testingTrainingValidation

September 17, 2019

1 Training, testing, and validation

The sum squares error **SSE** is a measure of how well a proposed model fits training data. But a major goal of regression, and statistics, is not to fit training data. A regression model is meant to generalize and predict future unseen data points well.

Suppose we have training data X_{train} and the corresponding values of interest y_{train}. Combining X and y together will be denoted D_{train}.

Also assume we have a prediction model $f(X)$

Then the **Mean Squared Error** is defined as

$$\text{MSE}(D, f) = \frac{\sum_{i=1}^{N}[y_i - f(x_i)]^2}{N}$$

If the MSE is computed on training data D_{train} we call this the **training MSE**

Our goal is not to perform well on data we've already collected, but to perform well on data our model was not trained from. We aim to minimize our **test MSE**

$$\text{MSE}(D_{\text{test}}, f)$$

where D_{test} is a data set containing X and y values our model (f) has not trained from.

1.1 $\text{MSE}_{\text{train}} \neq \text{MSE}_{\text{test}}$

It may be reasonable to assume minimizing the training MSE should also minimize the test MSE, but this is typically not the case. Let's look at our data from Class03, the polynomial regression data.

[92]:
```
data <- read.csv('polynomialData.csv')
print(head(data))
```

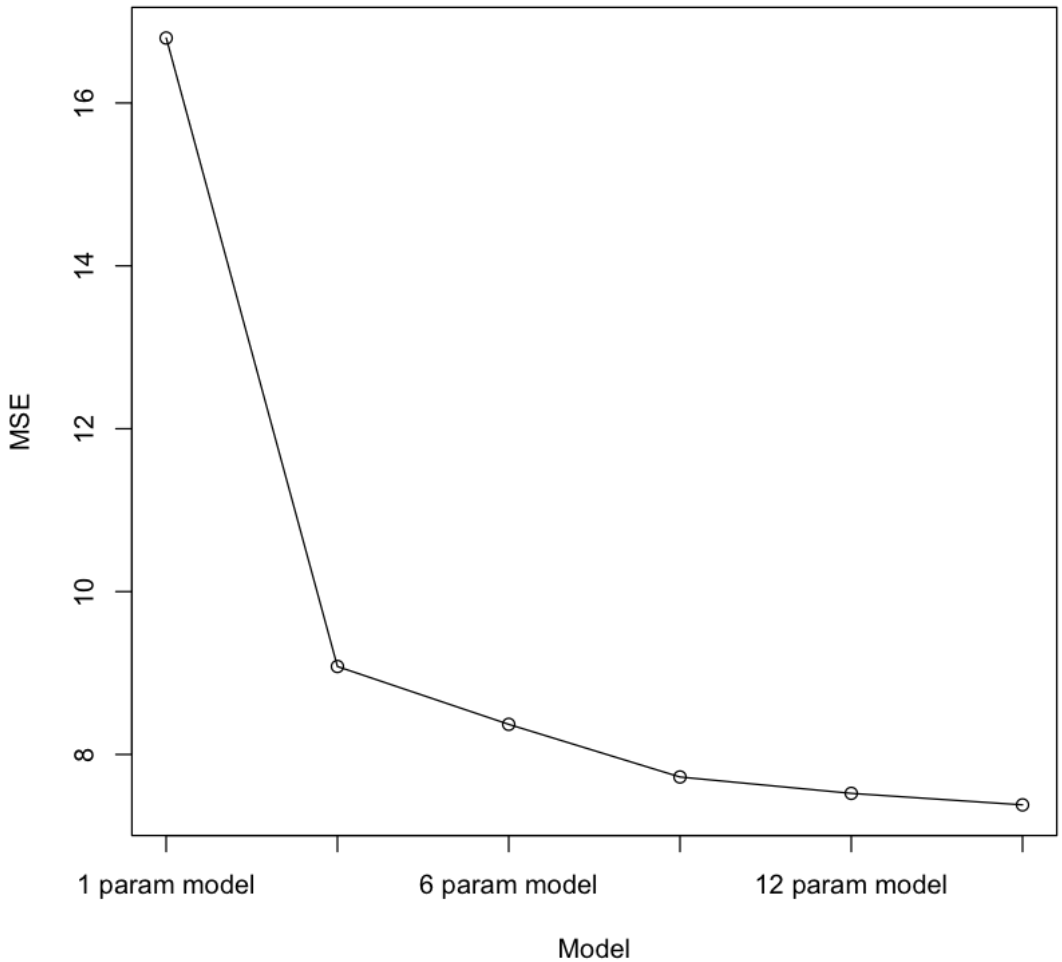
```
           x         y
1  0.9958723  8.2420054
2 -0.6556163  2.3114202
3 -0.9176787  4.0842076
```

```
4  0.1963727 -5.5386897
5  1.0309346  2.5166174
6  1.2610719 -0.5388713
```

