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]

1 Code for Functions that Give the Figures

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

```
fig3.2 <-
function(x=fCatWts){
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)
```

[1] Display of the figures can be suppressed, when processing this vignette through *knitr*, by placing an object `doFigs=FALSE` in the workspace.

```
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=fCatWts, 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=fCatWts, 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: Bbootstrap (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 (){
  ## 'cats' is from MASS
    y <- with(cats, na.omit(Bwt[Sex=="F"]))
    opar <- par(pty="s")
    qqnorm(y)
    par(opar)
}
```

```
fig3.8 <-
function ()
{
    opar <- par(fig=c(0, 1, 0.465, 1), 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$y)),
         col="gray", lwd=2, lty=2)
    lines(avdens)
    mtext(side=3, line=0.75, "A: Simulation (from a normal distribution)",
          adj=-0.1)
    legend("bottomright",
           legend=c("Source", "Sampling\ndistribution\nof mean"),
           col=c("gray", "black"), lty=c(2,1), lwd=c(2,1), bty="n",
           y.intersp=0.75, inset=c(0,0.2),
           cex=0.8)
    par(fig=c(0, 1, 0, 0.535), new=TRUE)
    y <- with(cats, na.omit(Bwt[Sex=="F"]))
    av <- numeric(1000)
    for (i in 1:1000)
        av[i] <- mean(sample(y, size=length(y), replace=TRUE))
    avdens <- density(av)
    plot(density(y), ylim=c(0, max(avdens$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 (from the sample data)", adj=-0.1)
    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(fig=c(0,1,0,1))
}
```

```
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 (plotit=TRUE)
{
    library(grid)
    parset1 <- simpleTheme(pch=1:6, alpha=0.8)
    plt1 <- xyplot(length ~ breadth, groups=species, data=cuckoos,
                   par.settings=parset1, aspect=1,
                   scales=list(tck=0.5),
                   auto.key=list(columns=2, alpha=1),
                   main=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$species)])
    parset2 <- simpleTheme(pch=c(0,6), alpha=0.8,
                           col=trellis.par.get()$superpose.symbol$col[c(7,6)])
    plt2 <- xyplot(length ~ breadth, groups=Species, data=cuckoos,
                   par.settings=parset2,
                   aspect=1, ylab="", scales=list(tck=0.25),
                   auto.key=list(columns=1, alpha=1),
                   main=textGrob("B:", x=unit(.05, "npc"),
                   y = unit(.25, "npc"), just="left",
                   gp=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 ()
{
    parset <- list(dot.symbol=list(pch=1, alpha=0.6))
    dotwren <- dotplot(species %in% "wren" ~ length, data=cuckoos,
                       scales=list(y=list(labels=c("Other", "Wren"))),
                       par.settings=parset, xlab="Length (mm)")
    dotwren
}
```

```
fig3.12 <-
function()
{
    avdiff <- numeric(100)
    for(i in 1:100){
        avs <- with(cuckoos, 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 (df=mcats)
{
    xyplot(Hwt ~ Bwt, data=df,
           type=c("p","r"))
}
```

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

```
fig3.15 <-
function(df=mcats, nrepeats=100)
{
    if(!require(car))stop("Package 'car' must be installed")
    bootmat <- bootreg(formula = Hwt ~ Bwt,
                       data = df,
                       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 (df=mcats, plotit=TRUE, nrepeats=100)
{
    bootmat <- bootreg(formula = Hwt ~ Bwt,
                       data = df[-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=df[-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

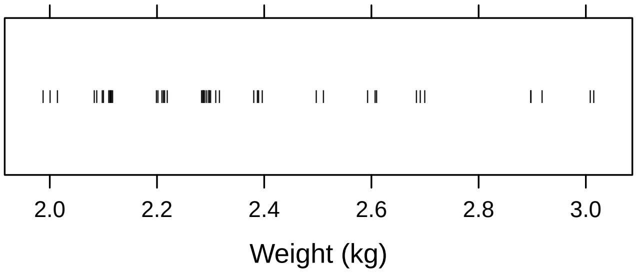
Unless doFigs is found in the workspace and is FALSE, then subject to checks that all necessary datasets and packages are available, the figures are now shown.

