3: Data-Based Generalization

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Ideas and issues illustrated by the graphs in this vignette

A central concern of data analysis is to generalize from results from the one data set that is available for analysis to some wider relevance. Ideas of sample and population are crucial for such generalization. A further important notion is that of a *sampling distribution*,

Mechanisms for assessing predictive accuracy include the use of theory, simulation (which extends the use of theory into areas where the calculations may be intractable), the training/test approach, cross-validation, and bootstrap methods.

Note: Figures 3.15 and 3.16 show results from repeated sampling – simulation or bootstrap sampling. The versions of these figures that are shown in Section 2 are for a substantially reduced number of repeat samples, relative to the text *Statistically Informed Data Mining.*

1 R Functions for Creating Chapter 3 Figures

```
fig3.1 <-
function (x=fCatBwt){
lattice::stripplot(jitter(x), pch='|', xlab="Weight (kg)",
                  aspect=0.25, col="black", border="gray")
}
```

```
fig3.2 <-
function(x=fCatBwt){
opar <- par(mfrow=c(2,2), xpd=TRUE,
            mar=c(3.6,3.1,3.6,1.1), mgp=c(2.25, 0.5, 0))
hist(x, labels=TRUE, xlim=c(2, 3),
     xlab="Height (cm)", main="", xpd=TRUE)
title(main="A: Frequency histogram", adj=0, line=1.5, cex.main=1.05)
hist(x, labels=TRUE, xlim=c(2,3),
     xlab="Weight (kg)", main="", freq=FALSE, xpd=TRUE)
title(main="B: Density histogram", adj=0, line=1.5, cex.main=1.05)
par(xpd=FALSE)
hist(x, xlim=c(2,3), xlab="Weight (kg)",
     main="", freq=FALSE)
axis(1)
lines(density(x), xlab="Weight (kg)", col="gray40")
title(main="C: Histogram, density is overlaid", adj=0, line=1.5,
      cex.main=1.05)
plot(density(x), xlim=c(2,3), xlab="Height (cm)",
     main="", sub="", bty="l", type="l")
av <- mean(x)
sdev <- sd(x)
xval <- pretty(c(2,3), n=40)
lines(xval, dnorm(xval, mean=av, sd=sdev), lty=2, col="gray40")
title(main="D: Density curve estimate", adj=0, line=1.5, cex.main=1.05)
par(opar)
par(mfrow=c(1,1))
}
```

```
fig3.3 <-
function (x=fCatBwt, plotit=TRUE){
    av <- mean(x); sdev <- sd(x); sampsize <- length(x)
    simmat <- cbind(x, matrix(rnorm(sampsize*5, mean=av, sd=sdev),
                                ncol=5))
    simdf <- as.data.frame(simmat)
    names(simdf) <- c("Source", paste("normal", 1:5, sep=""))
    simdf <- stack(simdf)
    names(simdf) <- c("height", "Sample")
    denplotSimple <- densityplot(~height, groups=Sample, data=simdf,
                                 xlab="Body weight (kg)")
    denplotn <- update(denplotSimple, scales=list(tck=0.5),
                       main=list(expression(plain("A: Simulation (Densities)")),
                       cex.title=0.9, x=0.05, just="left"),
                       par.settings=simpleTheme(lty=1:6))
    bwpltBasic <- bwplot(Sample ~ height, data=simdf,
                         xlab="Body weight (kg)",
                         auto.key=list(columns=3))
    bwplotn <- update(bwpltBasic, scales=list(tck=0.5),
                      main=list(expression(plain("B: Simulation (Boxplots)")),
                                cex.title=0.9, x=0.05, just="left"))
    if(plotit){
        print(denplotn, position=c(0,0,0.5,1))
        print(bwplotn, position=c(0.5,0,1,1),newpage=FALSE)
    }
    invisible(list(denplotn, bwplotn))
}
```

```
fig3.4 <-
function (x=fCatBwt, plotit=TRUE)
{
    sampsize <- length(x)
    bootmat <- cbind(x, matrix(0, ncol=5, nrow=sampsize))
    for(i in 2:6) bootmat[,i] <- sample(x, replace=TRUE)
    colnames(bootmat) <- c("Source", paste("normal", 1:5, sep=""))
    bootdf <- stack(as.data.frame(bootmat))
    names(bootdf) <- c("height", "Sample")
    denplotSimple <- densityplot(~ height, groups=Sample, data=bootdf,
                                 xlab="Body weight (kg)")
    legendA <- expression(plain("A: Bootstrap (Densities)"))
    denplot <- update(denplotSimple, scales=list(tck=0.5),
                      main=list(legendA, x=0.05, just="left"), cex.title=0.9,
                      par.settings=simpleTheme(lty=1:6))
    bwpltBasic <- bwplot(Sample ~ height, data=bootdf,
                         xlab="Body weight (kg)",
                         auto.key=list(columns=3))
    legendB <- expression(plain("B: Bootstrap (Boxplots)"))
    bwplot <- update(bwpltBasic, scales=list(tck=0.5),
                     main=list(legendB, x=0.05, just="left"), cex.title=0.9)
    if(plotit){
        print(denplot, position=c(0,0,0.5,1))
        print(bwplot, position=c(0.5,0,1,1),newpage=FALSE)
    }
    invisible(list(denplot, bwplot))
}
```

```
fig3.5 <-
function ()
{
    opar <- par(mgp=c(2,.75,0), mfrow=c(1,2))
    curve(dnorm(x), from = -3, to = 3,
          ylab=expression("dnorm("*italic(x)*")"),
          xlab=expression("Normal deviate "*italic(x)))
    curve(pnorm(x), from = -3, to = 3,
          ylab=expression("pnorm("*italic(x)*")"),
          xlab=expression("Normal deviate "*italic(x)))
    par(opar)
}
```

```
fig3.6 <-
function (){
    heights <- na.omit(subset(survey, Sex=="Female")$Height)
    plot(density(heights), bty="l", main="",
         cex.axis=1.15, cex.lab=1.15)
    av <- mean(heights); sdev <- sd(heights)
    abline(v=c(av-sdev, av, av+sdev), col="gray", lty=c(2,1,2))
    ## Show fitted normal curve
    xval <- pretty(heights, n=40)
    normal_den <- dnorm(xval, mean=av, sd=sdev)
