

Computational Statistics

An Introduction to 

Günther Sawitzki




CRC Press

Taylor & Francis Group

A CHAPMAN & HALL BOOK

Examples from
Computational Statistics

An Introduction to 

Günther Sawitzki
StatLab Heidelberg

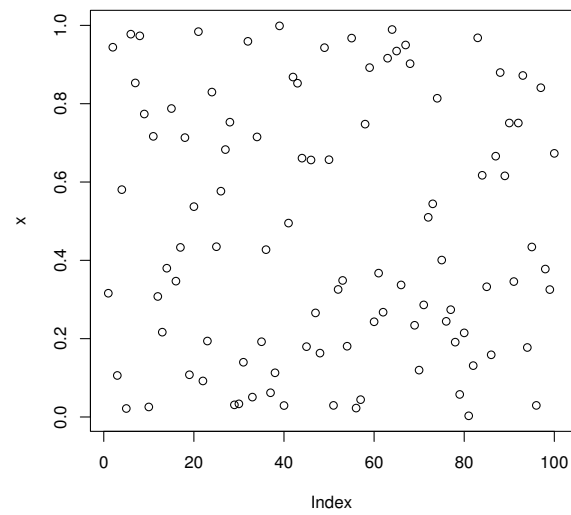
Chapman & Hall/CRC Press, Boca Raton (FL), 2009.
ISBN: 978-1-4200-8678-2.

<http://sintro.r-forge.r-project.org/>

Example 1.1: A Simple Plot

Input

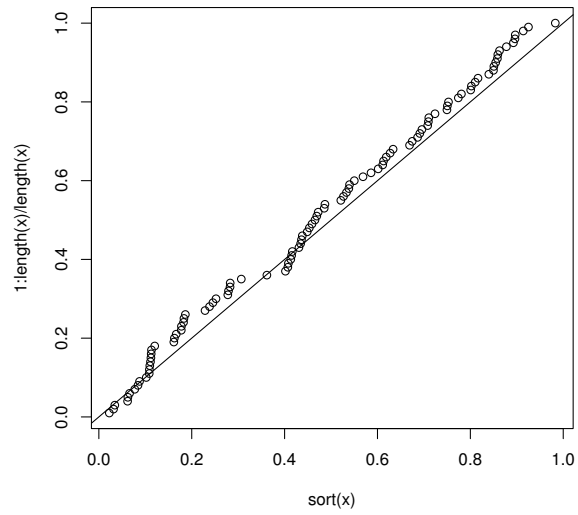
```
x <- runif(100)  
plot(x)
```



Example 1.5: Empirical Distribution Function

Input

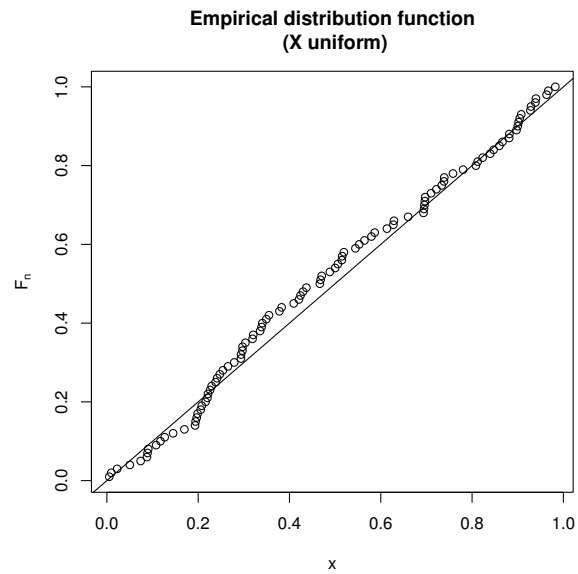
```
x <- runif(100)
plot(sort(x), 1:length(x)/length(x))
abline(0, 1)
```



Example 1.6: Empirical Distribution Function (Annotated Plot)