```r
if(!exists("doFigs")) doFigs <- TRUE
```

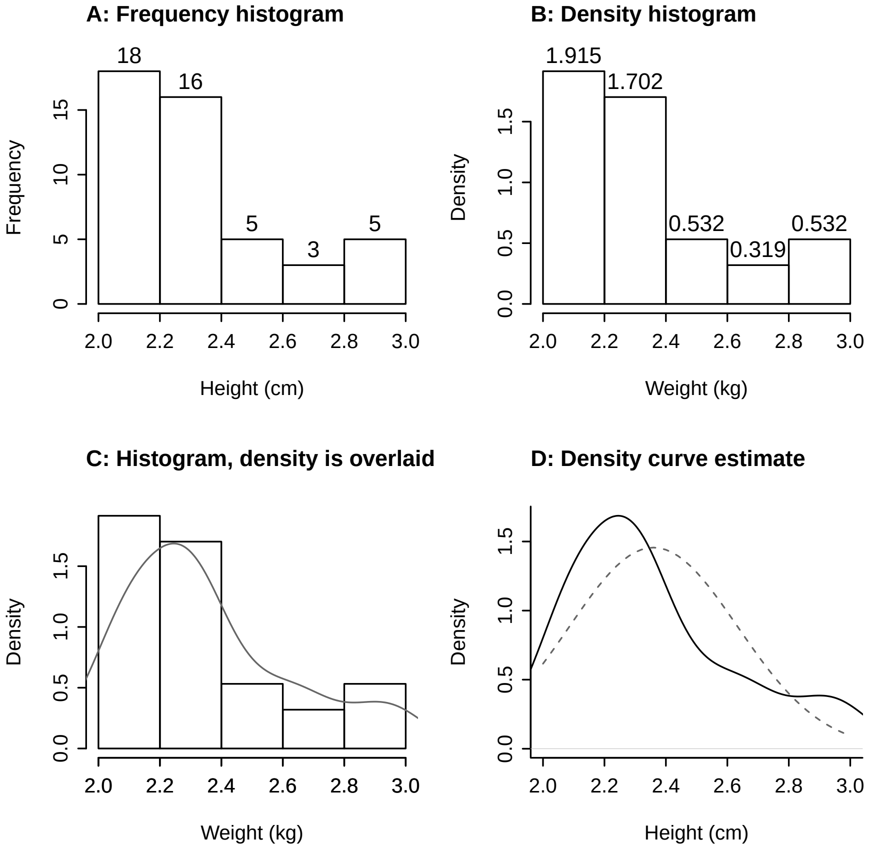
```r
pkgs <- c("lattice","DAAG","gamclass")
z <- sapply(pkgs, require, character.only=TRUE, warn.conflicts=FALSE)
if(any(!z)){
  notAvail <- paste(names(z)[!z], collapse=", ")
  stop(paste("The following packages should be installed:", notAvail))
}
```

```r
if(!exists("cats")){
  cat("Will load 'cats' dataset from MASS package")
  require(MASS)
}
fCatWts <- with(cats, na.omit(Bwt[Sex=="F"]))
mcats <- subset(cats, Sex=="M")
```

