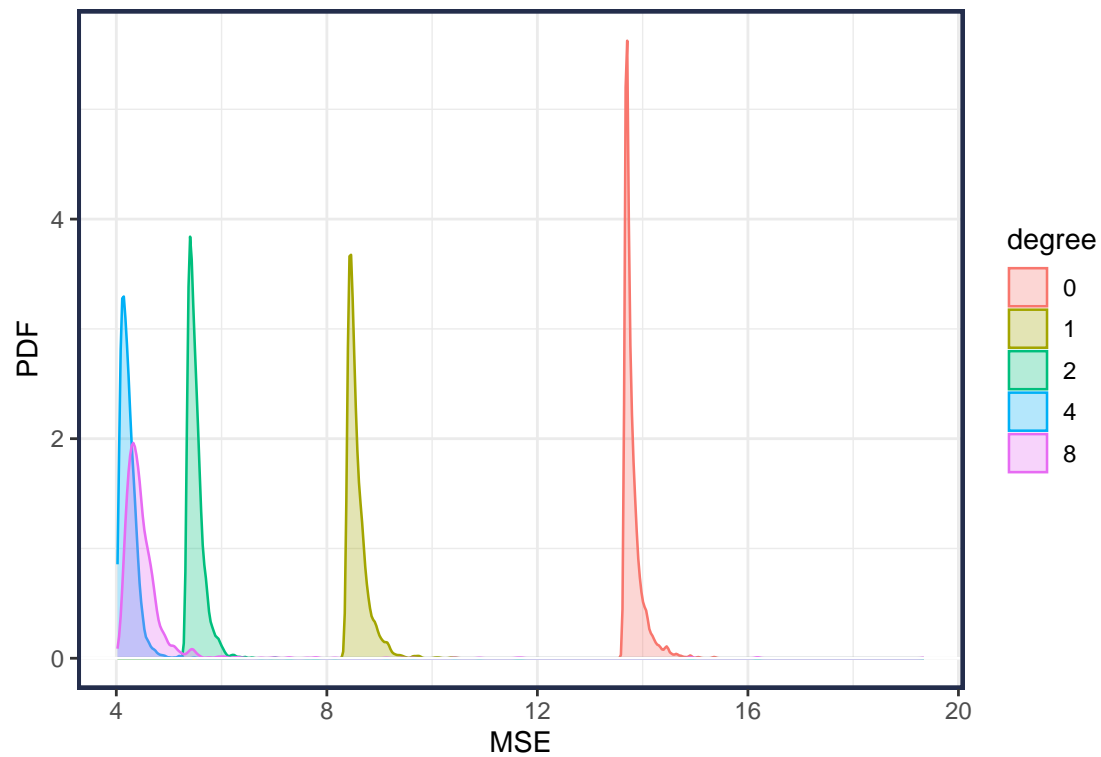
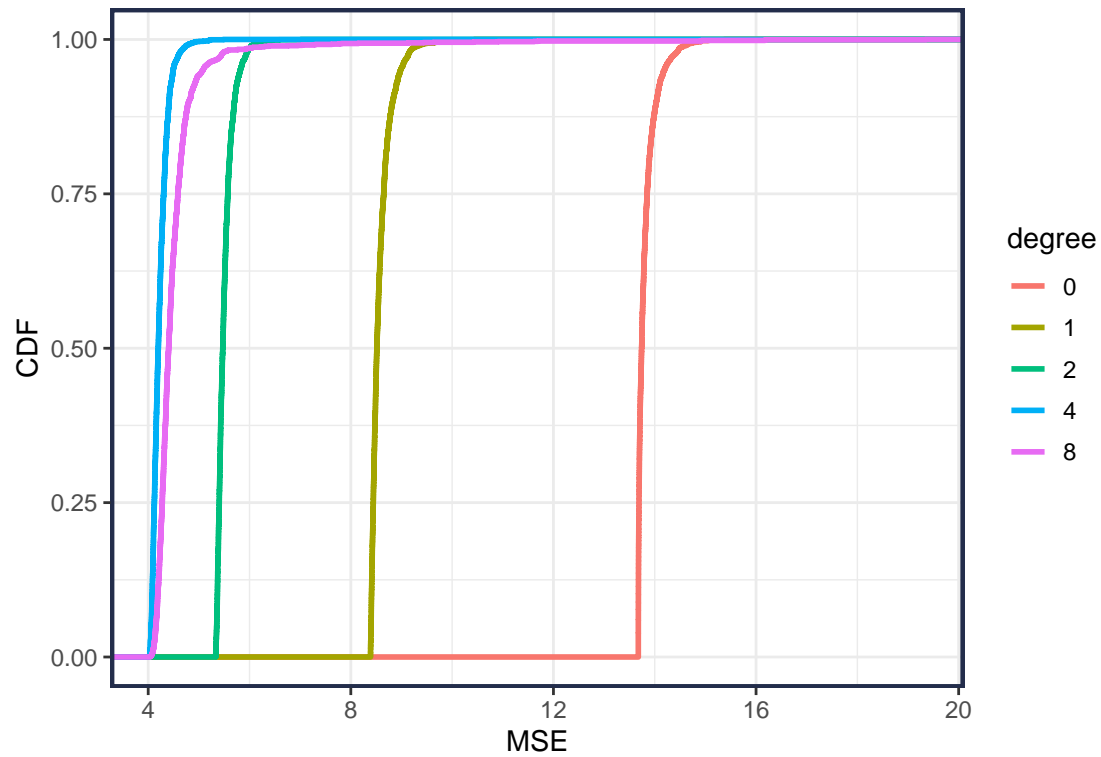
$$\begin{aligned} \text{MSE}(f) &= E_{D,Y,X}[(Y - \hat{f}_D(X))^2] \\ &= E_X[\text{MSE}_X(f)] \\ &= \int \text{MSE}_x(f) \Pr(dx) \end{aligned}$$

