Comparison over Multiple Samples

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<pre># This function calculates the average sum of squares # for prediction error, i.e. mean((y-yhat)^2) ave_y_mu_sq <- function(sample, predfun, na.rm = TRUE){ mean((sample\$y - predfun(sample\$x))^2, na.rm = na.rm) }</pre>	
<pre># Given two prediction functions predfun1 and predfun2, #this function calculates the mean of the difference squared ave_mu_mu_sq <- function(predfun1, predfun2, x, na.rm = TRUE){ mean((predfun1(x) - predfun2(x))^2, na.rm = na.rm) }</pre>	
<pre>### The function getSampleComp will return a logical vector ### (that way the complement is also recorded in the sample) getSampleComp <- function(pop, size, replace=FALSE) { N <- popSize(pop) samp <- rep(FALSE, N) samp[sample(1:N, size, replace = replace)] <- TRUE samp</pre>	

```
### This function will return a data frame containing
### only two variates, an x and a y
getXYSample <- function(xvarname, yvarname, samp, pop) {</pre>
  sampData <- pop[samp, c(xvarname, yvarname)]</pre>
  names(sampData) <- c("x", "y")</pre>
  sampData
}
popSize <- function(pop) {nrow(as.data.frame(pop))}</pre>
sampSize <- function(samp) {popSize(samp)}</pre>
age.unique = unique(Loblolly$age)
getmuFun <- function(pop, xvarname, yvarname){</pre>
  ## First remove NAs
  pop <- na.omit(pop[, c(xvarname, yvarname)])</pre>
  x <- pop[, xvarname]
  y <- pop[, yvarname]
  xks <- unique(x)
  muVals <- sapply(xks,
                    FUN = function(xk) {
                      mean(y[x==xk])
  ## Put the values in the order of xks
  ord <- order(xks)
  xks <- xks[ord]
  xkRange <-xks[c(1,length(xks))]</pre>
  minxk <- min(xkRange)</pre>
  maxxk <- max(xkRange)</pre>
  ## mu values
  muVals <- muVals[ord]</pre>
  muRange <- muVals[c(1, length(muVals))]</pre>
  muFun <- function(xVals){</pre>
    ## vector of predictions
    \#\# same size as xVals and NA in same locations
    predictions <- xVals
    ## Take care of NAs
    xValsLocs <- !is.na(xVals)
    ## Just predict non-NA xVals
    predictions[xValsLocs] <- sapply(xVals[xValsLocs],</pre>
                                FUN = function(xVal) {
                                    if (xVal < minxk) {</pre>
                                        result <- muRange[1]
                                    } else if (xVal > maxxk) {
                                        result <- muRange[2]
                                    } else if ( any(xVal == xks) ) {
                                      result <- muVals[xks == xVal]
```

```
} else {
                                         xlower <- max(c(minxk, xks[xks < xVal]))</pre>
                                         xhigher <- min(c(maxxk, xks[xks >= xVal]))
                                         mulower <- muVals[xks == xlower]</pre>
                                         muhigher <- muVals[xks == xhigher]</pre>
                                         interpolateFn <- approxfun(x=c(xlower, xhigher),</pre>
                                                                       y=c(mulower, muhigher))
                                         result <- interpolateFn(xVal)</pre>
                                     }
                                         result
                                         }
    ## Now return the predictions (including NAs)
    predictions
  }
  muFun
}
```

Note we are using the getmuhat function that does extrapolation using a constant.

```
getmuhat <- function(sampleXY, complexity = 1) {</pre>
  formula <- paste0("y ~ ",</pre>
                     if (complexity==0) {
                       "1"
                      } else
                      pasteO("poly(x, ", complexity, ", raw = FALSE)")
                       #pasteO("bs(x, ", complexity, ")")
  )
  fit <- lm(as.formula(formula), data = sampleXY)</pre>
  tx = sampleXY$x
  ty = fit$fitted.values
 range.X = range(tx)
  val.rY = c( mean(ty[tx == range.X[1]]),
               mean(ty[tx == range.X[2]]) )
  ## From this we construct the predictor function
  muhat <- function(x){</pre>
    if ("x" %in% names(x)) {
      ## x is a dataframe containing the variate named
      ## by xvarname
      newdata <- x
    } else
      ## x is a vector of values that needs to be a data.frame
    { newdata <- data.frame(x = x) }
    ## The prediction
    ##
    val = predict(fit, newdata = newdata)
    val[newdata$x < range.X[1]] = val.rY[1]</pre>
    val[newdata$x > range.X[2]] = val.rY[2]
    val
  ## muhat is the function that we need to calculate values
```

```
## at any x, so we return this function from getmuhat
muhat
}
```

5.3 Comparison Over Multiple Samples

• The inaccuracy of a predictor is measured by

$$APSE(\mathcal{P}, \widehat{\mu}_{\mathcal{S}}) = Ave_{u \in \mathcal{P}} (y_u - \widehat{\mu}_{\mathcal{S}}(\mathbf{x}_u))^2.$$

- where \mathcal{S} is the sample we used to fit the function, and
- $-\mathcal{T} := \mathcal{P} \mathcal{S}$ is the complement set of \mathcal{S} such that the population $\mathcal{P} = \{\mathcal{S}, \mathcal{T}\}$
- The function $\widehat{\mu}_{\mathcal{S}}(\mathbf{x})$ is based on a single sample \mathcal{S} and
 - its performance might be peculiar to the particular choice of sample.
 - the average prediction error might be very different from one sample to another sample (changing S).
 - It is important then to choose a predictor function that performs well no matter which sample was used to construct the predictor.
- Suppose that we have many samples, say $N_{\mathcal{S}}$ samples \mathcal{S}_j for $j = 1, \dots, N_{\mathcal{S}}$.
 - For each sample, we can calculate $\widehat{\mu}_{\mathcal{S}_i}(\mathbf{x})$ and

$$APSE(\mathcal{P}, \widehat{\mu}_{\mathcal{S}_i})$$

• The average APSE over all N_S samples should be a better measure of the quality of a predictor function.

$$\begin{split} APSE(\mathcal{P}, \widehat{\mu}) &= Ave_{j=1,\dots,N_{\mathcal{S}}} \ APSE(\mathcal{P}, \widehat{\mu}_{\mathcal{S}_{j}}) \\ &= \frac{1}{N_{\mathcal{S}}} \sum_{j=1}^{N_{\mathcal{S}}} \ APSE(\mathcal{P}, \widehat{\mu}_{\mathcal{S}_{j}}) \\ &= \frac{1}{N_{\mathcal{S}}} \sum_{j=1}^{N_{\mathcal{S}}} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_{i} - \widehat{\mu}_{\mathcal{S}_{j}}(\mathbf{x}_{i}))^{2}. \end{split}$$

• Note that in $APSE(\mathcal{P}, \widetilde{\mu})$, the **estimator** notation $\widetilde{\mu}$ is used to emphasize that the function is looking at the values of $\widehat{\mu}$ for all possible samples \mathcal{S}_{j} .