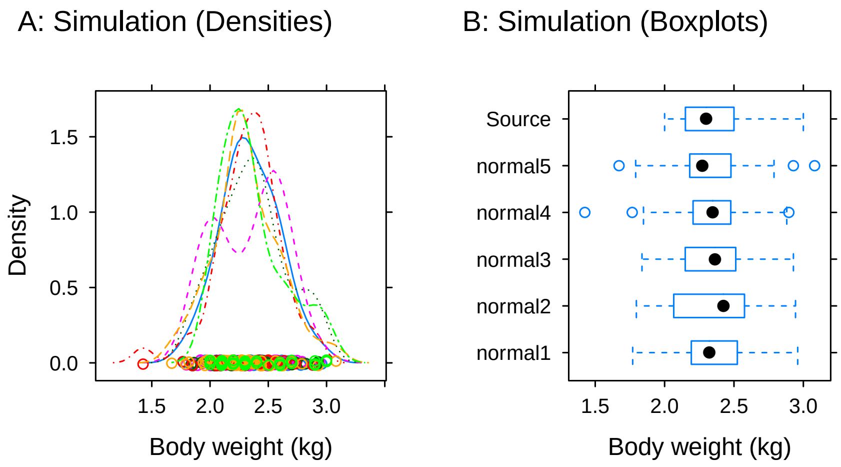
```r
fig3.1()
```



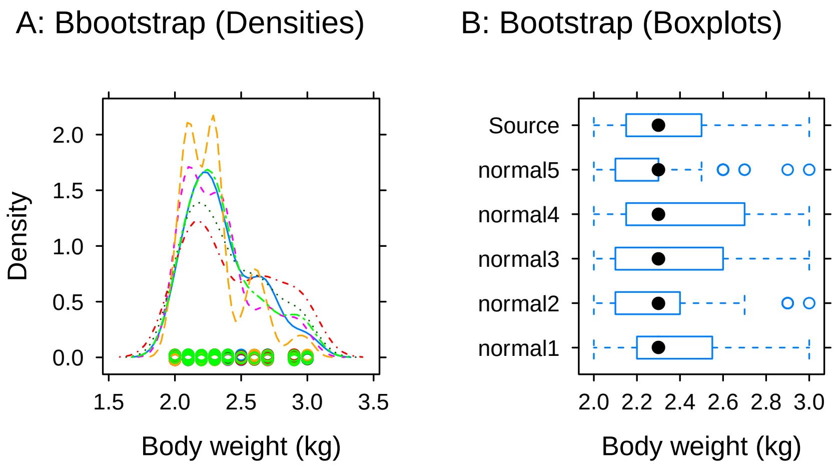
```r
fig3.2()
```


A: Frequency histogram
18
16
5
3
5
Frequency
0
5
10
15
2.0
2.2
2.4
2.6
2.8
3.0
Height (cm)
B: Density histogram
1.915
1.702
0.532
0.319
0.532
Density
0.0
0.5
1.0
1.5
2.0
2.2
2.4
2.6
2.8
3.0
Weight (kg)
C: Histogram, density is overlaid
Density
0.0
0.5
1.0
1.5
2.0
2.2
2.4
2.6
2.8
3.0
Weight (kg)
D: Density curve estimate
Density
0.0
0.5
1.0
1.5
2.0
2.2
2.4
2.6
2.8
3.0
Height (cm)

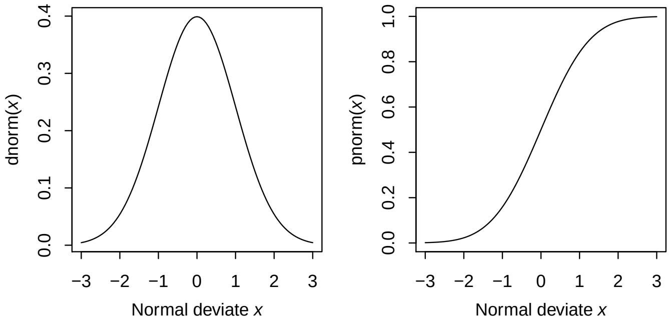