deg	bias.sq	var	mse
0	9.68	0.13	13.81
1	4.39	0.19	8.58
2	1.33	0.18	5.51
4	0.01	0.22	4.23
8	0.00	0.53	4.53

4.6 What does it all mean

The main point is that we desire to find a predictive model that has just the right *flexibility*. This will depend on both the true flexibility of the data as well as the sample size. A model that is too complex will have low bias, but potentially high variance. A model that is not complex enough will have high bias, but lower variance.

In a real setting, we will only observe one training data (a single curve) and will have to decide the optimal flexibility. The following plot shows the estimated distribution of MSE values.



While its possible that we could just happen to get a particular training data realization that favors a model other than the globally optimal model, this is unlikely for the bad models. However, it is not uncommon for “close” models.

Below is a table of the number of simulations that each model had the best MSE:

degree	n
0	0
1	0
2	0
3	397
4	1006
5	486
6	75
7	25
8	4
9	6
10	1

- While the degree=4 model does best, degree > 8 sometimes comes out best.
- **Conclusion 1:** In our toy example, a polynomial with degree=4 is the best model, in principal. However, for some data (i.e., some training data sets) the models with degree>4 and degree<4 would predict better.
- **Conclusion 2:** The above analysis is what is meant by the “bias-variance trade-off”.
 - In reality, we only get to observe one realization of the training data so we can never actually estimate the bias and variance the way we did above
 - But we can still estimate the Risk (e.g., MSE) by using resampling methods like cross-validation or statistical methods like BIC.
 - More loosely, when people mention bias-variance trade-off they are referring to the principal that the best model is one that has just the right flexibility.
 - If the model is too complex, it is unlikely to produce a good estimate (across the entire range of inputs) because it is likely to stray far from the expected mean at certain values.
 - If the model is not complex enough, then it will not track with the expected mean across the range of input values and thus produce poor overall performance.
- **Conclusion 3:** Performance of a model can vary across the input features X .
 - If you are only concerned about performance in a specific range of X , then emphasize these during training (e.g., weight observations close to X more heavily during model estimation).
 - If the test X values are coming from a different distribution than the training X values, then your model may not be optimal.