Input

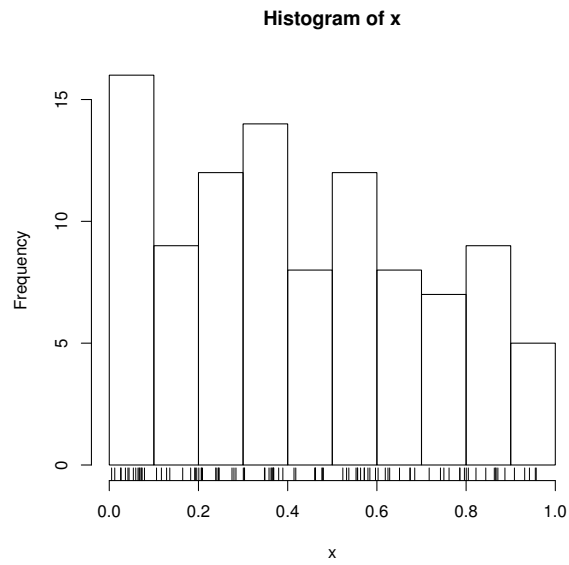
```
x <- runif(100)
plot(sort(x), (1:length(x))/length(x),
      xlab = "x", ylab = expression(F[n]),
      main = "Empirical distribution function\n (X uniform)"
)
abline(0, 1)
```



Example 1.7: Histogram with Rug

Input

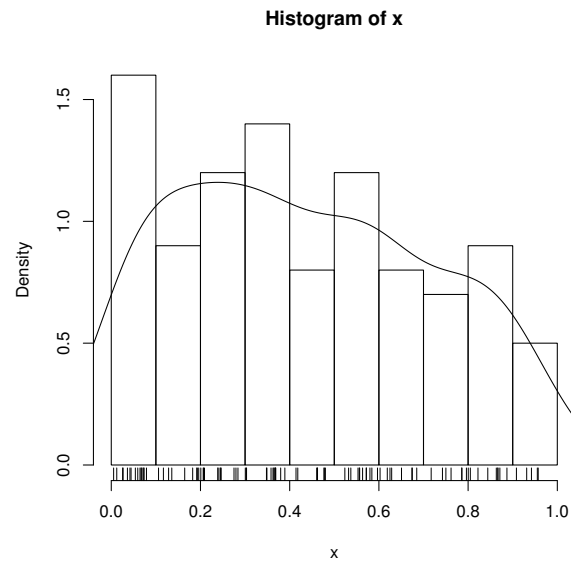
```
x <- runif(100)
hist(x)
rug(x)
```



Example 1.8: Augmented Histogram

Input

```
hist(x, probability = TRUE)  
rug(x)  
lines(density(x))
```



Example 1.9: Histogram Data Structure

Input

```
x <- runif(100)
whist <- hist(x)
whist
```

Output

```
$breaks
[1] 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0

$counts
[1] 11 13 13 12  8 14  6  6  9  8

$intensities
[1] 1.100000 1.300000 1.300000 1.200000 0.800000 1.400000 0.600000 0.600000
[9] 0.900000 0.800000

$density
[1] 1.100000 1.300000 1.300000 1.200000 0.800000 1.400000 0.600000 0.600000
[9] 0.900000 0.800000

$mids
[1] 0.05 0.15 0.25 0.35 0.45 0.55 0.65 0.75 0.85 0.95

$xname
[1] "x"

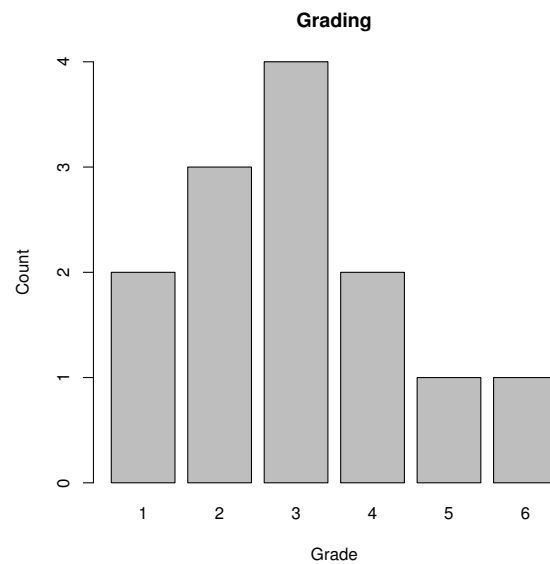
$equidist
[1] TRUE

attr(,"class")
[1] "histogram"
```