Notation

• It can be shown that the average predicted squared error, APSE, for the estimator $\widetilde{\mu}(\mathbf{x})$ is composed of three separate and interpretable pieces.

- But two bits of notation are needed before we discuss this decomposition.
- 1. We observe that $\mu(\mathbf{x})$ denotes a **conditional** average of y given \mathbf{x} , defined as the average of all y values in \mathcal{P} that share that value of \mathbf{x} . In other words, $\mu(\mathbf{x}) = E(Y|X = \mathbf{x})$.
 - Suppose that there are K different values of \mathbf{x} in the population \mathcal{P} so that \mathcal{P} can be partitioned according to the different values of k as

$$\mathcal{P} = \bigcup_{k=1}^{K} \mathcal{A}_k$$

where

$$\mathcal{A}_k = \{ u : u \in \mathcal{P}, \ \mathbf{x}_u = \mathbf{x}_k \}$$

and the unique values of \mathbf{x} are $\mathbf{x}_1, \dots, \mathbf{x}_K$

- (Note that $A_1 \dots A_K$ partition \mathcal{P} since $A_k \cap A_j = \emptyset$ for all $k \neq j$.)
- The conditional average $\mu(\mathbf{x})$ can now be expressed for each distinct x_k as

$$\mu(\mathbf{x}_k) = Ave_{i \in \mathcal{A}_k} \ y_i.$$

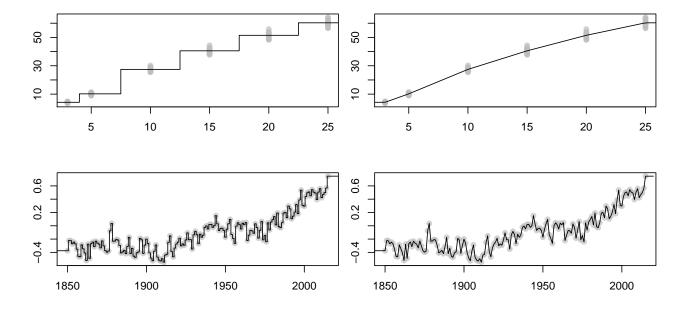
2. Let $\overline{\widehat{\mu}}(\mathbf{x})$ denote the average of the estimated predictor function over all samples

$$\overline{\widehat{\mu}}(\mathbf{x}) = \frac{1}{N_{\mathcal{S}}} \sum_{j=1}^{N_{\mathcal{S}}} \widehat{\mu}_{\mathcal{S}_j}(\mathbf{x}).$$

Example

- Growth of Loblolly pine trees and temperature data
 - This is conditional average of y given ${\bf x}$

$$\mu(\mathbf{x}_k) = Ave_{i \in \mathcal{A}_k} \ y_i. \text{ where } \mathcal{A}_k = \{u : u \in \mathcal{P}, \ \mathbf{x}_u = \mathbf{x}_k\}$$



5.4 Decomposing the $APSE(\mathcal{P}, \tilde{\mu})$

- As mentioned above, $APSE(\mathcal{P}, \widetilde{\mu})$ can be decomposed into three meaningful terms.
 - this is from the structure of the estimator $\widetilde{\mu}$ point of view.

$$\begin{split} &APSE(\mathcal{P}, \widehat{\mu}) \\ &= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \widehat{\mu}_{\mathcal{S}_j}(\mathbf{x}_i))^2 \\ &= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 \\ &= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 \\ &= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 \\ &= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 \\ &= \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 \\ &= \sum_{k=1}^{K} \frac{n_k}{N} \sum_{i \in \mathcal{A}_k} \frac{1}{n_k} (y_i - \mu(\mathbf{x}_k))^2 \\ &= \sum_{k=1}^{K} \frac{n_k}{N} \sum_{i \in \mathcal{A}_k} \frac{1}{n_k} (y_i - \mu(\mathbf{x}_k))^2 \\ &= Ave_{\mathbf{x}} (Var(Y|\mathbf{x})) \end{split} + \sum_{k=1}^{K} \frac{n_k}{N} \sum_{j=1}^{N_S} \frac{1}{N_S} (\widehat{\mu}_{\mathcal{S}_j}(\mathbf{x}_k) - \widehat{\mu}(\mathbf{x}_k))^2 \\ &+ Var(\widehat{\mu}) \end{split} + Var(\widehat{\mu}) \end{split} + Bias^2(\widehat{\mu}).$$

- Each term is an average over all x values and over all samples.
 - The first term is the average of the conditional variance of the response y,
 - the second term is the average of the variance of the estimator and
 - the last is term the squared bias.
- Note: The second last line accounts for units in the population with the same \mathbf{x} values. There are K unique values of \mathbf{x} in the population.

Another Decomposition of the APSE

• $APSE(\mathcal{P}, \widetilde{\mu})$ can be decomposed from the population's structure point of view as well.

$$APSE(\mathcal{P}, \widetilde{\mu})$$

$$= \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (y_i - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\widehat{\mu}_{\mathcal{S}_j}(\mathbf{x}_i) - \overline{\widehat{\mu}}(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{j=1}^{N_S} \frac{1}{N} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{i \in \mathcal{P}} (\overline{\widehat{\mu}}(\mathbf{x}_i) - \mu(\mathbf{x}_i))^2 + \frac{1}{N_S} \sum_{i \in \mathcal{P}} (\overline{\mu}(\mathbf{x}_i) - \mu(\mathbf{x}_i) - \mu(\mathbf{x}_i) - \mu(\mathbf{x}_i) - \mu(\mathbf{x}_i) - \mu(\mathbf{x}_i) - \mu(\mathbf{x}_i)$$

• We might write

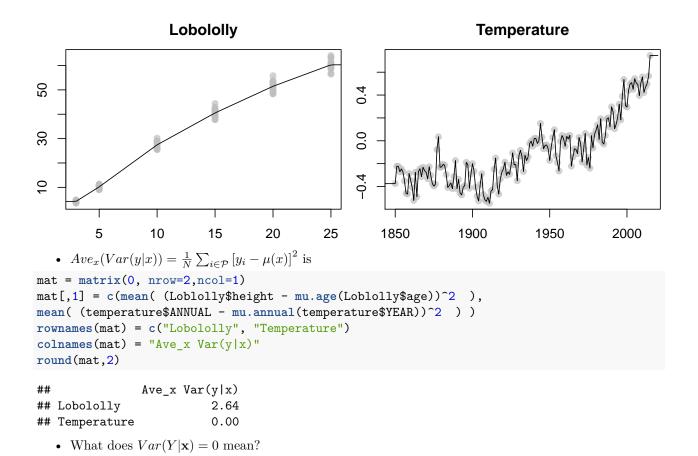
$$APSE(\mathcal{P}, \widetilde{\mu}) = \left(\frac{n}{N}\right) \left\{\widehat{APSE}(\mathcal{P}, \widetilde{\mu}) \text{ based on the same samples used by } \widehat{\mu}\right\} \\ + \left(1 - \frac{n}{N}\right) \left\{\widehat{APSE}(\mathcal{P}, \widetilde{\mu}) \text{ based on samples not used by } \widehat{\mu}\right\}$$

- If $n \ll N$, then the second term dominates.
 - Sometimes, even if $n \approx N$ we might also want to focus our evaluation only on the second term since this evaluation is based on values not used in the actual estimation process.