5 Appendix: R Code

5.1 Required R Packages

We will be using the R packages of:

- FNN for k nearest neighbor models
- tidyverse for data manipulation and visualization
- tidymodels (for optional tidymodels approach)

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

5.2 Training and Test Data

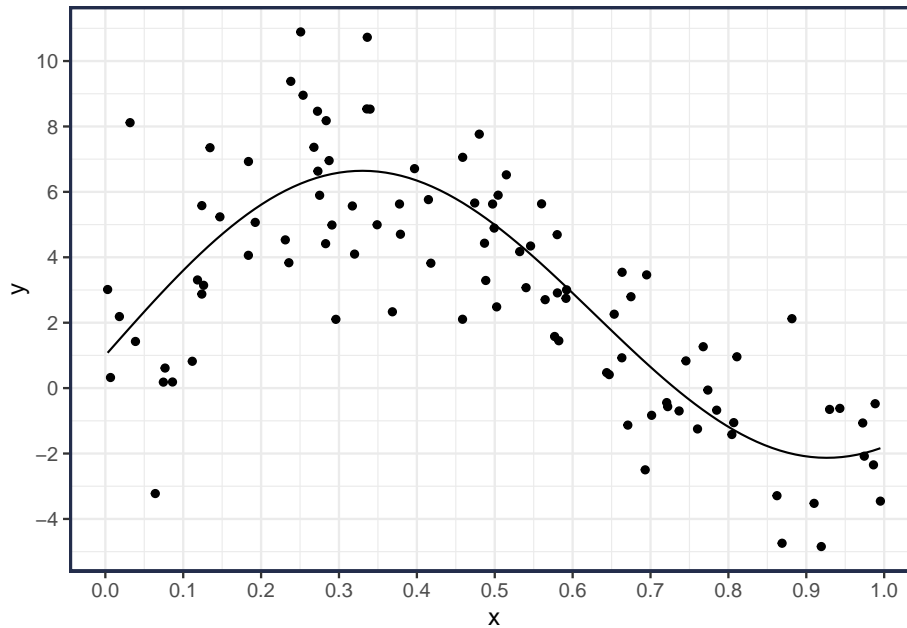
```
#-- Functions
sim_x <- function(n) runif(n) # U[0,1]
f <- function(x) 1 + 2*x + 5*sin(5*x) # true mean function
sim_y <- function(x, sd){ # generate Y|X from N{f(x),sd}
  n = length(x)
  f(x) + rnorm(n, sd=sd)
}

#-- Settings
n = 100 # number of observations
sd = 2 # stdev for error

#-- Generate Training Data
set.seed(825) # set seed for reproducibility
x = sim_x(n) # get x values
y = sim_y(x, sd=sd) # get y values
data_train = tibble(x, y) # training data tibble

#-- Generate Test Data
ntest = 50000 # Number of test samples
set.seed(235) # set *different* seed
xtest = sim_x(ntest) # generate test X's
ytest = sim_y(xtest, sd=sd) # generate test Y's
data_test = tibble(x=xtest, y=ytest) # test data

ggplot(data_train, aes(x,y)) +
  geom_point() +
  geom_function(fun = f) +
  scale_x_continuous(breaks=seq(0, 1, by=.10)) +
  scale_y_continuous(breaks=seq(-6, 10, by=2))
```

5.3 Evaluating Polynomial Models

We want to evaluate several polynomial models. For each tuning parameter (i.e., polynomial degree), we need to fit the model on the training data, make predictions on the test data, and score those predictions. Since we are going to repeat these steps for multiple tuning parameters, it's a good time to write a function!

```
#: Function to fit, predict, and evaluate a polynomial regression model
poly_eval <- function(deg, data_train, data_test){
  #: fit model with training data
  if(deg==0) m = lm(y~1, data=data_train) # intercept only model
  else m = lm(y~poly(x, degree=deg), data=data_train) # polynomial
  p = length(coef(m)) # number of parameters
  #: calculate training MSE
  mse_train = mean(m$residuals^2) # training MSE
  #: calculate test MSE
  yhat = predict(m, data_test) # predictions at test X's
  mse_test = mean((data_test$y - yhat)^2) # test MSE
  #: output a data frame of relevant info
  tibble(degree=deg, edf=p, mse_train, mse_test)
}
```

Let's try it out

```
poly_eval(deg = 2, data_train, data_test)
```

```
#> # A tibble: 1 x 4
#>   degree edf mse_train mse_test
#>   <dbl> <int>   <dbl>   <dbl>
#> 1     2     3     5.58     5.34
```

Looks good! Now we can iterate over a degree sequence.