Example 1.10: Barchart

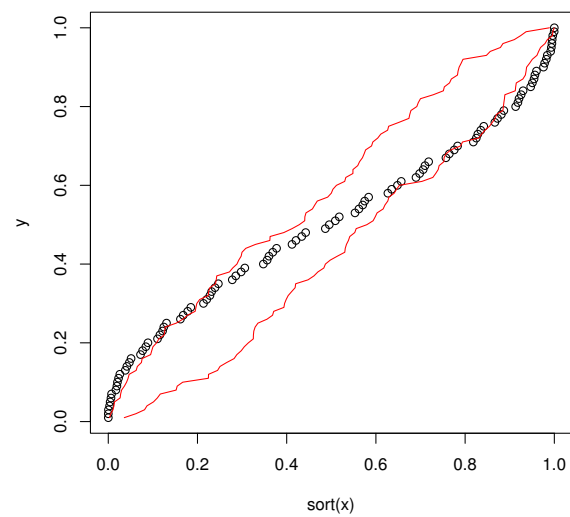
Input

```
grades <- c(2, 1, 3, 4, 2, 2, 3, 5, 1, 3, 4, 3, 6)
barplot(table(grades), xlab = 'Grade', ylab = 'Count',
        ylim = c(0, max(table(grades))),
        main = 'Grading')
```



Example 1.11: Monte Carlo Confidence Bands

```
Input
x <- (sin(1:100)+1)/2 # demo example only
y <- (1:length(x))/length(x)
plot(sort(x), y)
nrsamples <- 19 # no of simulations
samples <- matrix(data = runif(length(x)* nrsamples),
  nrow = length(x), ncol = nrsamples)
samples <- apply(samples, 2, sort)
envelope <- t(apply(samples, 1, range))
lines(envelope[, 1], y, col = "red")
lines(envelope[, 2], y, col = "red")
```

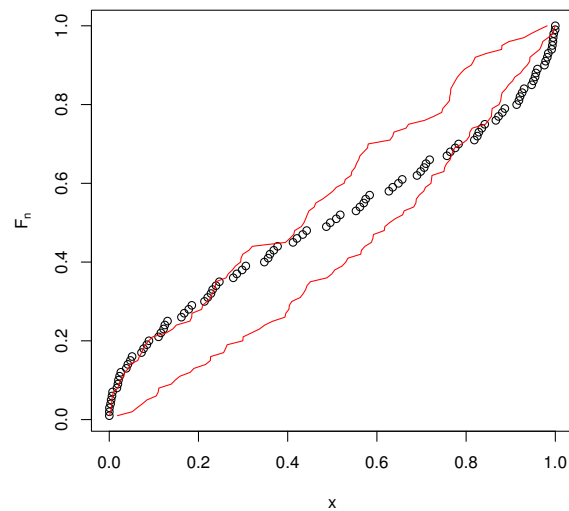


Example 1.12: Monte Carlo Confidence Bands (Augmented)

Input

```
plot(sort(x), y,  
     main = paste("Monte Carlo Band: ",  
                   bquote(.(nrsamples)), " Monte Carlo Samples"),  
     xlab = 'x', ylab = expression(F[n]))  
samples <- matrix(data = runif(length(x) * nrsamples),  
                  nrow = length(x), ncol = nrsamples)  
samples <- apply(samples, 2, sort)  
envelope <- t(apply(samples, 1, range))  
lines(envelope[, 1], y, col = "red")  
lines(envelope[, 2], y, col = "red")
```