    lines(xval, normal_den, col="gray40", lty=2)
    ytop <- par()$usr[4]-0.25*par()$cxy[2]
    text(c(av-sdev, av+sdev), ytop,
         labels=c("mean-SD","mean+SD"), col="gray40", xpd=TRUE)
}
```

```
fig3.7 <-
function (wts=fCatBwt){
    opar <- par(pty="s")
    qqnorm(wts)
    par(opar)
}
```

```
fig3.8 <-
function (wts=fCatBwt)
{
    opar <- par(mfrow=c(1,2), mar=c(2.1, 3.6, 3.6,2.6),
                mgp=c(2.25, 0.5,0))
    av <- numeric(1000)
    for (i in 1:1000)
        av[i] <- mean(rnorm(47, mean=2.36, sd=0.27))
    avdens <- density(av)
    xval <- pretty(c(2.36-3*0.27, 2.36+3*0.27), 50)
    den <- dnorm(xval, mean=2.36, sd=0.27)
    plot(xval, den, type="l", xlab="",  xlim=c(1.5, 3.75),
         ylab="Density", ylim=c(0,max(avdens$y)),
         col="gray", lwd=2, lty=2)
    lines(avdens)
    mtext(side=3, line=0.75, "A: Simulation (from a normal distribution)",
          adj=0)
    legend("bottomright",
           legend=c("Source", "Sampling\ndistribution\nof mean"),
           col=c("gray", "black"), lty=c(2,1), lwd=c(2,1), bty="n",
           y.intersp=0.75, inset=c(0,0.2),
           cex=0.8)
    av <- numeric(1000)
    for (i in 1:1000)
        av[i] <- mean(sample(wts, size=length(wts), replace=TRUE))
    avdens <- density(av)
    plot(density(wts), ylim=c(0, max(avdens$y)),
         xlab="", ylab="Density", xlim=c(1.5, 3.75),
         col="gray", lwd=2, lty=2, main="")
    lines(avdens)
    mtext(side=3, line=0.75,
          "B: Bootstrap samples (resample sample)", adj=0)
    legend("bottomright",
           legend=c("Source",
                      "Sampling\ndistribution\nof mean"),
           col=c("gray", "black"), lty=c(2,1), lwd=c(2,1), bty="n",
           y.intersp=0.75, inset=c(0,0.2),
           cex=0.8)
    par(opar)
    par(mfrow=c(1,1))
}
```

```
fig3.9 <-
function ()
{
    xleft <- 0:3; xrt <- 1:4
    ybot <- rep(0,4); ytop <- rep(1,4) - 0.05
    opar <- par(mar=rep(0.1,4))
    plot(c(0,5), c(-1,4), xlab="", ylab="", axes=F, type="n")
    for(i in 0:3){
        i1 <- i+1
        rect(xleft, ybot+i, xrt, ytop+i)
        xli <- xleft[i+1]; xri <- xrt[i+1];
        yboti <- (ybot+i)[i+1]; ytopi <- (ytop+i)[i+1]
        rect(xli, yboti, xri, ytopi, col="gray80")
        text(0.5*(xli+xri), 0.5*(yboti+ytopi), "TEST")
        text(0.5*(xleft[-i1]+xrt[-i1]), 0.5*(ybot[-i1]+ytop[-i1])+i, "Training")
        text(4+strwidth("TE"), i+0.475, paste("Fold", i1), adj=0)
}
}
```

```
fig3.10 <-
function (dset=cuckoos, plotit=TRUE)
{
    parset1 <- lattice::simpleTheme(pch=1:6, alpha=0.8)
    plt1 <- lattice::xyplot(length ~ breadth, groups=species, data=dset,
                   par.settings=parset1, aspect=1,
                   scales=list(tck=0.5),
                   auto.key=list(columns=2, alpha=1),
                   main=grid::textGrob("A:", x=unit(.025, "npc"),
                   y = unit(.25, "npc"), just="left",
                   gp=gpar(cex=1))
                   )
    Species <- factor(c(rep("other", 5), "wren")[unclass(cuckoos$species)])
    parset2 <- lattice::simpleTheme(pch=c(0,6), alpha=0.8,
                           col=trellis.par.get()$superpose.symbol$col[c(7,6)])
    plt2 <- lattice::xyplot(length ~ breadth, groups=Species, data=dset,
                   par.settings=parset2,
                   aspect=1, ylab="", scales=list(tck=0.25),
                   auto.key=list(columns=1, alpha=1),
                   main=grid::textGrob("B:", x=unit(.05, "npc"),
                   y = unit(.25, "npc"), just="left",
                   gp=grid::gpar(cex=1))
                   )
    plt2 <- update(plt2,
                   par.settings=list(layout.heights=list(key.top=1.5)))
    if(plotit){
        print(plt1, position=c(0,0,0.515,1))
        print(plt2, position=c(0.485,0,1,1), newpage=FALSE)
    }
    invisible(list(plt1, plt2))
}
```

```
fig3.11 <-
function (dset=cuckoos)
{
    parset <- list(dot.symbol=list(pch=1, alpha=0.6))
    dotwren <- dotplot(species %in% "wren" ~ length, data=dset,
                       scales=list(y=list(labels=c("Other", "Wren"))),
                       par.settings=parset, xlab="Length (mm)")
    dotwren
}
```

```
fig3.12 <-
function(dset=cuckoos)
{
    avdiff <- numeric(100)
    for(i in 1:100){
        avs <- with(dset, sapply(split(length, species %in% "wren"),
                                    function(x)mean(sample(x, replace=TRUE))))
        avdiff[i] <- avs[1] - avs[2]  # FALSE (non-wren) minus TRUE (wren)
    }
    xtxt <- paste("Means of bootstrap samples of length difference,\n",
                  "non-wren - wren (mm)")
    dotdiff <- dotplot(~ avdiff, xlab=xtxt,
                       par.settings=list(dot.symbol=list(pch=1, alpha=0.6)))
    dotdiff
}
```

```
fig3.13 <-
function (dset=mcats)
{
    xyplot(Hwt ~ Bwt, data=dset,
           type=c("p","r"))
}
```

```
fig3.14 <-
function(dset=mcats)
{
    mcats.lm <- lm(Hwt ~ Bwt, data=dset)
    res <- resid(mcats.lm)
    plot(density(res), main="")
    rug(res, col="gray")
}
```

```
fig3.15 <-
function(dset=mcats, nrepeats=100)
{
    bootmat <- bootreg(formula = Hwt ~ Bwt,
                       data = dset,
                       nboot = nrepeats)
    bootdf <- as.data.frame(bootmat)
    names(bootdf) <- c("Intercept","Slope")
    colr <- adjustcolor(rep("black",3),
                        alpha.f=0.25)
    scatterplot(Slope ~ Intercept, col=colr,
                data=bootdf, boxplots="xy",
                reg.line=NA, smooth=FALSE)
}
```