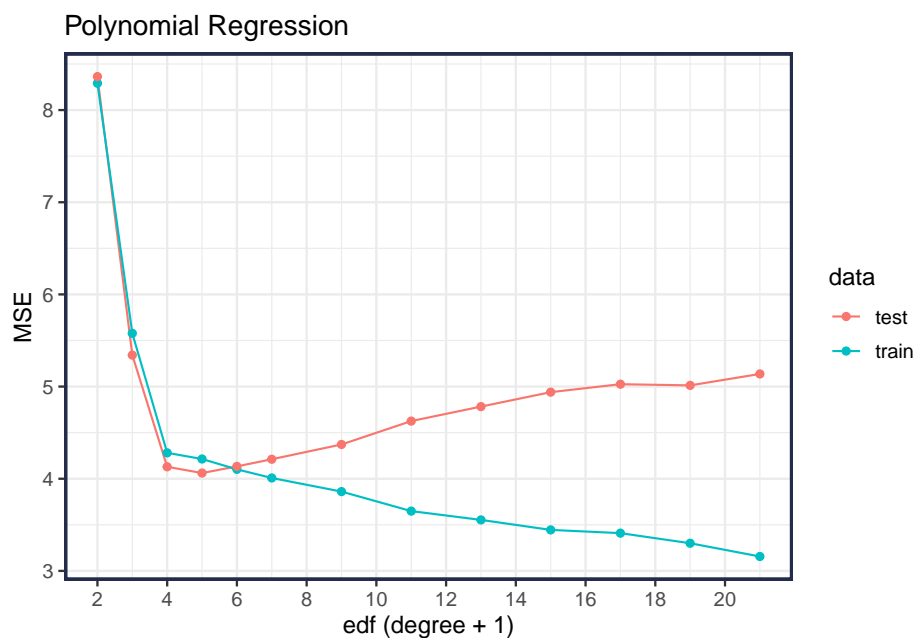
```
#: degree sequence
deg_seq = c(1:6, seq(8, 20, by=2)) # sequence of Degrees

# Using purrr::map_df()
perf_poly = map_df(deg_seq, ~poly_eval(., data_train=data_train, data_test=data_test))
```

```
# Using a loop
perf_poly = vector("list", length(deg_seq))
for(deg in deg_seq){
  tmp = poly_eval(deg, data_train=data_train, data_test=data_test)
  perf_poly = bind_rows(perf_poly, tmp)
}
```

Now for the plots

```
perf_poly %>%
  # make long:
  pivot_longer(starts_with("mse"), names_to="data", values_to="mse") %>%
  # remove 'mse_' from values:
  mutate(data = str_remove(data, "mse_")) %>%
  # plot:
  ggplot(aes(edf, mse, color=data)) + geom_line() + geom_point() +
  labs(title="Polynomial Regression", x = 'edf (degree + 1)', y="MSE") +
  scale_x_continuous(breaks=seq(2, 30, by=2))
```



```
#: base R plot alternative
with(perf_poly, plot(edf, mse_train, type='l', las=1))
with(perf_poly, lines(edf, mse_test, col=2))
```

And we can find the best polynomial degree for our test data

```
perf_poly %>% slice_min(mse_test)

#> # A tibble: 1 x 4
#>   degree   edf mse_train mse_test
#>   <dbl> <int>   <dbl>   <dbl>
#> 1     4     5     4.21     4.06
```

5.3.1 Tidymodels

We can repeat the process with tidymodels. The tidymodels approach has a nice helper function called `tune_grid()` that lets us fit and evaluate models in one function.