Example of $\mu(x)$

- Growth of Loblolly pine trees and temperature data
 - One difference between the two data-sets is that in the Loblolly data, we have multiple y measurements for any given \mathbf{x} .
 - This facilitates computation of **conditional** average of $Var(Y|\mathbf{x})$.

$$\mu(\mathbf{x}_k) = Ave_{i \in \mathcal{A}_k} \ y_i.$$
 where $\mathcal{A}_k = \{u : u \in \mathcal{P}, \ \mathbf{x}_u = \mathbf{x}_k\}$



One sample (S) and the complement set (T)

- Consider the global temperature data.
- Generate one sample of size n=25 and its complement set.

```
xnam <- "YEAR"
ynam <- "ANNUAL"
pop <- temperature
n <- 25

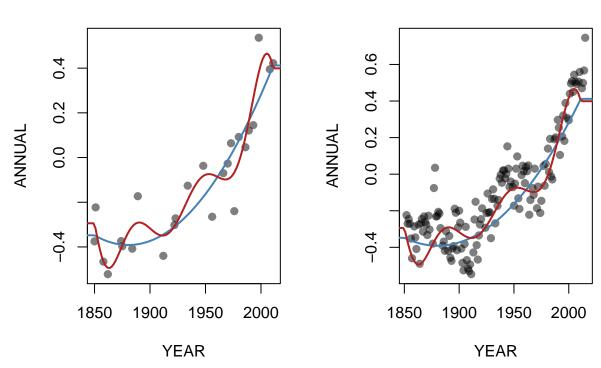
set.seed(341) # for reproducibility
samp <- getSampleComp(pop, n)
Ssamp <- getXYSample(xnam, ynam, samp, pop)
Tsamp <- getXYSample(xnam, ynam, !samp, pop)
muhat2 <- getmuhat(Ssamp, 2)
muhat9 <- getmuhat(Ssamp, 9)

xlim <- extendrange(pop[, xnam])
par(mfrow=c(1,2))</pre>
```

```
plot(Ssamp,
     main=paste0("muhat (p=2,9) on S"),
     xlab = xnam, ylab = ynam,
     pch=19, col= adjustcolor("black", 0.5))
curve(muhat2, from = xlim[1], to = xlim[2],
      add = TRUE, col="steelblue", lwd=2)
curve(muhat9, from = xlim[1], to = xlim[2],
      add = TRUE, col="firebrick", lwd=2)
plot(Tsamp,
     main=paste0("muhat (p=2,9) on T"),
     xlab = xnam, ylab = ynam,
     pch=19, col= adjustcolor("black", 0.5))
curve(muhat2, from = xlim[1], to = xlim[2],
      add = TRUE, col="steelblue", lwd=2)
curve(muhat9, from = xlim[1], to = xlim[2],
      add = TRUE, col="firebrick", lwd=2)
```

muhat (p=2,9) on S

muhat (p=2,9) on T



Nine samples and complements

• Set some variables and generate $N_{\mathcal{S}}=9$ samples of size n=25

```
xnam <- "YEAR"</pre>
ynam <- "ANNUAL"</pre>
pop <- temperature
    <- 25
N_S <- 9
set.seed(1) # for reproducibility
samples <- lapply(1:N_S, FUN= function(i){getSampleComp(pop, n)})</pre>
         <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, Si, pop)})</pre>
         <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, !Si, pop)})</pre>
Tsam
   • The function to construct \overline{\mu}(x)
getmubar <- function(muhats) {</pre>
  function(x) {
    Ans <- sapply(muhats, FUN=function(muhat){muhat(x)})</pre>
    apply(Ans, MARGIN=1, FUN=mean)
  }
}
   • Fit polynomials of degree 2 and 9 on all samples and get the average function.
muhats2 <- lapply(Ssam, getmuhat, complexity = 2)</pre>
```

The fitted polynomials on S

mubar2 <- getmubar(muhats2)</pre>

mubar9 <- getmubar(muhats10)</pre>

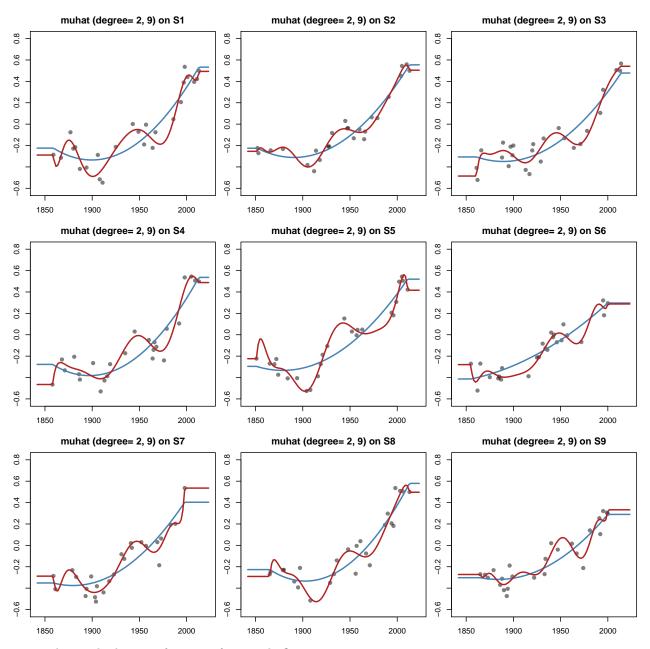
muhats9 <- lapply(Ssam, getmuhat, complexity = 10)</pre>

```
par(mfrow=c(3,3), mar=2.5*c(1,1,1,0.1))

xlim <- extendrange(temperature[, xnam])
ylim <- extendrange(temperature[, ynam])

for (i in 1:N_S) {
    plot(Ssam[[i]],
        main=paste("muhat (degree= 2, 9) on S", i, sep=""),
        xlab = xnam, ylab = ynam,
        pch=19, col= adjustcolor("black", 0.5), ylim=ylim, xlim=xlim)

    tempfn = muhats2[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="steelblue", lwd=2)
    tempfn = muhats9[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="firebrick", lwd=2)
}</pre>
```



• The residuals sum of squares from each S_i

```
Smat = matrix(0, nrow=2,ncol= N_S+1 )

for (j in 1:N_S) {
    tempfn = muhats2[[j]]
    Smat[1,j] = mean( (Ssam[[j]]$y - tempfn(Ssam[[j]]$x))^2 )

    tempfn = muhats9[[j]]
    Smat[2,j] = mean( (Ssam[[j]]$y - tempfn(Ssam[[j]]$x))^2 )
}

rownames(Smat) = c("Degree = 2", "Degree = 9")
colnames(Smat) = c(paste("S", 1:N_S, sep=""), "Avg.")
Smat[,N_S+1] = apply(Smat[,1:N_S],1,mean)
```

```
round(Smat,3)

## S1 S2 S3 S4 S5 S6 S7 S8 S9 Avg.
## Degree = 2 0.015 0.007 0.014 0.016 0.013 0.007 0.013 0.011 0.009 0.012
## Degree = 9 0.005 0.002 0.006 0.006 0.002 0.003 0.003 0.007 0.005 0.004
```