```
fig3.3()
```


A: Simulation (Densities)
Density
0.0
0.5
1.0
1.5
1.5
2.0
2.5
3.0
Body weight (kg)
B: Simulation (Boxplots)
Source
normal5
normal4
normal3
normal2
normal1
1.5
2.0
2.5
3.0
Body weight (kg)

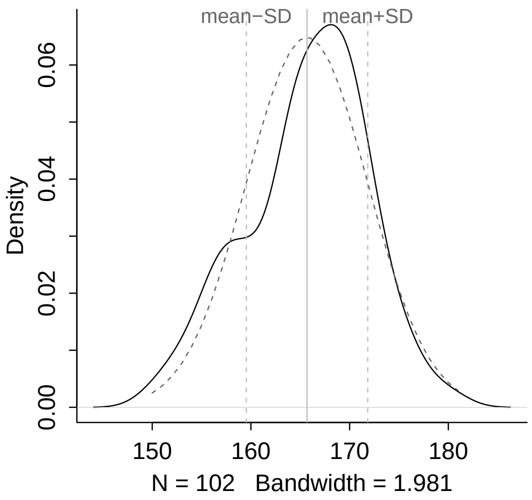
```
fig3.4()
```



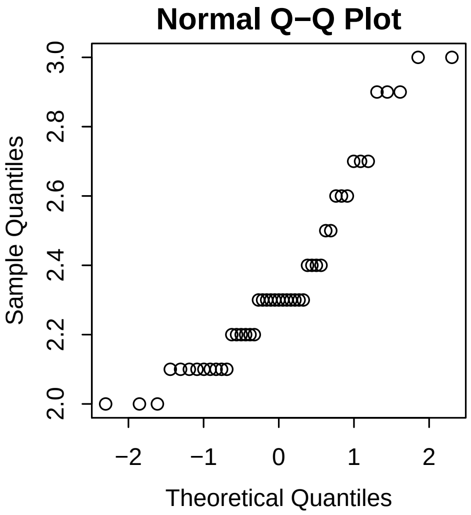
```
fig3.5()
```



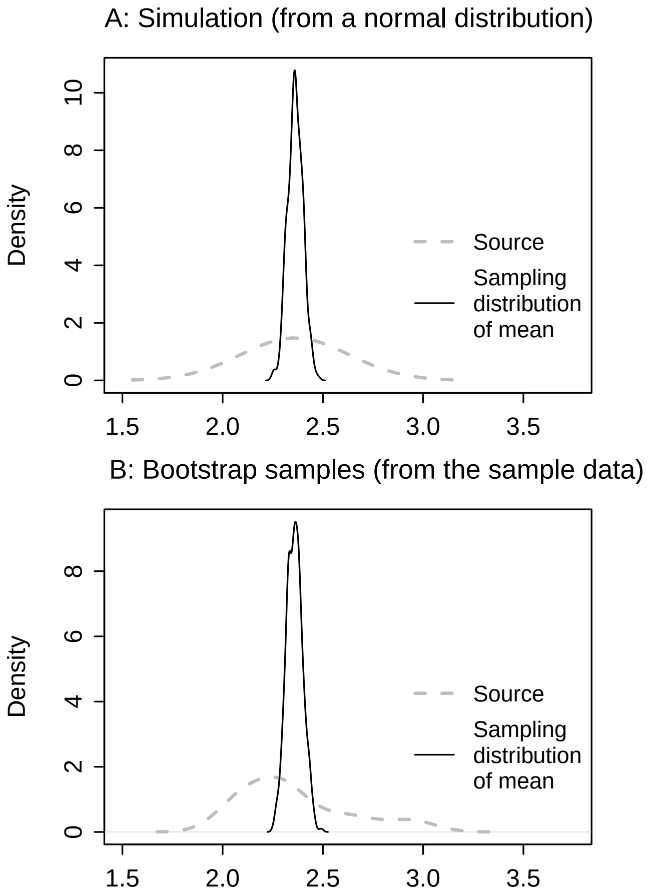
```
fig3.6()
```


mean−SD
mean+SD
Density
0.00
0.02
0.04
0.06
150
160
170
180
N = 102   Bandwidth = 1.981

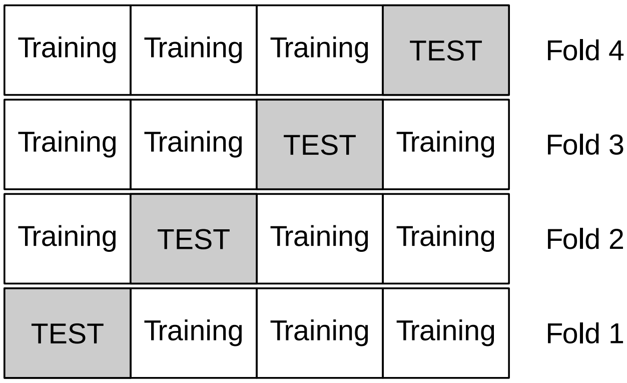