One small nuisance step. We have to create a `rset` object that contains the information about the training and testing sets. In the future we will use functions like `vfold_cv()` instead of the manual process we need to do now.

```
library(tidymodels)

# manually create an `rset` object
# Note: normally we would use initial_split() to make train/test split.
#       However since we are doing things a bit differently (i.e., we can
#       generate as much evaluation data as we want), we have to force things
#       a bit.
#       Long answer short: you probably won't have to do this step for any
#       real analysis.
splits = make_splits(data_train, data_test) %>%
  list %>%
  manual_rset("train/test")
```

Next we set up a *workflow* for polynomial regression with tunable degree. Notice it the `step_poly()` function that `degree = tune()` which indicates the degree needs to be specified.

```
poly_wf = workflow(
  preprocessor = recipe(y~x, data = data_train) %>%
    step_poly(x, degree = tune()), # note the tune() for degree
  spec = linear_reg()
)
```

Now we will use the `tune_grid()` function. All tunable parameters (i.e., those indicated by `tune()`) need to be supplied in the `grid =` argument. In this case, it is `degree`.

```
poly_tune = tune_grid(
  # specify workflow
  object = poly_wf,

  # specify the grid for all parameters that have tune().
  grid = expand_grid(degree = c(1:6, seq(8, 20, by=2))),

  # pass in the `rset` object
  resamples = splits,

  # specify the metrics to calculate. The package doesn't give use MSE,
  # so we'll use RMSE and later take the squared value.
  metrics = metric_set(rmse)
)
```

The output doesn't look very informative at this point.

```
poly_tune

#> # A tibble: 1 x 4
#>   splits          id      .metrics      .notes
#>   <list>         <chr>    <list>      <list>
#> 1 <split [100/50000]> train/test <tibble [13 x 5]> <tibble [0 x 3]>
```

Notice that we have a tibble with *list columns*. We can extract the relevant information using `collect_metrics()`.

```
poly_tune %>%
  collect_metrics(summarize = FALSE)

#> # A tibble: 13 x 6
#>   id      degree .metric .estimator .estimate .config
#>   <chr>    <dbl> <chr>    <chr>      <dbl> <chr>
#> 1 train/test      1 rmse     standard      2.89 Preprocessor01_Model1
#> 2 train/test      2 rmse     standard      2.31 Preprocessor02_Model1
#> 3 train/test      3 rmse     standard      2.03 Preprocessor03_Model1
#> 4 train/test      4 rmse     standard      2.02 Preprocessor04_Model1
#> 5 train/test      5 rmse     standard      2.03 Preprocessor05_Model1
#> 6 train/test      6 rmse     standard      2.05 Preprocessor06_Model1
#> # i 7 more rows
```

The relevant columns are degree and .estimate. But remember the function is returning RMSE, but we want our results in $MSE = RMSE^2$.

```
poly_tune %>%
  collect_metrics(summarize = FALSE) %>%
  mutate(
    mse = .estimate^2 # recall the estimate is RMSE
  ) %>%
  select(degree, mse)
```

```
#> # A tibble: 13 x 2
#>   degree  mse
#>   <dbl> <dbl>
#> 1     1  8.36
#> 2     2  5.34
#> 3     3  4.13
#> 4     4  4.06
#> 5     5  4.13
#> 6     6  4.21
#> # i 7 more rows
```

5.4 Evaluating k nearest neighbor models

Here is a function that fits a knn model on the training data for a particular k , makes predictions on the test data, and evaluates the MSE.

```
#: Function to evaluate kNN
knn_eval <- function(k, data_train, data_test){
  # fit model and eval on training data
  knn = knn.reg(data_train[, 'x', drop=FALSE],
                y = data_train$y,
                test = data_train[, 'x', drop=FALSE],
                k = k)
  r = data_train$y - knn$pred # residuals on training data
  mse_train = mean(r^2) # training MSE

  # fit model and eval on test data
  knn.test = knn.reg(data_train[, 'x', drop=FALSE],
                    y = data_train$y,
                    test = data_test[, 'x', drop=FALSE],
                    k = k)
  r.test = data_test$y - knn.test$pred # residuals on test data
  mse_test = mean(r.test^2) # test MSE
  # results
  edf = nrow(data_train)/k # effective dof (edof)
```

```
tibble(k=k, edf=edf, mse_train, mse_test)
}
```

Let's try it out

```
knn_eval(k = 10, data_train, data_test)
```

```
#> # A tibble: 1 x 4
#>       k    edf mse_train mse_test
#>   <dbl> <dbl>   <dbl>   <dbl>
#> 1     10     10     3.86     4.42
```

Set up a grid of neighborhood size (k).