We can lower our training MSE by fitting more and more complicated polynomials.

[93]:

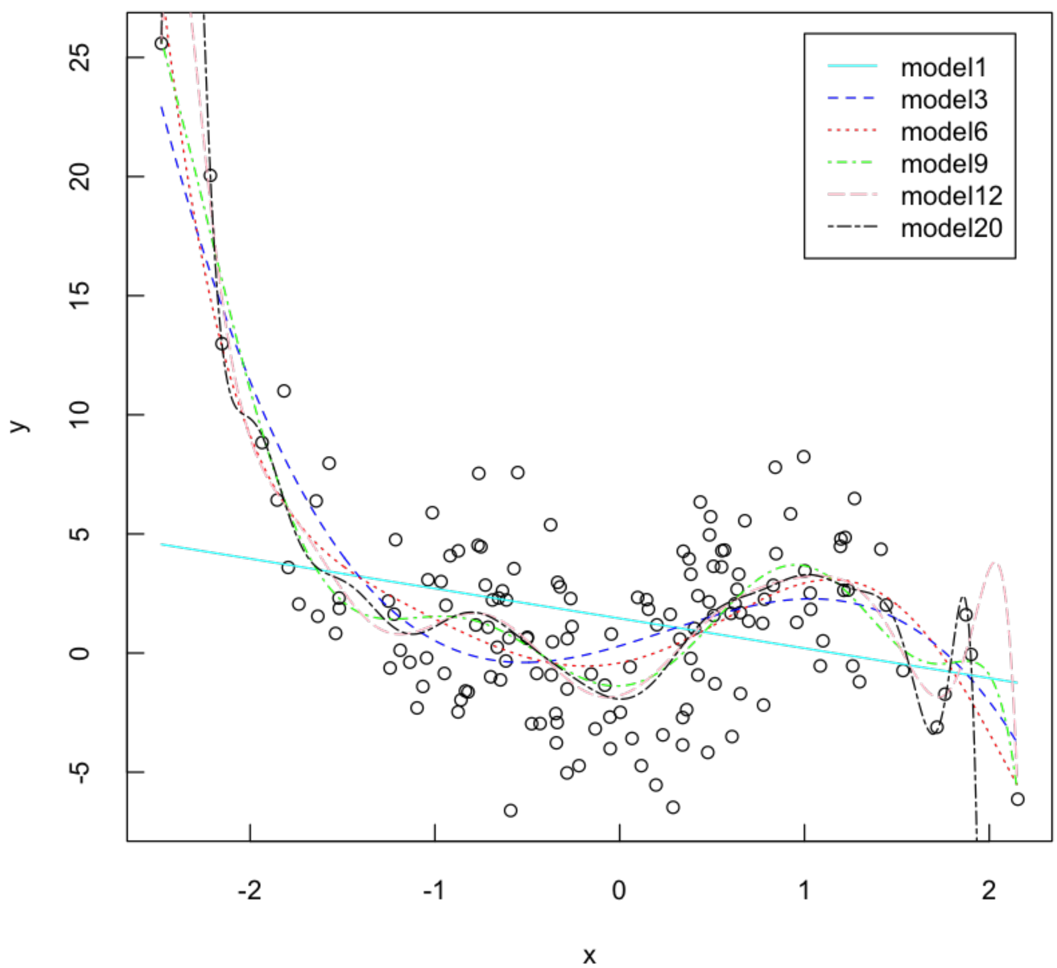
```
model1 <- lm(y~x,data=data)
model3 <- lm(y~x+I(x^2)+I(x^3),data=data)
model6 <- lm(y~x+I(x^2)+I(x^3)+I(x^4)+I(x^5)+I(x^6),data=data)
model9 <-␣
 ↪lm(y~x+I(x^2)+I(x^3)+I(x^4)+I(x^5)+I(x^6)+I(x^7)+I(x^8)+I(x^9),data=data)
model12 <-␣
 ↪lm(y~x+I(x^2)+I(x^3)+I(x^4)+I(x^5)+I(x^6)+I(x^7)+I(x^8)+I(x^9)+I(x^10)+I(x^11)+I(x^12),data=d
model20 <-␣
 ↪lm(y~x+I(x^2)+I(x^3)+I(x^4)+I(x^5)+I(x^6)+I(x^7)+I(x^8)+I(x^9)+I(x^10)+I(x^11)+I(x^12)
                 +I(x^13)+I(x^14)+I(x^15)+I(x^16)+I(x^17)+I(x^18)+I(x^19)+I(x^20)
              ,data=data)


MSE = function(model,data){
     N = nrow(data)
     return( sum((predict(model,data) - data$y)^2)/N )
}

fromString2Model = function(string){
    return(eval(parse(text=string)))
}

i<-1
MSEs <- rep(0,6)
for (model in c("model1","model3","model6","model9","model12","model20")){
    MSEs[i] <- MSE(fromString2Model(model),data)
    i=i+1
}

plot(MSEs,xlab="Model",ylab="MSE",xaxt = "n")
lines(MSEs)
axis(1, at=c(1,2,3,4,5,6)
     , labels=c("1 param model","3 param model","6 param model","9 param␣
 ↪model","12 param model","20 param model"))
```