```
fig3.7()
```


Normal Q−Q Plot
Sample Quantiles
2.0
2.2
2.4
2.6
2.8
3.0
−2
−1
0
1
2
Theoretical Quantiles

```
fig3.8()
```

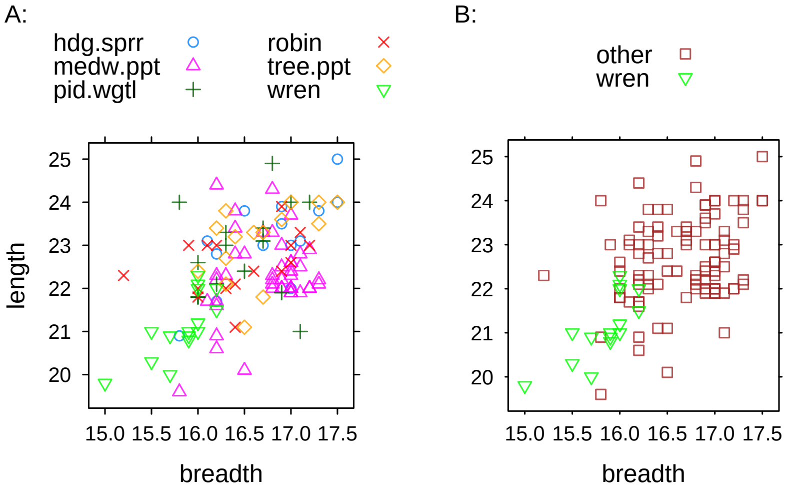

A: Simulation (from a normal distribution)
Density
0
2
4
6
8
10
Source
Sampling distribution of mean
1.5
2.0
2.5
3.0
3.5
B: Bootstrap samples (from the sample data)
Density
0
2
4
6
8
Source
Sampling distribution of mean
1.5
2.0
2.5
3.0
3.5

```
fig3.9()
```

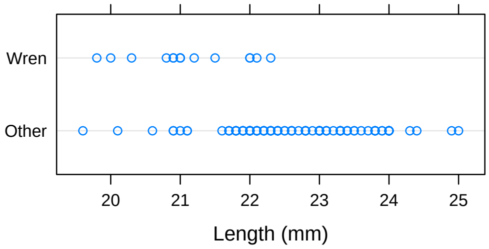


Training	Training	Training	TEST	Fold 4