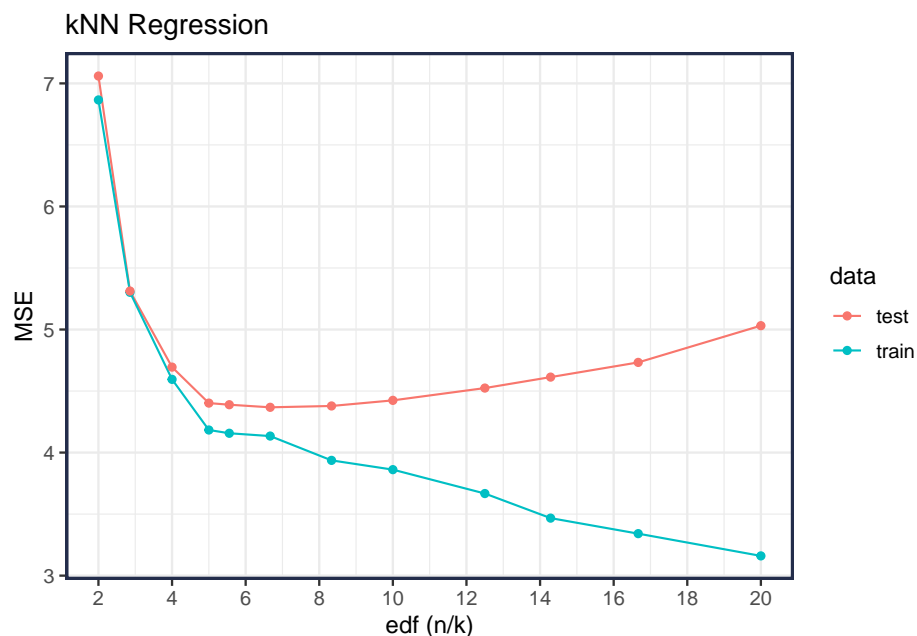
```
K = c(50, 35, 25, 20, 18, 15, 12, 10, 8, 7, 6, 5)
```

And let it run

```
# Using purrr::map_df()
perf_knn = map_df(K, knn_eval, data_train=data_train, data_test=data_test)

# Using a loop
perf_knn = tibble()
for(k in K){
  tmp = knn_eval(k, data_train=data_train, data_test=data_test)
  perf_knn = bind_rows(perf_knn, tmp)
}
```

```
#: Plot Results
perf_knn %>%
  # make long:
  pivot_longer(starts_with("mse"), names_to="data", values_to="mse") %>%
  # remove 'mse_' from values:
  mutate(data = str_remove(data, "mse_")) %>%
  # plot:
  ggplot(aes(edf, mse, color=data)) + geom_line() + geom_point() +
  labs(title="kNN Regression", x='edf (n/k)', y="MSE") +
  scale_x_continuous(breaks=seq(2, 30, by=2))
```



```
#- base R plot
with(perf_knn, plot(edf, mse_train, type='l', las=1))
with(perf_knn, lines(edf, mse_test, col=2))
grid()
```

And we can find the best neighborhood size for our test data

```
#: best knn
perf_knn %>% slice_min(mse_test)

#> # A tibble: 1 x 4
#>       k     edf mse_train mse_test
#>   <dbl> <dbl>   <dbl>   <dbl>
#> 1     15   6.67     4.13     4.37
```

5.4.1 Tidymodels

We can slightly modify the `tune_grid()` we used for polynomials.