This looks like a more complicated model, one with more parameters, should always be better. Lets look at the functions graphically.

[94]:
```
# plot data

plot(data$x,data$y
      ,xlab="x"
      ,ylab="y"
      ,tck=0.02
)

# plot model predictions
minX <- min(data$x)
```

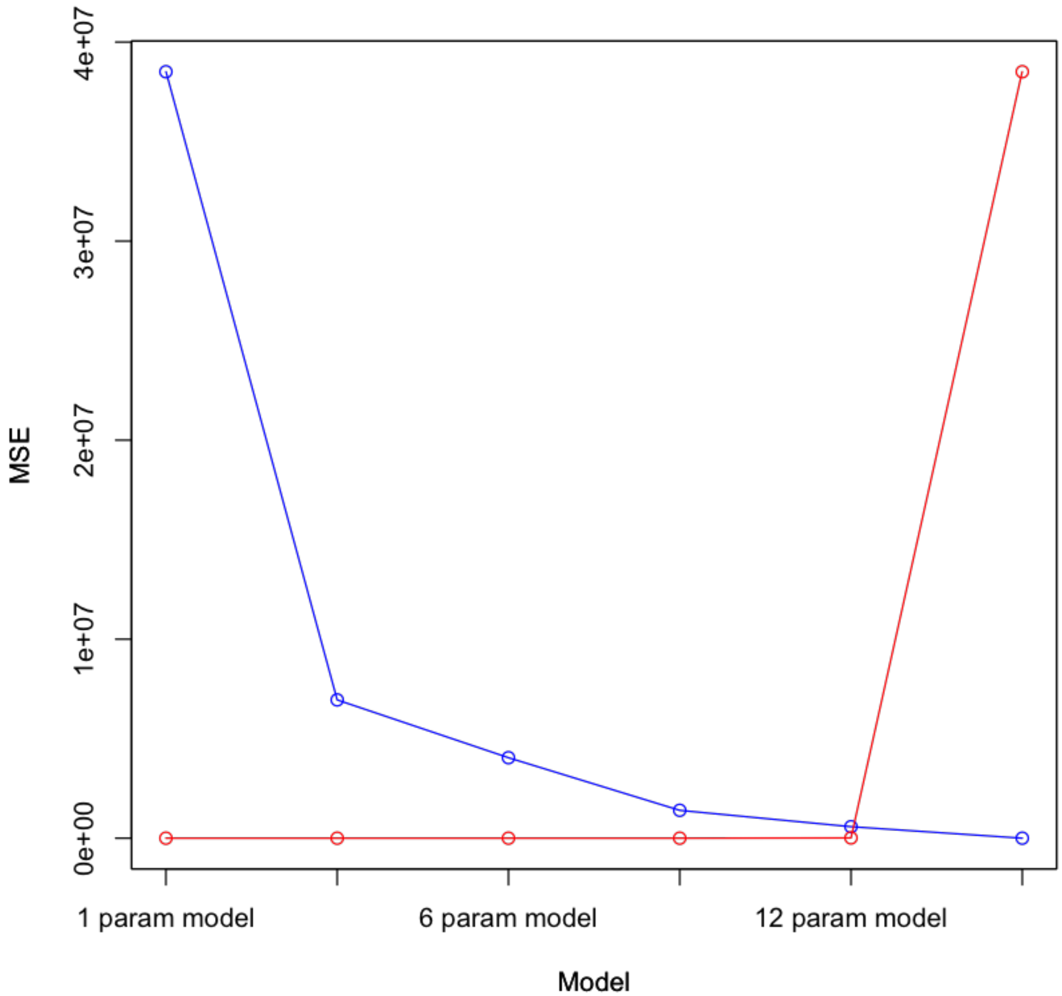
```r
maxX <- max(data$x)
newdata <- data.frame(x=seq(minX,maxX,0.01))

i<-1
colors = c('cyan','blue','red','green','pink','black')
for (model in c("model1","model3","model6","model9","model12","model20")){
    predictions <- predict(fromString2Model(model),newdata)
    lines(newdata$x,predictions,col=colors[i], lty=i)
    i<-i+1
}

legend(1,26,legend=c("model1","model3","model6","model9","model12","model20")
                     ,col=colors
                     ,lty=1:6
)
```



The more complicated models have smaller MSE, but also look like they may be learning the training data to well. We can evaluate the MSE on a set of test data the model hasn't trained on.

[106]:
```
testData <- read.csv('testData.csv')
print(head(data))

i<-1
tstMSEs <- rep(0,6)
for (model in c("model1","model3","model6","model9","model12","model20")){
    tstMSEs[i] <- MSE(fromString2Model(model),testData) # notice change here␣
 ↪from training to test data
    i=i+1
}
plot(MSEs,xlab="Model",ylab="MSE",xaxt = "n",yaxt = "n",col="blue")
lines(MSEs,xaxt = "n",col="blue")

par(new=TRUE)
plot(tstMSEs,xlab="Model",ylab="MSE",xaxt = "n",col="red")
lines(tstMSEs,col="red")

axis(1, at=c(1,2,3,4,5,6)
     , labels=c("1 param model","3 param model","6 param model","9 param␣
 ↪model","12 param model","20 param model"))

#legend()
```

```
           x          y
1  0.9958723  8.2420054
2 -0.6556163  2.3114202
3 -0.9176787  4.0842076
4  0.1963727 -5.5386897
5  1.0309346  2.5166174
6  1.2610719 -0.5388713
```



Though the training error gets better with more model complexity, the more complicated the model the higher the test mse. More complicated models **overfit** the training data. instead of learning to generalize, the model learns fluctuations in the training data.