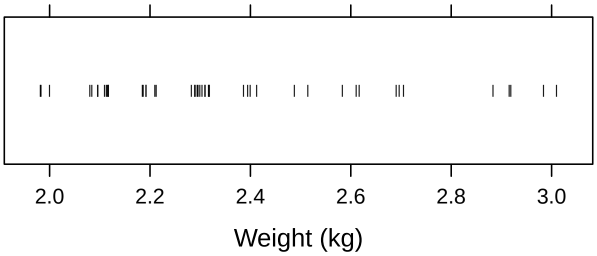
```
fig3.16 <-
function (dset=mcats, plotit=TRUE, nrepeats=100)
{
    bootmat <- bootreg(formula = Hwt ~ Bwt,
                       data = dset[-97, ],
                       nboot = nrepeats)
    bootdf0 <- as.data.frame(bootmat)
    names(bootdf0) <- c("Intercept","Slope")
    gphA <- xyplot(Slope ~ Intercept, data=bootdf0, alpha=0.25,
                   main=paste("A:", nrepeats, "bootstrap samples"),
                   cex.title=1.1)
        simmat <- simreg(formula = Hwt ~ Bwt,
                         data=dset[-97, ], nsim=nrepeats)
    simdf <- as.data.frame(simmat)
    names(simdf) <- c("Intercept","Slope")
    gphB <- xyplot(Slope ~ Intercept, data=simdf, alpha=0.25,
                   main=paste("B:", nrepeats, "simulations"),
                   cex.title=1.1)
    if(plotit){
        print(gphA, position=c(0,0,0.515,1))
        print(gphB, position=c(0.485,0,1,1), newpage=FALSE)
    }
    invisible(list(gphA, gphB))
}
```