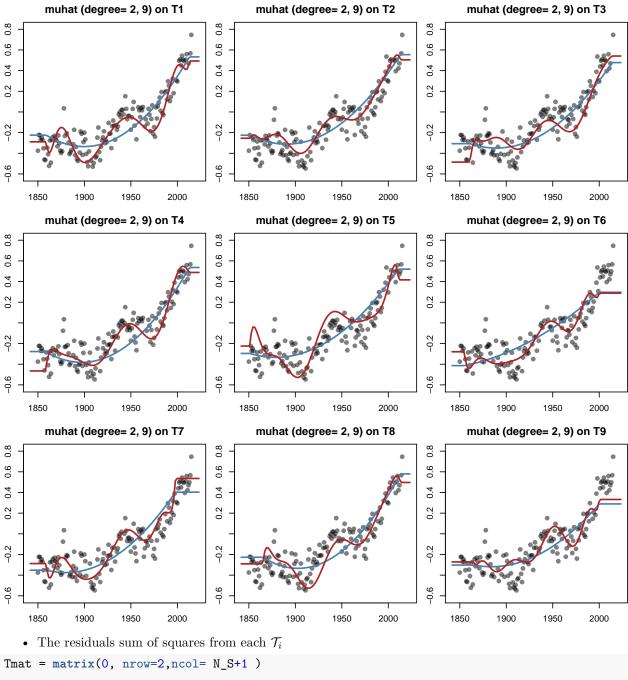
Fitted polynomials on \mathcal{T}

```
par(mfrow=c(3,3), mar=2.5*c(1,1,1,0.1))

dset = c(2,4,10)
xlim <- extendrange(temperature[, xnam])
ylim <- extendrange(temperature[, ynam])

for (i in 1:N_S) {
    plot(Tsam[[i]],
        main=paste("muhat (degree= 2, 9) on T", i, sep=""),
        xlab = xnam, ylab = ynam,
        pch=19, col= adjustcolor("black", 0.5), ylim=ylim, xlim=xlim)

tempfn = muhats2[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="steelblue", lwd=2)
    tempfn = muhats9[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="firebrick", lwd=2)
}</pre>
```



```
Tmat = matrix(0, nrow=2,ncol= N_S+1 )

for (j in 1:N_S) {
    tempfn = muhats2[[j]]
    Tmat[1,j] = mean( (Tsam[[j]]$y - tempfn(Tsam[[j]]$x))^2 )

    tempfn = muhats9[[j]]
    Tmat[2,j] = mean( (Tsam[[j]]$y - tempfn(Tsam[[j]]$x))^2 )
}

rownames(Tmat) = c("Degree = 2", "Degree = 9")
colnames(Tmat) = c(paste("T", 1:N_S, sep=""), "Avg.")
Tmat[,N_S+1] = apply(Tmat[,1:N_S],1,mean)
```

round(Tmat,3) ## T1 T2 T3 T4 T5 T6 T7 T8 T9 Avg. ## Degree = 2 0.016 0.017 0.016 0.017 0.016 0.023 0.019 0.018 0.020 0.018 ## Degree = 9 0.014 0.013 0.016 0.013 0.025 0.019 0.013 0.017 0.018 0.016

• Comparing this slide with the previous one what do you learn?

Sampling Variability

• Let us compare the fits across the 9 samples from above.

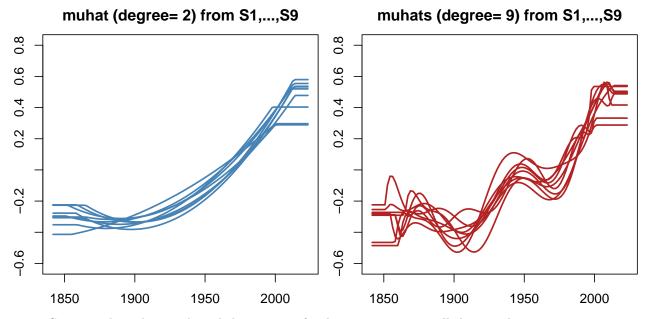
```
par(mfrow=c(1,2), mar=2.5*c(1,1,1,0.1))

plot(Ssam[[i]], main="muhat (degree= 2) from S1,...,S9", xlab = xnam,
        ylab = ynam, pch=19, col=0, ylim=ylim, xlim=xlim)

for (i in 1:N_S) {
    tempfn = muhats2[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="steelblue", lwd=2)
}

plot(Ssam[[i]], main="muhats (degree= 9) from S1,...,S9", xlab = xnam,
        ylab = ynam, pch=19, col=0, ylim=ylim, xlim=xlim)

for (i in 1:N_S) {
    tempfn = muhats9[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="firebrick", lwd=2)
}
```

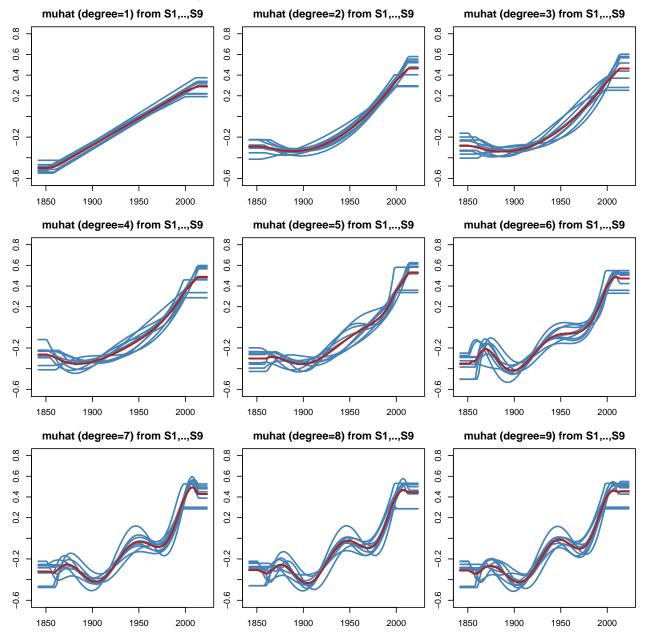


• Generate the polynomials and the averages for degrees 1 to 9 over all the samples.

```
cset = 1:9
muhats <- Map( function(i) {lapply(Ssam, getmuhat, complexity = i)}, cset)</pre>
mubars <- Map( function(muhati) { getmubar(muhati) } , muhats)</pre>
```

- The average function is different from the function fitted on the whole population.