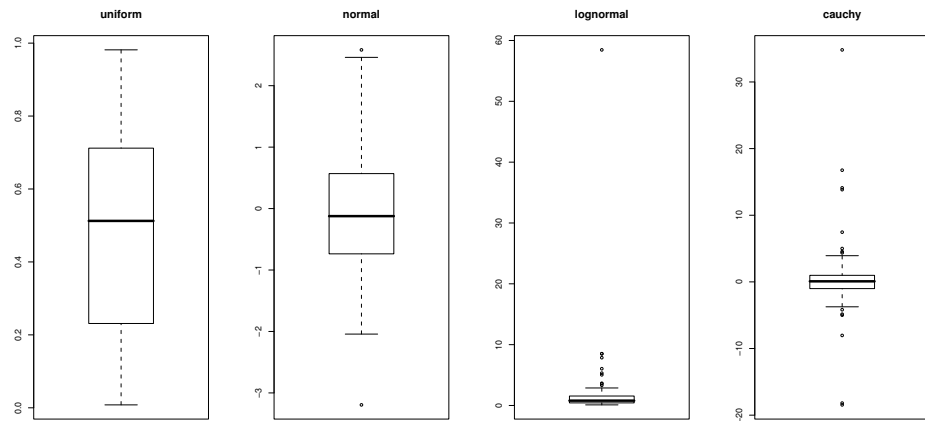
Monte Carlo Band: 19 Monte Carlo Samples



Example 1.13: Box-and-Whisker Plot

Input

```
oldpar <- par(mfrow = c(1, 4))
boxplot(runif(100), main = "uniform")
boxplot(rnorm(100), main = "normal")
boxplot(exp(rnorm(100)), main = "lognormal")
boxplot(rcauchy(100), main = "cauchy")
par(oldpar)
```



Example 1.14: Distribution Functions (Various Distributions)

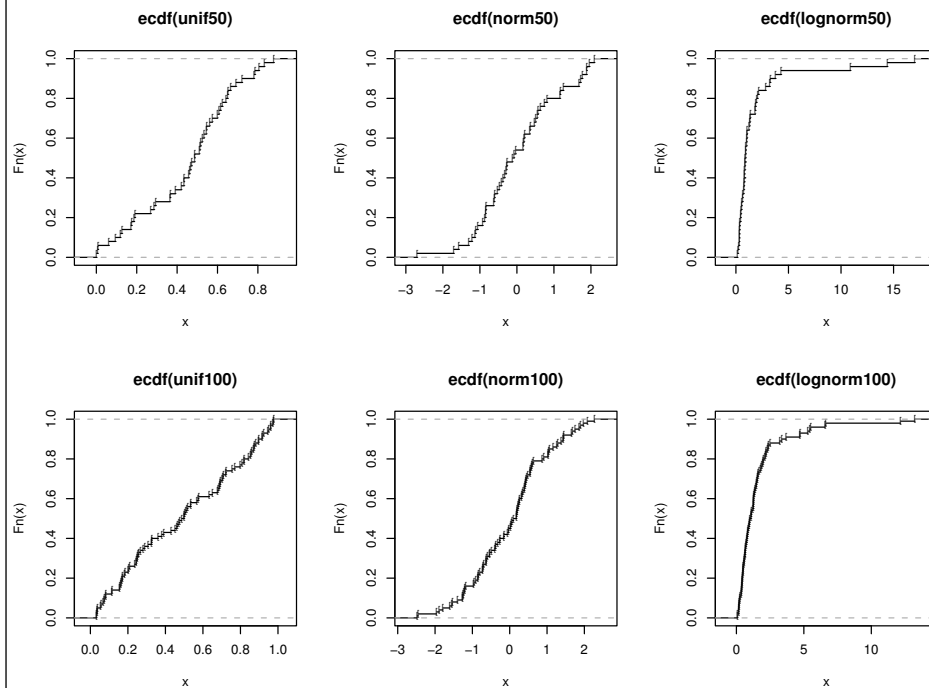
Input

```
oldpar <- par(mfrow = c(2, 3))

plot(ecdf(unif50), pch = "")
plot(ecdf(norm50), pch = "")
plot(ecdf(lognorm50), pch = "")

plot(ecdf(unif100), pch = "")
plot(ecdf(norm100), pch = "")
plot(ecdf(lognorm100), pch = "")

par(oldpar)
```



Example 1.15: Normal QQ Plots (Various Distributions)