2 Show the Figures

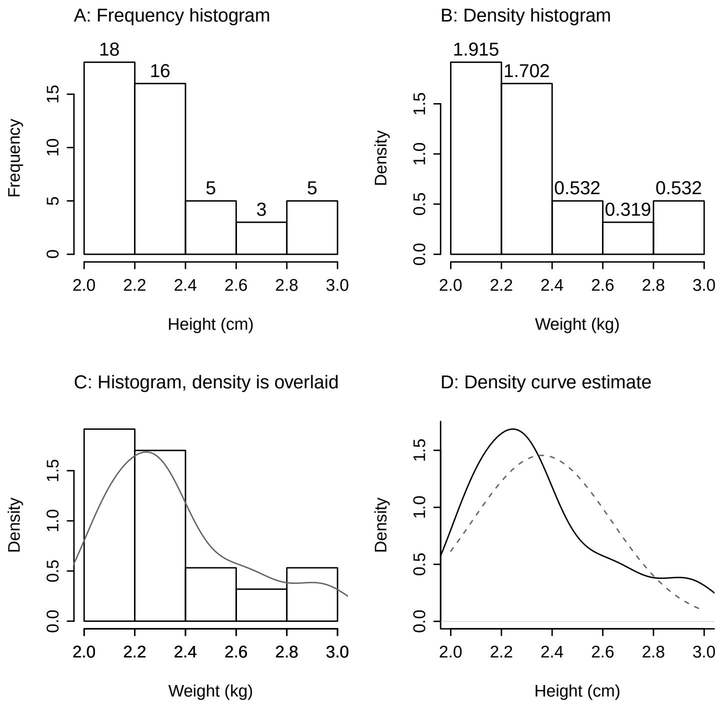
```
pkgs <- c("lattice","DAAG","gamclass","MASS","car","grid")
z <- sapply(pkgs, require, character.only=TRUE,
            warn.conflicts=FALSE, quietly=TRUE)
if(any(!z)){
  notAvail <- paste(names(z)[!z], collapse=", ")
  print(paste("The following packages should be installed:", notAvail))
}
```

```
msg <- "Data object 'cats', from 'MASS', may not be available"
if(!requireNamespace("MASS"))print(msg) else {
  mcats <- subset(MASS::cats, Sex=="M")
  fcats <- subset(MASS::cats, Sex=="F")
  fCatBwt <- na.omit(fcats[, "Bwt"])
}
if(!exists("cuckoos")){
        msg <- "Cannot find either 'cuckoos' or 'DAAG::cuckoos',"
if(requireNamespace("DAAG"))cuckoos <- DAAG::cuckoos else
          print(msg)
      }
```