First we will specify the knn workflow. In this workflow, the model specification has the tunable parameter `neighbors`.

```
knn_wf = workflow(
  preprocessor = recipe(y~x, data = data_train),
  spec = nearest_neighbor(neighbors = tune(), # tune this parameter
    mode = "regression", # regression / classification
    weight_func = "rect" # using unweighted knn
  )
)

knn_tune = tune_grid(
  #: specify model
  object = knn_wf,

  #: specify the grid for all parameters that have tune().
  grid = expand_grid(neighbors = c(50, 35, 25, 20, 18, 15, 12, 10, 8, 7, 6, 5)),

  #: pass in the 'rset' object
  resamples = splits,

  #: specify the metrics to calculate. The package doesn't give use MSE,
  # so we'll use RMSE and later take the squared value.
  metrics = metric_set(rmse)
)
```

The output doesn't look very informative at this point.

```
knn_tune

#> # A tibble: 1 x 4
#>   splits          id      .metrics      .notes
#>   <list>         <chr>    <list>    <list>
#> 1 <split [100/50000]> train/test <tibble [12 x 5]> <tibble [0 x 3]>
```

Notice that we have a tibble with *list columns*. We can extract the relevant information using `collect_metrics()`.

```
knn_tune %>%
  collect_metrics(summarize = FALSE)
```

```
#> # A tibble: 12 x 6
#>   id      neighbors .metric .estimator .estimate .config
#>   <chr>      <dbl> <chr>   <chr>      <dbl> <chr>
#> 1 train/test      5 rmse    standard    2.24 Preprocessor1_Model01
#> 2 train/test      6 rmse    standard    2.18 Preprocessor1_Model02
#> 3 train/test      7 rmse    standard    2.15 Preprocessor1_Model03
#> 4 train/test      8 rmse    standard    2.13 Preprocessor1_Model04
#> 5 train/test     10 rmse    standard    2.10 Preprocessor1_Model05
#> 6 train/test     12 rmse    standard    2.09 Preprocessor1_Model06
#> # i 6 more rows
```

Extract relevant columns and transform RMSE to MSE.

```
knn_tune %>%
  collect_metrics(summarize = FALSE) %>%
  mutate(
    mse = .estimate^2 # recall the estimate is RMSE
  ) %>%
  select(neighbors, mse)
```

```
#> # A tibble: 12 x 2
#>   neighbors  mse
#>   <dbl> <dbl>
#> 1      5  5.03
#> 2      6  4.73
#> 3      7  4.61
#> 4      8  4.52
#> 5     10  4.42
#> 6     12  4.38
#> # i 6 more rows
```

5.5 Comparison of best models

The optimal models (i.e., the model with optimal tuning parameters) have about the same edf.

```
(best_poly = perf_poly %>% slice_min(mse_test))
```

```
#> # A tibble: 1 x 4
#>   degree edf mse_train mse_test
#>   <dbl> <int>   <dbl>   <dbl>
#> 1      4      5    4.21    4.06
```

```
(best_knn = perf_knn %>% slice_min(mse_test))
```

```
#> # A tibble: 1 x 4
#>     k edf mse_train mse_test
#>   <dbl> <dbl>   <dbl>   <dbl>
#> 1    15  6.67    4.13    4.37
```

Let's see how the resulting predictions appear. We will re-fit each model on the training data and make predictions on a grid.

```
data_grid = tibble(x = seq(0, 1, length = 100))
```

```
#: optimal polynomial model
opt_poly = lm(y~poly(x, degree=best_poly$degree), data=data_train) # polynomial
yhat_poly = predict(opt_poly, data_grid) # predictions at test X's
```

```
#: optimal knn
opt_knn = FNN::knn.reg(select(data_train, x),
  y = data_train$y,
```