 - Blue lines are $\widehat{\mu}_{\mathcal{S}_i}(x)$ for $i=1,\ldots,N_{\mathcal{S}}$ Red line is $\overline{\widehat{\mu}}(x) = \frac{1}{N_{\mathcal{S}}} \sum_{i=1}^{N_{\mathcal{S}}} \widehat{\mu}_{\mathcal{S}_i}(x)$

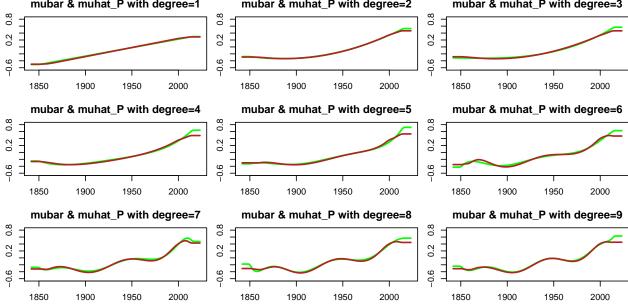


• What do you observe in these plots?

Aside

- The average function is different from the function fitted on the whole population.
- For the same degree, each plot shows a
 - Red line, representing the average fitted function $\overline{\widehat{\mu}}(x) = \frac{1}{N_S} \sum_{i=1}^{N_S} \widehat{\mu}_{S_i}(x)$ and Green line, representing the fitted function using the population denoted by $\widehat{\mu}_{\mathcal{P}}(x)$.

```
par(mfrow=c(3,3), mar=2.5*c(1,1,1,0.1))
for (i in 1:length(cset) ) {
   plot(Ssam[[i]], main=paste0("mubar & muhat_P with degree=", cset[i],""),
        xlab = xnam, ylab = ynam, pch=19, col=0, ylim=ylim, xlim=xlim)
   tempfn = getmuhat(getXYSample(xnam, ynam, rep(TRUE, 166), pop), complexity = cset[i])
   curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="green", lwd=2)
   tempfn = mubars[[i]]
   curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="firebrick", lwd=2)
}
   mubar & muhat_P with degree=1
                                   mubar & muhat_P with degree=2
                                                                   mubar & muhat_P with degree=3
0.8
                                0.8
                                                               0.8
```



- But what is $\mu(x)$?
 - it is NOT the green line!
 - it is the piecewise function (at least, that is our best guess of it).

Bias

The bias concerns the difference

$$\overline{\widehat{\mu}}(\mathbf{x}_k) - \mu(\mathbf{x}_k)$$

- Let's compare the average function over the samples, i.e. $\overline{\widehat{\mu}}(x)$, to the piecewise function defined on the whole population. Each plot shows a

 - Red line representing $\overline{\widehat{\mu}}(x) = \frac{1}{N_S} \sum_{i=1}^{N_S} \widehat{\mu}_{S_i}(x)$ Black line representing $\mu(x)$: the piecewise function defined on \mathcal{P}

```
par(mfrow=c(3,3), mar=2.5*c(1,1,1,0.1))
for (i in 1:length(cset) ) {
   plot(Ssam[[i]], main=paste0("mubar (degree=", cset[i],") and piecewise fn"),
          xlab = xnam, ylab = ynam, pch=19, col=0, ylim=ylim, xlim=xlim)
   tempfn = getmuFun(temperature, xnam, ynam)
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="black", lwd=2)
    tempfn = mubars[[i]]
    curve(tempfn, from = xlim[1], to = xlim[2], add = TRUE, col="firebrick", lwd=2)
}
   mubar (degree=1) and piecewise fn
                                         mubar (degree=2) and piecewise fn
                                                                              mubar (degree=3) and piecewise fn
0.8
                                     0.8
                                                                           0.8
                                     0.2
                                                                           0.2
0.2
                                     9.0-
                                                                           9.0
    1850
            1900
                     1950
                             2000
                                          1850
                                                  1900
                                                                  2000
                                                                               1850
                                                                                                        2000
                                                          1950
                                                                                       1900
                                                                              mubar (degree=6) and piecewise fn
   mubar (degree=4) and piecewise fn
                                         mubar (degree=5) and piecewise fn
0.8
                                     0.8
                                                                           0.8
0.2
                                     0.2
                                                                           0.2
                                     9.0
                                                                           9.0
    1850
            1900
                     1950
                             2000
                                          1850
                                                  1900
                                                                               1850
   mubar (degree=7) and piecewise fn
                                         mubar (degree=8) and piecewise fn
                                                                              mubar (degree=9) and piecewise fn
0.8
                                     0.8
0.2
                                     0.2
                                                                           0.2
                                     9.0-
    1850
            1900
                     1950
                             2000
                                          1850
                                                  1900
                                                          1950
                                                                  2000
                                                                               1850
                                                                                       1900
                                                                                                1950
                                                                                                        2000
```

• It might be easier to view the bias by plotting the difference

```
\overline{\widehat{\mu}}(x) - \mu(x)
par(mfrow=c(3,3), mar=2.5*c(1,1,1,0.1))
for (i in 1:length(cset) ) {
   plot(Ssam[[i]], main=paste0("bias for mubar (degree=", cset[i],")"),
```

```
xlab = xnam, ylab = ynam, pch=19, col=0, ylim=c(-0.4, 0.4), xlim=xlim)
   tempfn1 = getmuFun(temperature, xnam, ynam)
   tempfn2 = mubars[[i]]
   tempnew = function(z) { tempfn1(z) - tempfn2(z)}
   curve(tempnew, from = xlim[1], to = xlim[2], add = TRUE, col="black", lwd=2)
   abline(h=0, lty=2)
}
       bias for mubar (degree=1)
                                           bias for mubar (degree=2)
                                                                               bias for mubar (degree=3)
0.4
                                    0.4
                                    0.0
0.0
    1850
            1900
                                        1850
                                                                            1850
                    1950
                            2000
                                                1900
                                                        1950
                                                                2000
                                                                                    1900
                                                                                            1950
                                                                                                    2000
       bias for mubar (degree=4)
                                           bias for mubar (degree=5)
                                                                               bias for mubar (degree=6)
0.4
                                    0.4
                                                                        0.4
                                    0.0
                                                                        -0.4
    1850
            1900
                    1950
                            2000
                                        1850
                                                1900
                                                        1950
                                                                2000
                                                                            1850
                                                                                            1950
                                                                                                    2000
       bias for mubar (degree=7)
                                           bias for mubar (degree=8)
                                                                               bias for mubar (degree=9)
0.4
                                    0.4
                                    0.0
                                                                        0.0
                                    -0.4
    1850
            1900
                    1950
                            2000
                                        1850
                                                1900
                                                        1950
                                                                2000
                                                                            1850
                                                                                    1900
                                                                                            1950
                                                                                                    2000
   • To calculate the bias numerically, we need the following function.
bias2_mutilde <- function(Ssamples, Tsamples, mu, complexity) {</pre>
  ## get the predictor function for every sample S
  muhats <- lapply(Ssamples,
                      FUN=function(sample) getmuhat(sample, complexity)
  )
  ## get the average of these, mubar
  mubar <- getmubar(muhats)</pre>
  ## average over all samples S
  N_S <- length(Ssamples)</pre>
  mean(sapply(1:N_S,
                FUN=function(j){
                   ## average over (x_i,y_i) in a
                   ## single sample T_j the squares
                   ## (y - muhat(x))^2
                   T_j <- Tsamples[[j]]</pre>
                   ave_mu_mu_sq(mubar, mu, T_j$x)
  )
  )
}
```