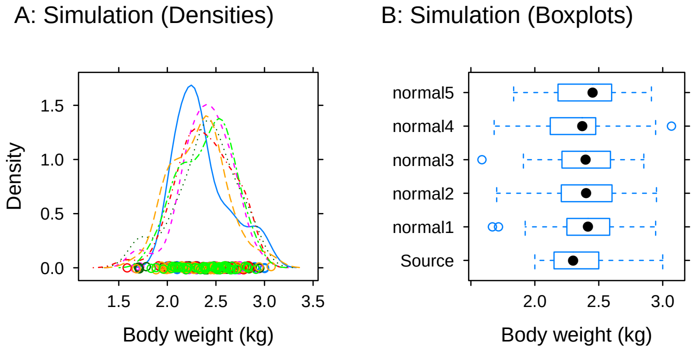
```
if(exists('fCatBwt'))fig3.1() else
    print("Object 'fCatBwt' is not available; get from 'MASS::cats'")
```



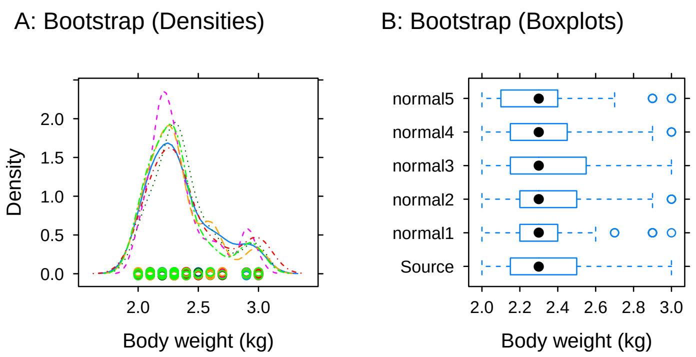
```
if(exists('fCatBwt'))fig3.2() else
    print("Object 'fCatBwt' is not available; get from 'MASS::cats'")
```



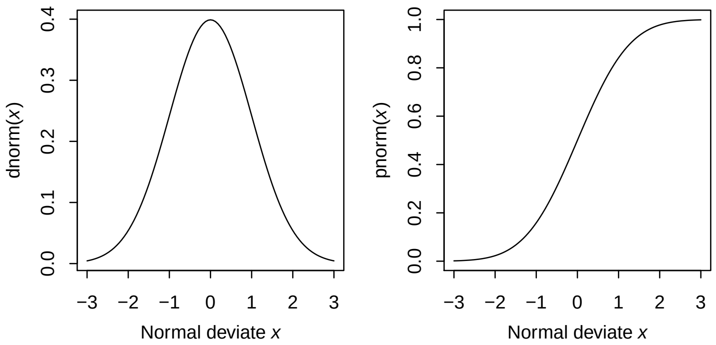
```
if(exists('fCatBwt'))fig3.3() else
    print("Object 'fCatBwt' is not available; get from 'MASS::cats'")
```



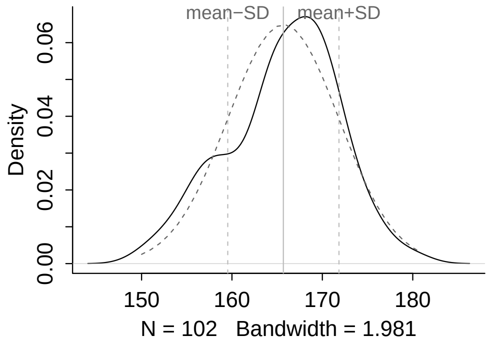
```
if(exists('fCatBwt'))fig3.4() else
    print("Object 'fCatBwt' is not available; get from 'MASS::cats'")
```