Training	Training	TEST	Training	Fold 3
Training	TEST	Training	Training	Fold 2
TEST	Training	Training	Training	Fold 1

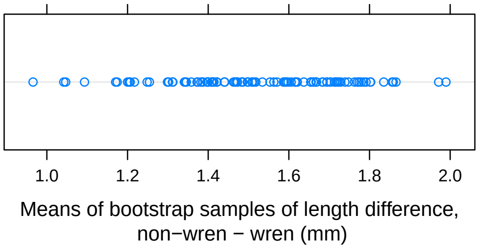
```
fig3.10()
```



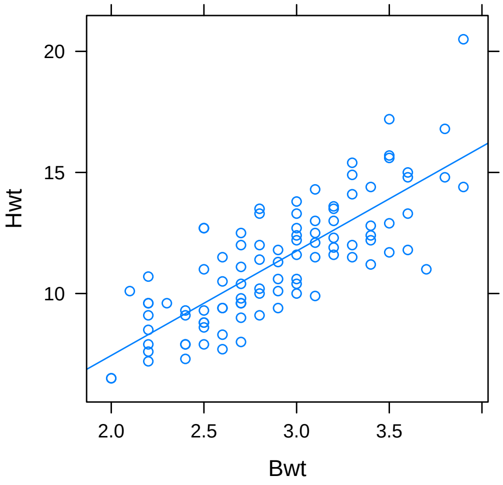
```
fig3.11()
```



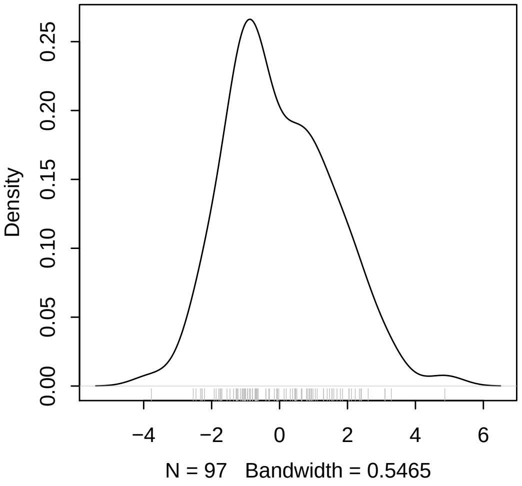
```
fig3.12()
```



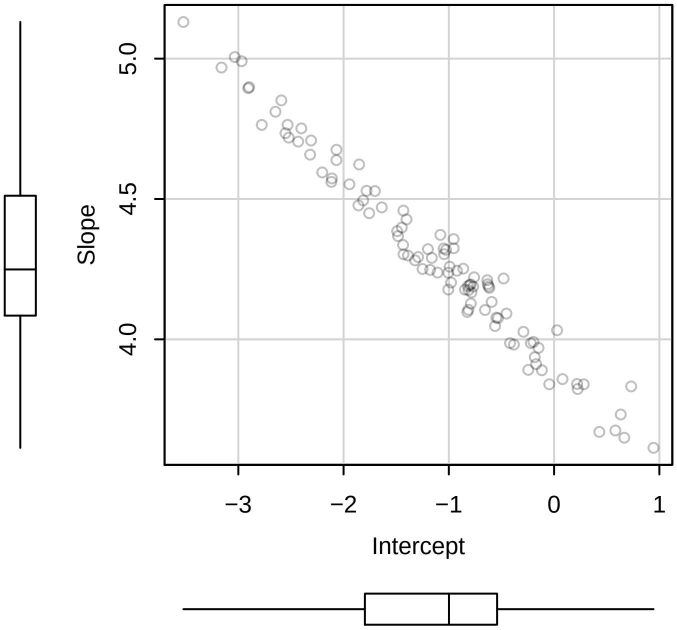
```
fig3.13()
```



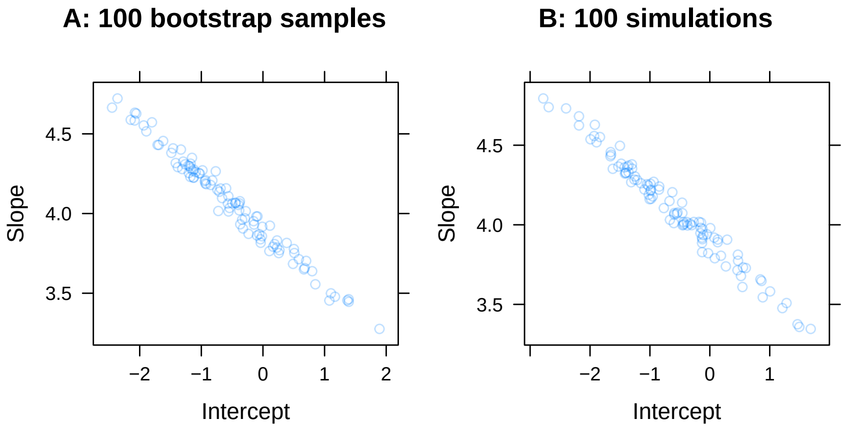
```
fig3.14()
```



```
fig3.15(nrepeats=100)
```



```
fig3.16(nrepeats=100)
```


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