1.2 Bias-variance tradeoff

More complicated models tend to not only learn the true function f, our signal, but the noise too. On the other hand, simpler models may not learn the true function f, but the model is less likely to change if fit to a different set of training data. The trade off between choosing a complicated, but not too complicated model is called the Bias-Variance trade off. A model with low bias is closer to the true f. A model with low variance will not drastically change if fitted to different training data.

Assume we have a response variable y we're interesting in understanding as a function of x. Further assume that y has the following form $y = f(x) + \epsilon$, where $f(x)$ is the **true** function. Then we can write our MSE as

$$\begin{aligned}
\text{MSE} &= E_{XY}[y - \hat{f}(x)]^2 && (1)\\
&= E[f(x) + \epsilon - \hat{f}(x)]^2 && (2)\\
&= E[f(x) - E(\hat{f}) + E(\hat{f}) - \hat{f}(x) + \epsilon]^2 && (3)\\
&= [f(x) - E(\hat{f})]^2 + E[E\hat{f} - \hat{f}(x)]^2 + \epsilon^2 && (4)\\
&= \text{Bias}^2 + \text{Variance} + \text{Error} && (5)
\end{aligned}$$

Our expectation is over the probability of (X,y) pairs, our training data. Intuitively, you can imagine this expectation as the average over all possible training data sets we could have received.

Bias

The bias measures how far our predicted function $\hat{f}$ is from the true function f.

Variance

The variance measures how much our predicted model changes for changes in our training set.

ϵ^2

This an irreducible error made by assumptions about the form of the problem, a quantity we cannot change.

1.3 Cross-Validation

In a best-case scenario you can fit a model to a set of training data and collect additional data for testing. Your model can be fit to training data, used to predict your target variable (y) on the testing set, and those predictions $(\hat{y})$ can be compared to the truth (y).

Because of financial limitations, time burden, and other constraints, statistical modelers are typically unable to collect additional testing data. Instead resort to splitting our data set into training and testing. Our model can learn from the training dataset and test predictions on the test dataset.

Hold-out A straight-forward method is to split our data into a single training **Tr** and testing **Tst** dataset. The model is trained on **Tr** and tested on **Tst**. But splitting our data into a single training/testing dataset may bias our model. We want to assess the model fit independent of how we split our data into training and testing.

K-fold Cross-validation splits the all the data into K distinct sets at random. The total dataset (D) is then a union of K data pieces (P_k)

$$D = \cup_{i=1}^{K} P_k$$

From $i = 1$ to K, remove the ith dataset P_i from the total dataset D. Train the model on $D - P_i$, compute test statistics of the model on P_i, and store those test statistics in a list L. Summary statistics can be computed from L.

For example, we can compute the MSE on every train/test split and append all the MSEs to L. A common summary statistics, called the cv_{error} is the average MSE over all train/test splits.

[25]:
```
data <- read.csv('polynomialData.csv')

#split into K  random pieces
K=10

dataPieces = split(data[sample(nrow(data)),],1:10)

sapply(dataPieces
       ,function(P){
           traiingData <- data[ -  ]

           model <- lm(y~x,data=data)
           MSE = function(model,data){
             N = nrow(data)
             return( sum((predict(model,data) - data$y)^2)/N )
            }

            return(MSE())



       })
```

$'1' NULL

$'2' NULL

$'3' NULL

$'4' NULL

$'5' NULL

$'6' NULL

$'7' NULL

$'8' NULL

$'9' NULL

$'10' NULL

[28]:
```
data[ -row.names(dataPieces[[1]]) ]
```

```
    Error in -row.names(dataPieces[[1]]): invalid argument to unary operator
Traceback:
```

1. `data[-row.names(dataPieces[[1]])]`
2. `` `[.data.frame`(data, -row.names(dataPieces[[1]])) ``

[ ]:

```
```

[ ]:

```
```