• Then we can also calculate the bias for the global temperature data

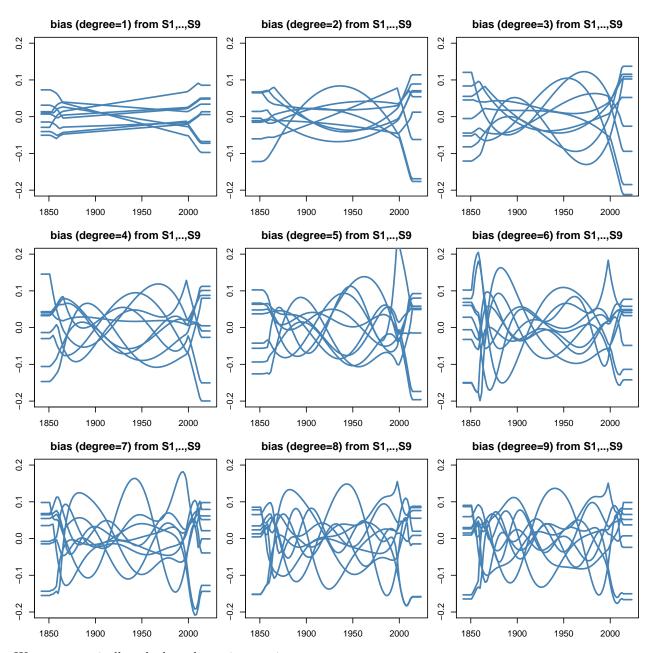
• Which estimate has the smallest bias?

Variance of the $\widetilde{\mu}_{\mathcal{S}}(x)$

• Here we examine the variability of

$$\widehat{\mu}_{\mathcal{S}_i}(x) - \overline{\widehat{\mu}}_{\mathcal{S}}(x)$$

for each S_i , where $i = 1, ..., N_S$ and varying degree of the polynomial.



We can numerically calculate the variance using

```
FUN=function(j){
    ## get muhat based on sample S_j
    muhat <- muhats[[j]]
    ## average over (x_i,y_i) in a
    ## single sample T_j the squares
    ## (y - muhat(x))^2
    T_j <- Tsamples[[j]]
    ave_mu_mu_sq(muhat, mubar, T_j$x)
}
)
)
)</pre>
```

Applying the function to our example.

Putting it all together

- We can combine the three measurements
 - Sampling Variability
 - Bias
 - Variance of the $\widetilde{\mu}_{\mathcal{S}}(x)$

into a single measure to obtain the APSE.

```
BVmat = rbind(0,Bmat, Vmat, Bmat+Vmat)
rownames(BVmat)[1] = "Var(y|x)"
rownames(BVmat)[4] = "APSE"
round(BVmat,3)
##
                deg=1 deg=2 deg=3 deg=4 deg=5 deg=6 deg=7 deg=8 deg=9
## Var(y|x)
                0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## [Bias(mu)]^2 0.026 0.016 0.016 0.015 0.013 0.011 0.010 0.010 0.010
               0.001 0.002 0.003 0.003 0.004 0.005 0.004 0.004 0.004
## Var(mu)
## APSE
               0.027 0.018 0.019 0.018 0.017 0.016 0.015 0.014 0.014
  • Note that Var(y|x) = 0. Why?
plot( 1:9, BVmat[2,], xlab="Degree", ylab="", type='l', ylim=c(0, 0.1), col="firebrick", lwd=2 )
lines( 1:9, (BVmat[1,]^2), xlab="Degree", ylab="", col="black", lwd=2 )
lines( 1:9, BVmat[3,], xlab="Degree", ylab="", col="steelblue", lwd=2 )
```

```
lines( 1:9, BVmat[4,], col="purple", lwd=2)
text(2,0.08,'APSE',col="purple")
text(2,0.07,'Bias^2',col="firebrick")
text(2,0.06,'var(mu.tilde)',col="steelblue")
text(2,0.05, 'aver.var(y|x)',col="black")
0.10
0.08
              APSE
             Bias^2
90.0
          var(mu.tilde)
          aver.var(y|x)
0.04
0.02
0.00
                2
                                  4
                                                    6
                                                                      8
                                        Degree
```

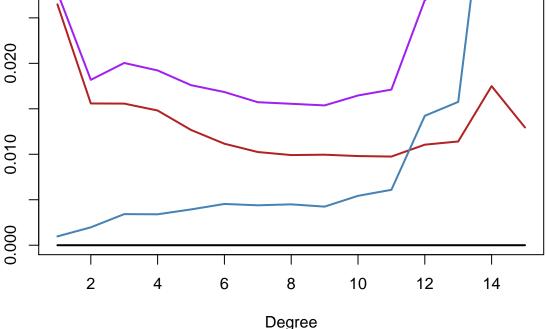
APSE

• We can calculate all components of APSE at once with the following code:

```
T_j \leftarrow na.omit(T_j)
                      y \leftarrow T_j y
                      x \leftarrow T_j x
                      mu_x \leftarrow mu(x)
                      muhat_x <- muhat(x)</pre>
                      mubar_x <- mubar(x)</pre>
                      ## apse
                      ## average over (x_i,y_i) in a
                      ## single sample T_j the squares
                      ## (y - muhat(x))^2
                      apse <- (y - muhat_x)</pre>
                      ## bias2:
                      ## average over (x_i,y_i) in a
                      ## single sample T_j the squares
                      ## (y - muhat(x))^2
                      bias2 <- (mubar_x -mu_x)</pre>
                      ## var_mutilde
                      ## average over (x_i,y_i) in a
                      ## single sample T_j the squares
                      ## (y - muhat(x))^2
                      var_mutilde <- (muhat_x - mubar_x)</pre>
                      ## var_y :
                      ## average over (x_i,y_i) in a
                      ## single sample T_j the squares
                      ## (y - muhat(x))^2
                      var_y \leftarrow (y - mu_x)
                      ## Put them together and square them
                      squares <- rbind(apse, var_mutilde, bias2, var_y)^2</pre>
                      ## return means
                      rowMeans(squares)
 ))
}
```

• We extend the polynomial range as well.

```
##
              deg=1 deg=2 deg=3 deg=4 deg=5 deg=6 deg=7 deg=8 deg=9 deg=10
              0.028 0.018 0.020 0.019 0.018 0.017 0.016 0.016 0.015
## apse
## var mutilde 0.001 0.002 0.003 0.003 0.004 0.005 0.004 0.004 0.004
              0.026 0.016 0.016 0.015 0.013 0.011 0.010 0.010 0.010 0.010
## bias2
              0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000
## var_y
##
              deg=11 deg=12 deg=13 deg=14 deg=15
               0.017 0.027 0.029 0.066 0.063
## apse
## var_mutilde 0.006 0.014 0.016 0.045 0.047
## bias2
               0.010 0.011 0.011 0.017 0.013
## var_y
               0.000 0.000 0.000 0.000 0.000
plot( degrees, apse_vals[3,], xlab="Degree", ylab="", type='l',
     ylim=c(0, 0.026), col="firebrick", lwd=2 )
lines(degrees, apse_vals[2,], xlab="Degree", ylab="", col="steelblue", lwd=2 )
lines(degrees, apse_vals[1,], col="purple", lwd=2)
lines(degrees, apse_vals[4,], col="black", lwd=2)
```