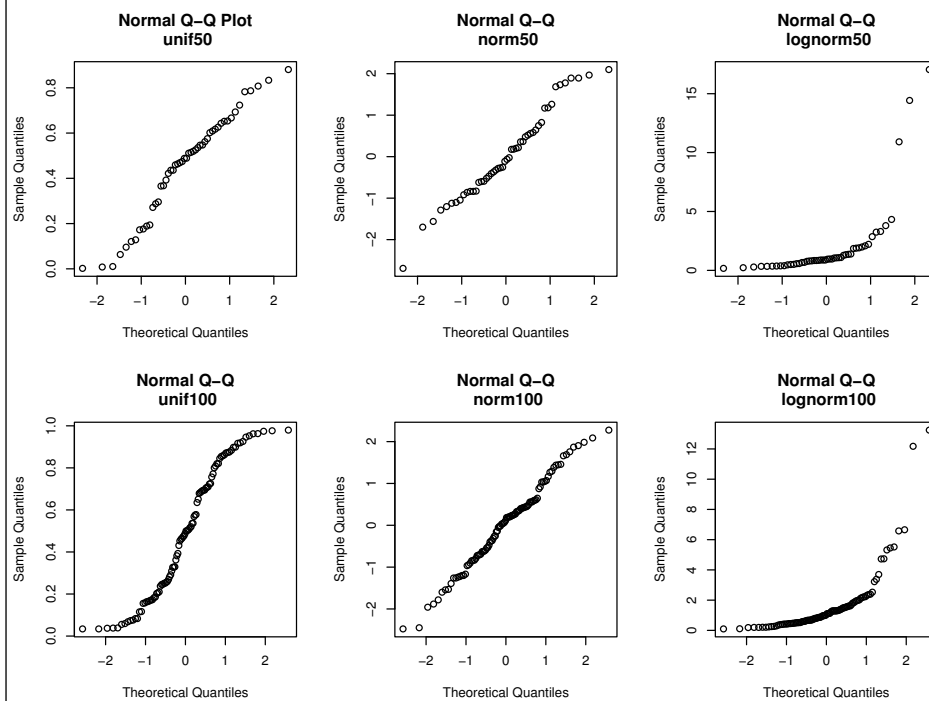
Input

```
oldpar <- par(mfrow = c(2, 3))

qqnorm(unif50, main = "Normal Q-Q Plot\n unif50")
qqnorm(norm50, main = "Normal Q-Q\n norm50")
qqnorm(lognorm50, main = "Normal Q-Q\n lognorm50")

qqnorm(unif100, main = "Normal Q-Q\n unif100")
qqnorm(norm100, main = "Normal Q-Q\n norm100")
qqnorm(lognorm100, main = "Normal Q-Q\n lognorm100")

par(oldpar)
```



Exercise 1.26	
	Use <i>PP</i> plots instead of distribution functions to illustrate the χ^2 - and Kolmogorov-Smirnov approximations.

Exercise 1.27	
	Use <i>QQ</i> plots instead of distribution functions. Can you add confidence regions to these plots with the help of the χ^2 - resp. Kolmogorov-Smirnov statistics?

To get an impression of the fluctuation, we have to compare the empirical plots with typical plots of a model distribution. A plot matrix is a simple way to do this. Here is an example for the normal *QQ* plot, implemented as a function:

Input

```
qqnormx <- function(x, nrow = 5, ncol = 5, main = deparse(substitute(x))) {
  oldpar <- par(mfrow = c(nrow, ncol))
  qqnorm(x, main = main)
  for (i in 1:(nrow*ncol-1))
    qqnorm(rnorm(length(x)), main = "N(0, 1)", xlab="", ylab="")
  par(oldpar)
}
```