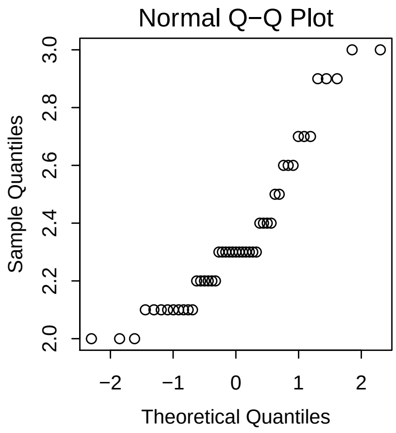
```r
fig3.5()
```



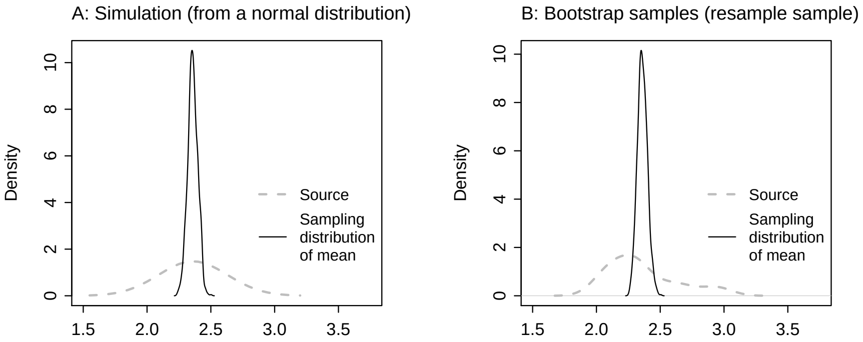
```r
fig3.6()
```



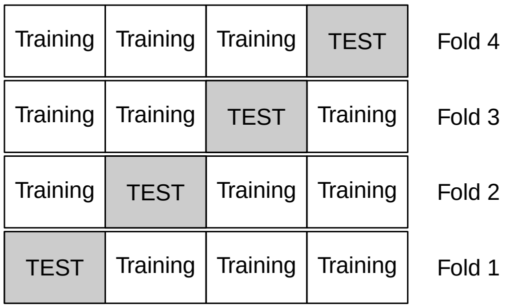
```r
if(exists("fCatBwt"))fig3.7() else
    print("Object 'fCatBwt' was not found; get from 'MASS::cats'")
```



```
if(exists("fCatBwt"))fig3.8() else
    print("Object 'fCatBwt' was not found; get from 'MASS::cats'")
```

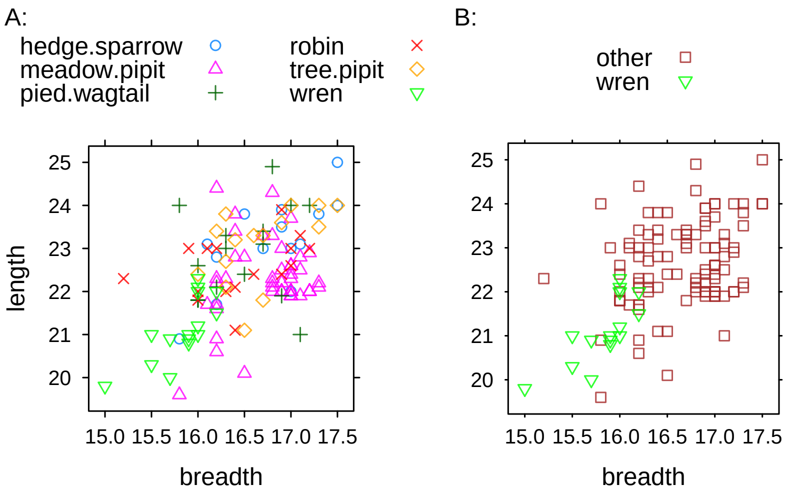


```
fig3.9()
```

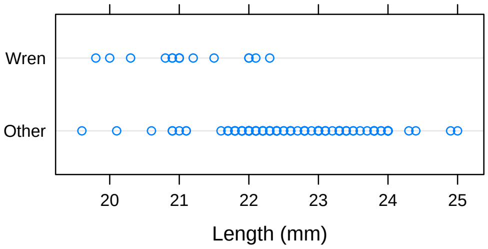


Training	Training	Training	TEST	Fold 4
Training	Training	TEST	Training	Fold 3
Training	TEST	Training	Training	Fold 2
TEST	Training	Training	Training	Fold 1

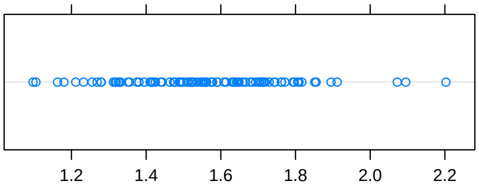
```
if(exists("cuckoos"))fig3.10() else
    print("Object 'cuckoos' was not found; get 'DAAG::cuckoos'")
```



```
if(exists("cuckoos"))fig3.11() else
    print("Object 'cuckoos' was not found; get 'DAAG::cuckoos'")
```