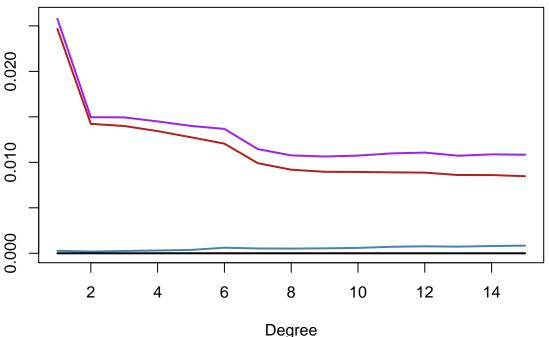
Changing n and N_S

• We might want to vary N_S and n to see our conclusion is sensitive to these inputs.

```
- Here we set N_S = 25 and n = 100.
```

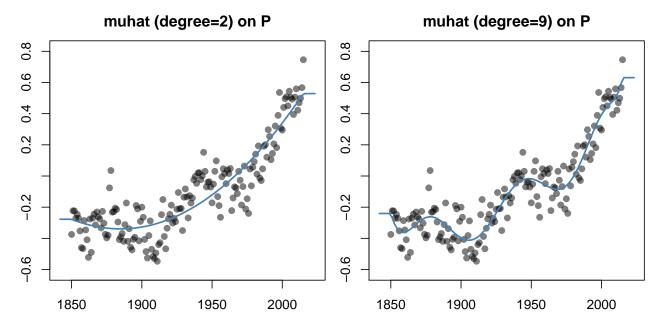
```
N_S <- 25
xnam <- "YEAR"
ynam <- "ANNUAL"
pop <- temperature
n <- 100</pre>
```

```
set.seed(341) # for reproducibility
samples <- lapply(1:N_S, FUN= function(i){getSampleComp(pop, n)})</pre>
        <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, Si, pop)})</pre>
        <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, !Si, pop)})</pre>
Tsam
degrees <- 1:15
muhat = getmuFun(pop, xnam, ynam)
apse_vals <- sapply(degrees,</pre>
                     FUN = function(deg){
                        apse_all(Ssam, Tsam,
                                 complexity = deg, mu = muhat)
                     }
)
colnames(apse_vals) = paste("deg=", degrees, sep="")
#round(apse_vals,5)
plot( degrees, apse_vals[3,], xlab="Degree", ylab="", type='1',
      ylim=c(0, 0.026), col="firebrick", lwd=2 )
lines(degrees, apse_vals[2,], xlab="Degree", ylab="", col="steelblue", lwd=2 )
lines(degrees, apse_vals[1,], col="purple", lwd=2)
lines(degrees, apse_vals[4,], col="black", lwd=2)
```



- Can you guess which colour is which by just looking at the trends?
 - black: $ave_{x}[var(y|x)]$
 - blue: $var(\widetilde{\mu}(x))$
 - $\text{ red: } Bias^2$
 - purple: APSE

Plot of Temperature



Examples

Set getmuhat back to the original function.

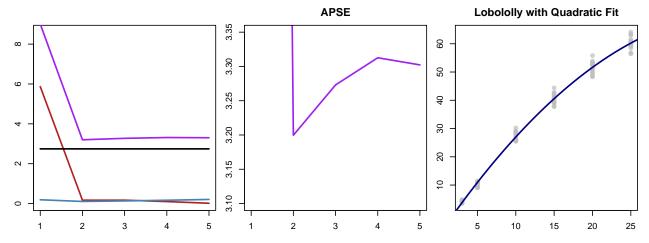
```
} else
    ## x is a vector of values that needs to be a data.frame
{newdata <- data.frame(x = x) }
    ## The prediction
    predict(fit, newdata = newdata)
}
## muhat is the function that we need to calculate values
## at any x, so we return this function from getmuhat
muhat
}</pre>
```

Growth of Loblolly pine trees.

- Here we set $N_S = 25$ and n = 40.
- With n = 40 means we are using 0.6 of the population in each sample

Then we fit polynomials of different degrees to all the samples and calculate the APSE.

```
## deg=1 deg=2 deg=3 deg=4 deg=5
## apse 9.0085 3.1996 3.2730 3.3126 3.3023
## var_mutilde 0.1897 0.1055 0.1310 0.1662 0.2065
## bias2 5.8694 0.1684 0.1692 0.0986 0.0150
## var y 2.7440 2.7440 2.7440 2.7440 2.7440
```



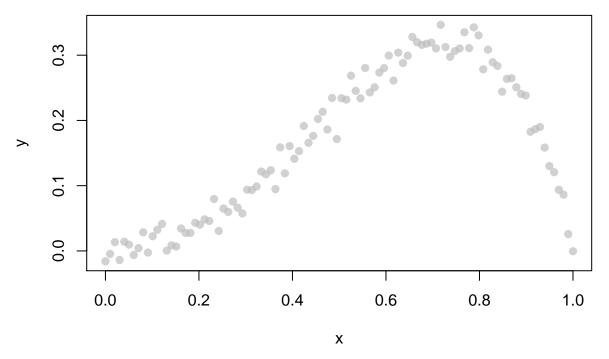
- Here we form samples by selecting units without replacement.
 - What other way could we be selecting units?

Polynomial with degree = 5

- Here we demonstrate that the chosen/fitted function is an approximation to the underlying true function (if a true function exists).
 - Recall that, in real world, "all models are wrong, but some are useful."
 - In this particular example though, we will work with simulated data, so "the true model" does actually exist.
- Suppose that $\mu(x) = x^2 x^5$ (true model) and we generate apopulation with N = 100

$$y_i = \mu(x_i) + r_i = x_i^2 - x_i^5 + r_i$$

```
set.seed(341)
x = seq(0,1, length.out=100)
y = x^2 - x^5 + rnorm(100, sd=.015)
plot(x, y, col=adjustcolor("grey", 0.7), pch=19)
```



• We will start with $N_S = 25$ samples each of size n = 25.