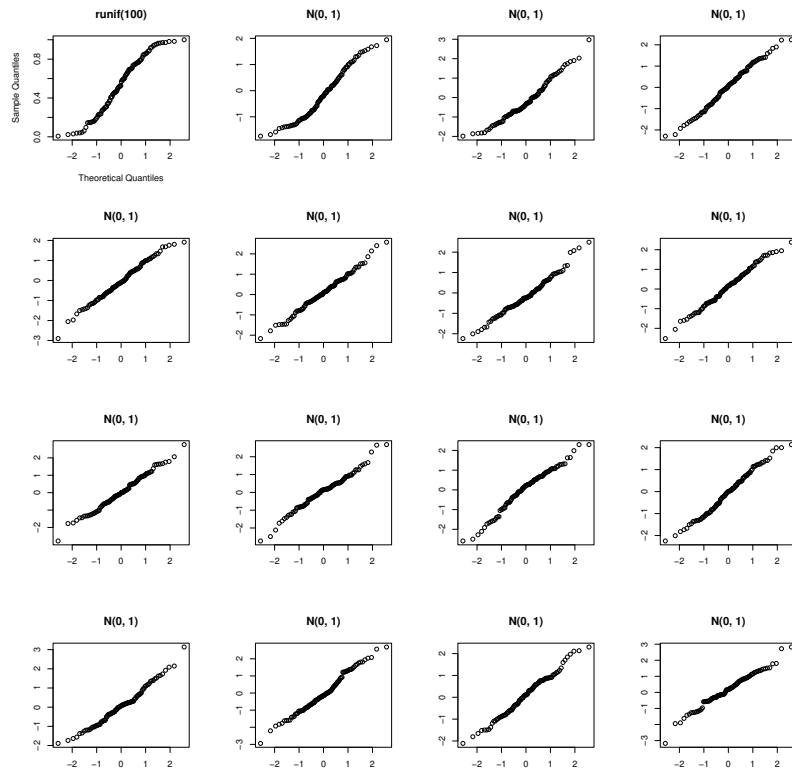
In this example we used a *for* loop. Like all programming languages, R has control structures such as loops or conditional statements. In R, however, loops should be avoided if possible in favor of more efficient language constructs (see [?]). A summary of control structures in R can be found in Appendix ?? (page ??).

Exercise 1.28	
	Generate a matrix of dimensions $(nrow * ncol - 1), length(x)$ with random numbers and use apply() to avoid the loop. <i>Hint:</i> See Example 1.11 (page 32).

Deviations from a linear structure should be considered as fluctuations if they stay within the frame of the simulated examples. If the data set under investigation is too extreme in comparison with the simulated examples, this indicates a contradiction with the model assumptions. Because of space limitations of the printing area, we use only a small number of comparison plots here.

Example 1.16: Graphical Monte Carlo Test

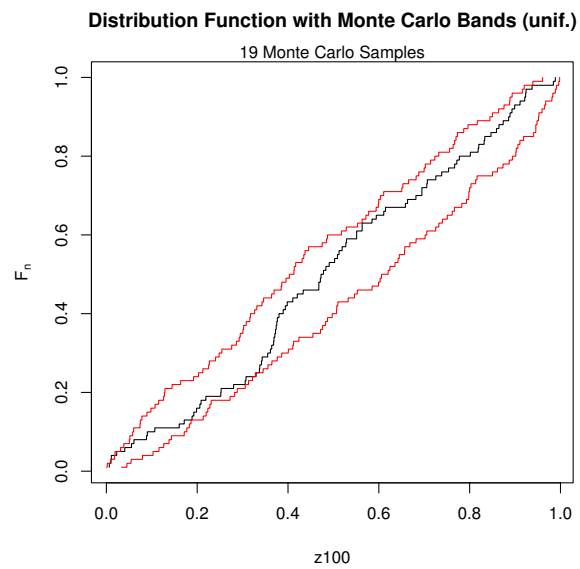
`qqnormx(runif(100), nrow=4, ncol=4)` *Input*