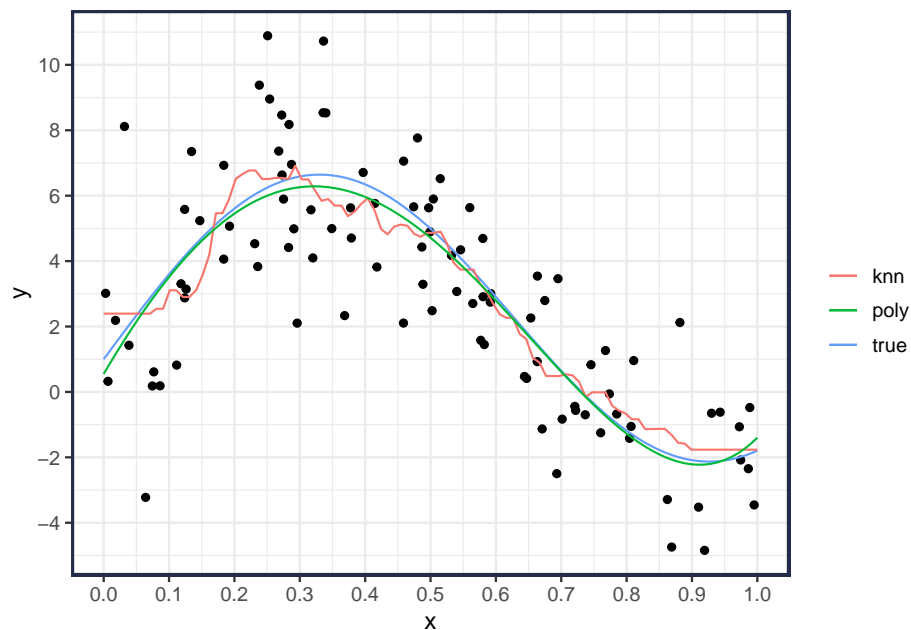
```

      k = best_knn$k,
      test = data_grid)
yhat_knn = opt_knn$pred

preds = data_grid %>%
  mutate(
    poly = yhat_poly,
    knn = yhat_knn
  ) %>%
  pivot_longer(cols = c(poly, knn), names_to = "model", values_to = ".pred")

ggplot(data_train, aes(x, y)) +
  geom_point() +
  geom_function(fun = f, aes(color = "true")) +
  geom_line(data = preds, aes(x = x, y = .pred, color = model)) +
  scale_x_continuous(breaks = seq(0, 1, by = .10)) +
  scale_y_continuous(breaks = seq(-6, 10, by = 2)) +
  labs(color = "")

```



5.5.1 Tidymodels

Use `show_best()` to see the best models.

```
show_best(poly_tune)
```

```

#> # A tibble: 5 x 7
#>   degree .metric .estimator mean      n std_err .config
#>   <dbl> <chr>    <chr>    <dbl> <int>   <dbl> <chr>
#> 1     4 rmse     standard  2.02     1    NA Preprocessor04_Model1
#> 2     3 rmse     standard  2.03     1    NA Preprocessor03_Model1
#> 3     5 rmse     standard  2.03     1    NA Preprocessor05_Model1
#> 4     6 rmse     standard  2.05     1    NA Preprocessor06_Model1
#> 5     8 rmse     standard  2.09     1    NA Preprocessor07_Model1

```

```
show_best(knn_tune)
```

```
#> # A tibble: 5 x 7
```



```
#>   neighbors .metric .estimator  mean      n std_err .config
#>      <dbl> <chr>   <chr>      <dbl> <int>   <dbl> <chr>
#> 1       15 rmse    standard    2.09     1      NA Preprocessor1_Model07
#> 2       12 rmse    standard    2.09     1      NA Preprocessor1_Model06
#> 3       18 rmse    standard    2.09     1      NA Preprocessor1_Model08
#> 4       20 rmse    standard    2.10     1      NA Preprocessor1_Model09
#> 5       10 rmse    standard    2.10     1      NA Preprocessor1_Model05
```

Use `finalize_workflow()` and `select_best()` to make the final models.

```
poly_wf %>%
  finalize_workflow(select_best(poly_tune)) %>%
  fit(data = data_train) %>%
  predict(data_grid)
```

```
#> # A tibble: 100 x 1
#>   .pred
#>   <dbl>
#> 1 0.549
#> 2 0.890
#> 3 1.22
#> 4 1.54
#> 5 1.86
#> 6 2.16
#> # i 94 more rows
```

```
knn_wf %>%
  finalize_workflow(select_best(knn_tune)) %>%
  fit(data = data_train) %>%
  predict(data_grid)
```

```
#> # A tibble: 100 x 1
#>   .pred
#>   <dbl>
#> 1  2.39
#> 2  2.39
#> 3  2.39
#> 4  2.39
#> 5  2.39
#> 6  2.39
#> # i 94 more rows
```