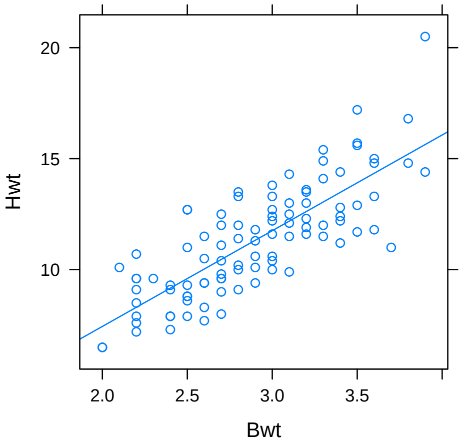


```
if(exists("cuckoos"))fig3.12() else
    print("Object 'cuckoos' was not found; get 'DAAG::cuckoos'")
```

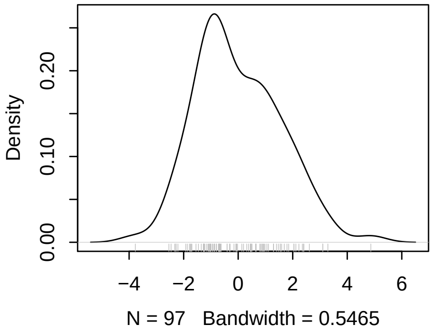


Means of bootstrap samples of length difference,
non−wren − wren (mm)

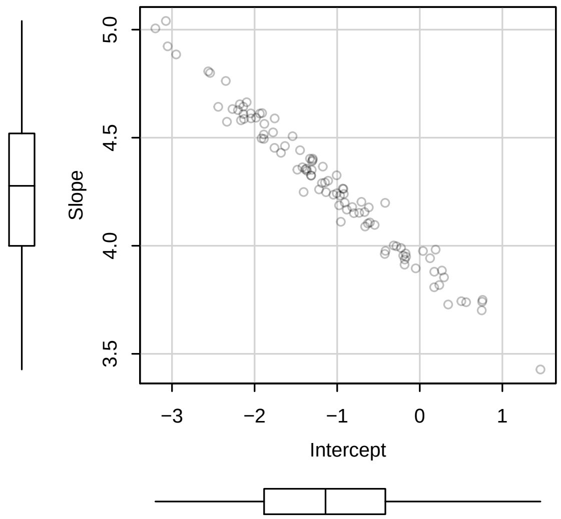
```
if(exists('mcats'))fig3.13() else
    print("Object 'mcats' was not found; subset from 'MASS::cats'")
```



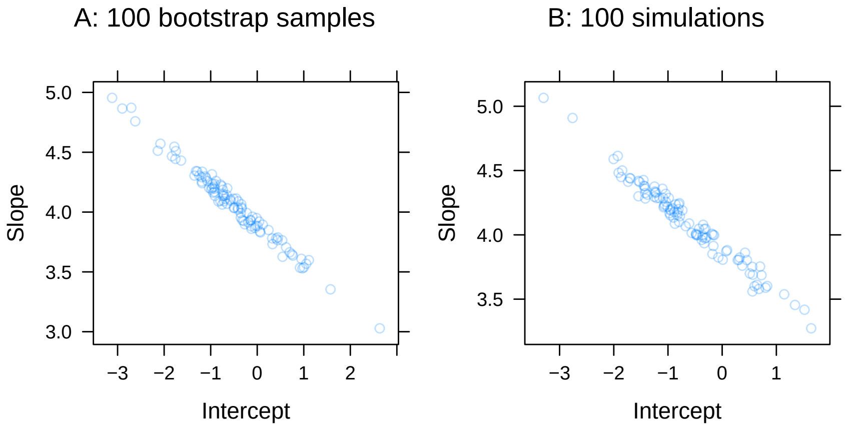
```
if(exists('mcats'))fig3.14() else
    print("Object 'mcats' was not found; subset from 'MASS::cats'")
```



```
if(!require(car)){
    print("Figure 3.15 requires the 'car' package")
    return("The 'car' package needs to be installed.")
}
if(exists("mcats"))fig3.15(nrepeats=100) else
    print("Object 'mcats' was not found; subset from 'MASS::cats'")
```



```
if(exists('mcats'))fig3.16() else
    print("Object 'mcats' was not found; subset from 'MASS::cats'")
```


A: 100 bootstrap samples
B: 100 simulations
Slope
Intercept
Slope
Intercept