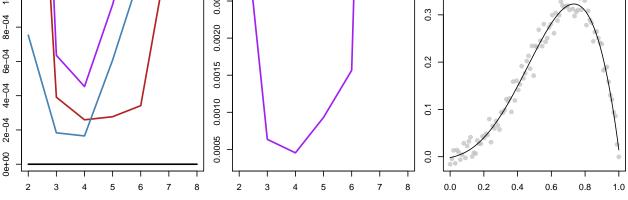
```
datax = data.frame(x=x,y=y)
N_S <- 25
xnam <- "x"</pre>
ynam <- "y"</pre>
pop <- datax
     <- 25
set.seed(341) # for reproducibility
samples <- lapply(1:N_S, FUN= function(i){getSampleComp(pop, n)})</pre>
         <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, Si, pop)})</pre>
Ssam
Tsam
         <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, !Si, pop)})</pre>
```

• Calculate the APSE

bias2

```
degrees <- 2:8
muhat = getmuFun(pop, xnam, ynam)
apse_vals <- sapply(degrees,</pre>
                     FUN = function(deg){
                        apse_all(Ssam, Tsam,
                                 complexity = deg, mu = muhat)
                     }
)
colnames(apse_vals) = paste("deg=", degrees, sep="")
round(apse_vals,5)
##
                 deg=2
                          deg=3
                                  deg=4
                                          deg=5
                                                   deg=6
                                                           deg=7
               0.00429 0.00064 0.00045 0.00093 0.00156 0.01459 0.07619
## apse
```

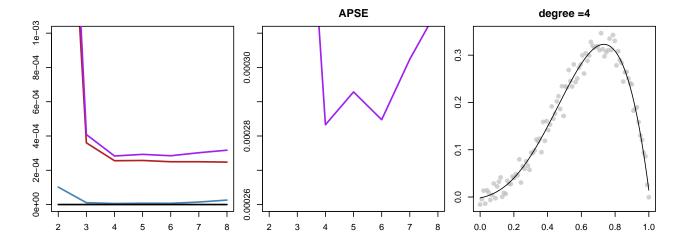
```
0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
par(mfrow=c(1,3), mar=2.5*c(1,1,1,0.1))
plot( degrees, apse_vals[3,], xlab="Degree", ylab="", type='1',
     ylim=c(0, 0.001),
      col="firebrick", lwd=2 )
lines(degrees, apse_vals[2,], xlab="Degree", ylab="", col="steelblue", lwd=2)
lines(degrees, apse_vals[1,], col="purple", lwd=2)
lines(degrees, apse_vals[4,], col="black", lwd=2)
plot( degrees, apse_vals[1,], xlab="Degree", ylab="", type='l',
      col="purple", lwd=2, ylim=c(0.00030, 0.00261), main="APSE" )
plot(datax$x, datax$y, xlab="x", ylab="y", col=adjustcolor("grey", 0.7), pch=19, main="degree =4")
samL = rep(TRUE, nrow(datax))
sample.Data <- getXYSample(xnam, ynam, samL, datax)</pre>
mu.age = getmuhat(sample.Data, complexity = 4)
curve(mu.age, 0, 1, add=TRUE, n=100)
                                            APSE
                                                                          degree =4
                               0.0025
```



 $N_S = 25$ and n = 75

• Let us keep $N_S = 25$ but increase the sample size from n = 25 to n = 75.

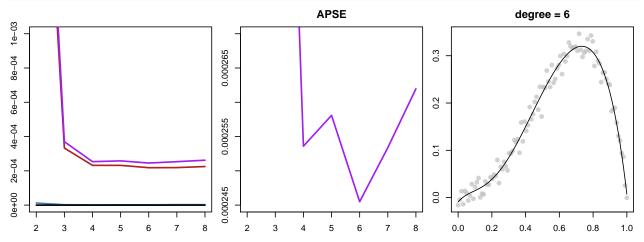
```
Tsam
        <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, !Si, pop)})</pre>
degrees <- 2:8
muhat = getmuFun(pop, xnam, ynam)
apse_vals <- sapply(degrees,</pre>
                     FUN = function(deg){
                       apse all(Ssam, Tsam,
                                complexity = deg, mu = muhat)
                     }
)
colnames(apse_vals) = paste("deg=", degrees, sep="")
round(apse_vals,5)
##
                 deg=2
                         deg=3
                                 deg=4 deg=5
                                                 deg=6
                                                         deg=7
## apse
              0.00369 0.00041 0.00028 0.00029 0.00028 0.00030 0.00032
## var_mutilde 0.00010 0.00001 0.00001 0.00001 0.00001 0.00003
              0.00322\ 0.00036\ 0.00026\ 0.00026\ 0.00025\ 0.00025\ 0.00025
## bias2
              0.00000\ 0.00000\ 0.00000\ 0.00000\ 0.00000\ 0.00000
## var_y
par(mfrow=c(1,3), mar=2.5*c(1,1,1,0.1))
plot( degrees, apse_vals[3,], xlab="Degree", ylab="", type='l',
     ylim=c(0, 0.001), col="firebrick", lwd=2 )
lines(degrees, apse_vals[2,], xlab="Degree", ylab="", col="steelblue", lwd=2 )
lines(degrees, apse_vals[1,], col="purple", lwd=2)
lines(degrees, apse_vals[4,], col="black", lwd=2)
plot( degrees, apse_vals[1,], xlab="Degree", ylab="", type='l',
      col="purple", lwd=2, ylim=c(0.00026, 0.00031), main="APSE" )
plot(datax$x, datax$y, xlab="x", ylab="y",
     col=adjustcolor("grey", 0.7), pch=19, main="degree =4")
samL = rep(TRUE, nrow(datax))
sample.Data <- getXYSample(xnam, ynam, samL, datax)</pre>
mu.age = getmuhat(sample.Data, complexity = 4)
curve(mu.age, 0, 1, add=TRUE, n=100)
```



```
N_S = 25 and n = 95
```

• Again, we'll keep $N_S = 25$ but increase the sample size from n = 75 to n = 95.

```
datax = data.frame(x=x,y=y)
N_S <- 25
xnam <- "x"</pre>
ynam <- "y"</pre>
pop <- datax
     <- 95
set.seed(341) # for reproducibility
samples <- lapply(1:N_S, FUN= function(i){getSampleComp(pop, n)})</pre>
        <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, Si, pop)})</pre>
Ssam
Tsam
        <- lapply(samples, FUN= function(Si){getXYSample(xnam, ynam, !Si, pop)})</pre>
degrees <- 2:8
muhat = getmuFun(pop, xnam, ynam)
apse_vals <- sapply(degrees,</pre>
                     FUN = function(deg){
                        apse_all(Ssam, Tsam,
                                 complexity = deg, mu = muhat)
                     }
)
colnames(apse_vals) = paste("deg=", degrees, sep="")
round(apse_vals,5)
##
                 deg=2
                          deg=3
                                  deg=4
                                          deg=5
                                                   deg=6
                                                           deg=7
               0.00340\ 0.00037\ 0.00025\ 0.00026\ 0.00025\ 0.00025\ 0.00026
## apse
## var_mutilde 0.00001 0.00000 0.00000 0.00000 0.00000 0.00000
               0.00314 0.00033 0.00023 0.00023 0.00022 0.00022 0.00023
## bias2
               0.00000 0.00000 0.00000 0.00000 0.00000 0.00000
## var_y
```



- Note that this time the APSE has chosen polynomial degree 6 for the data.
 - However, the mount of decrease in the APSE from degree 4 to degree 6 is not really significant: notice the vertical axis scale.