Example 1.17: R Function Call

Input

```
z100 <- runif(100)
ppdemo(z100)
```



Example 1.18: R Function Listing

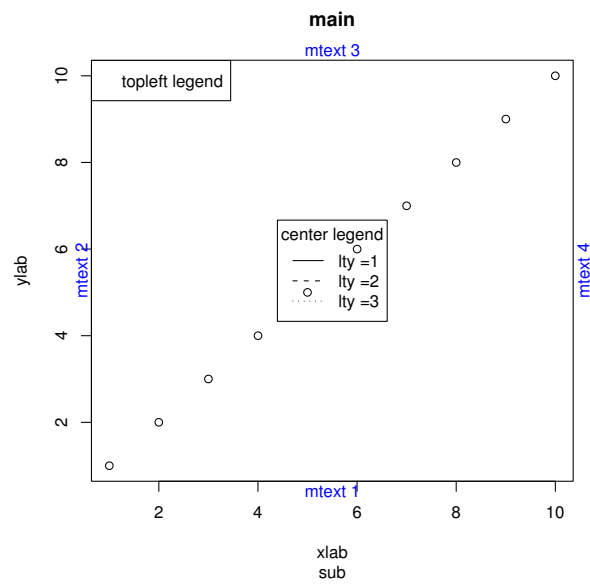
ppdemo *Input*

Output

```
function (x, samps = 19) {      # samps: nr of simulations
  y <- (1:length(x))/length(x)
  plot(sort(x), y, xlab = substitute(x), ylab = expression(F[n]),
        main = "Distribution Function with Monte Carlo Bands (unif.)",
        type = "s")
  mtext(paste(samps, "Monte Carlo Samples"), side = 3)
  samples <- matrix(runif(length(x)* samps),
                    nrow = length(x), ncol = samps)
  samples <- apply(samples, 2, sort)
  envelope <- t(apply(samples, 1, range))
  lines(envelope[, 1], y, type = "s", col = "red");
  lines(envelope[, 2], y, type = "s", col = "red")
}
```

Example 1.19: Margin Text

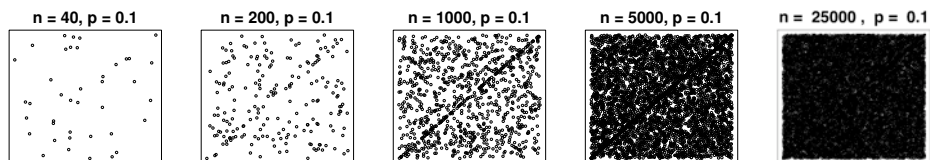
```
plot(1:10, xlab = "xlab", ylab = "ylab", main = "main", sub = "sub")
mtext("mtext 1", side = 1, col = "blue")
mtext("mtext 2", side = 2, col = "blue")
mtext("mtext 3", side = 3, col = "blue")
mtext("mtext 4", side = 4, col = "blue")
legend("topleft", legend = "topleft legend")
legend("center", legend = c("lty =1", "lty =2", "lty =3"),
      lty = 1:3, title = "center legend")
```



Example 1.20: Needle in the Haystack

```
NeedleInTheHayStack <- function(nn, Input p=0.1, col="black", ... ) {  
  oldpar <- par(mfrow=c(1,length(nn)))  
  on.exit(par(oldpar))  
  for (n in nn){  
    nhay <- n-round(p*n); xhay <- runif(nhay); yhay <- runif(nhay)  
    needle <- runif(round(p*n))  
    plot( x = c(xhay, needle), y = c(yhay,needle),  
          main = paste("n = ", n, ", p = ", p, sep=""),  
          cex.main=3.0,  
          axes=FALSE, frame.plot=TRUE,  
          xlab="", ylab="",  
          col= col, ...)  
  }  
}
```

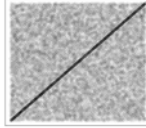
`NeedleInTheHayStack(c(40, 200,1000, 5000, 25000))`



Example 1.21: Needle in the Haystack

Input
`NeedleInTheHayStack(25000, col = rgb(red=0, blue=0, green=0, alpha=0.1))`

n = 25000, p = 0.1



Example 2.3: Least Squares Estimator

`lm(y ~ x)`

Input

Call:

`lm(formula = y ~ x)`

Output

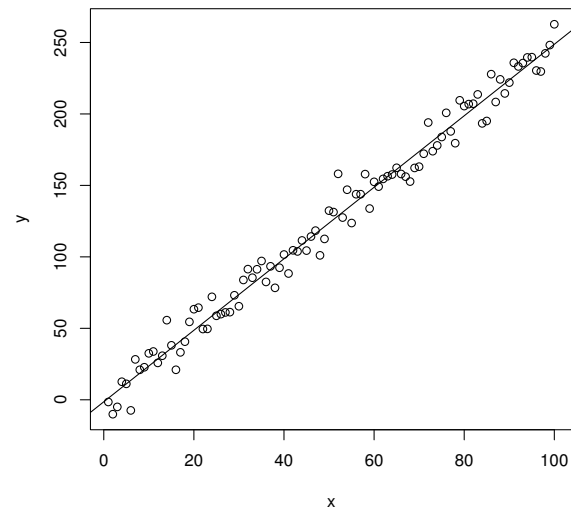
Coefficients:

(Intercept)	x
-1.416	2.502

Example 2.4: Linear Model Plot

Input

```
lmres <- lm(y ~ x)
plot(x, y)
abline(lmres)
```



Example 2.5: Linear Model Summary

Input

```
summary(lm( y ~ x))
```

Output

Call:

```
lm(formula = y ~ x)
```

Residuals:

Min	1Q	Median	3Q	Max
-21.0700	-6.7568	0.4417	5.6749	29.3925

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-1.41598	1.92062	-0.737	0.463
x	2.50154	0.03302	75.762	<2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 9.531 on 98 degrees of freedom

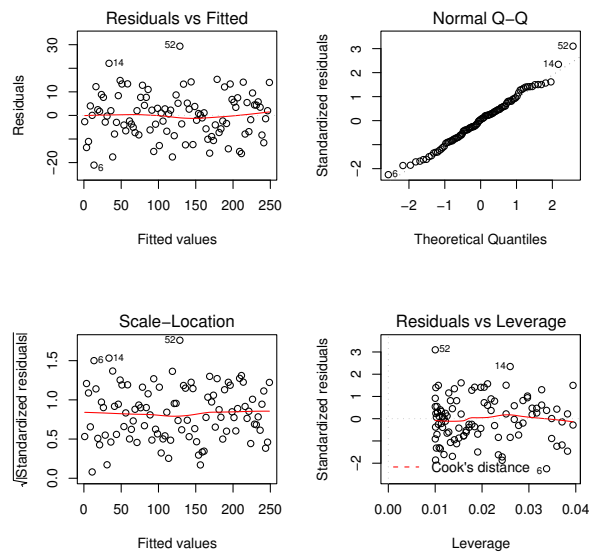
Multiple R-squared: 0.9832, Adjusted R-squared: 0.983

F-statistic: 5740 on 1 and 98 DF, p-value: < 2.2e-16

Example 2.6: Linear Model Plot

Input

```
plot(lm(y ~ x))
```



Example 2.7: Linear Model ANOVA Summary

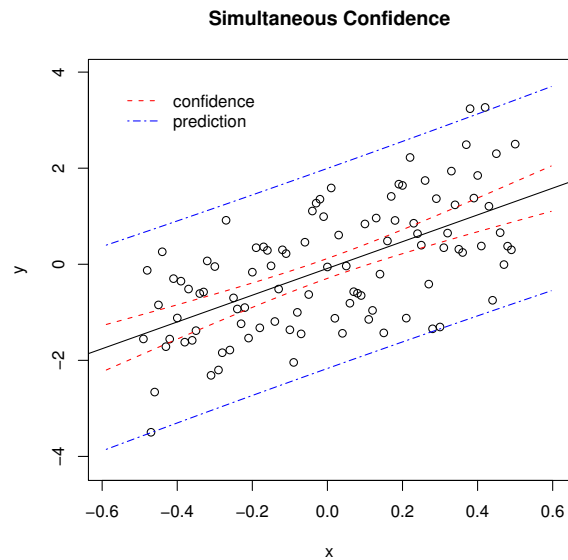
```
summary(aov(lmres))
```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
x	1	521421	521421	5739.8	< 2.2e-16 ***
Residuals	98	8903	91		

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Example 2.8: Linear Model Confidence Bands

```
plot(x, y, xlim = xlim, ylim = ylim)
abline(lmxy)
matplot(newx$x,
        cbind(pred.w.clim[, -1], pred.w.plim[, -1]),
        lty = c(2, 2, 6, 6),
        col = c(2, 2, 4, 4),
        type = "l", add = TRUE)
title(main = "Simultaneous Confidence")
legend("topleft",
       lty = c(2, 6),
       legend = c("confidence", "prediction"),
       col = c(2, 4),
       inset = 0.05, bty = "n")
```



Example 2.9: Tukey's Multiple Comparison

Input

```
library(multcomp)
lhtres <- glht(lmres, linfct=mcp(Tmt="Tukey"))
summary(lhtres) # multiple tests
```

Output

Simultaneous Tests for General Linear Hypotheses

Multiple Comparisons of Means: Tukey Contrasts

Fit: $\text{lm}(\text{formula} = y \sim 0 + \text{Tmt}, \text{data} = \text{s35})$

Linear Hypotheses:

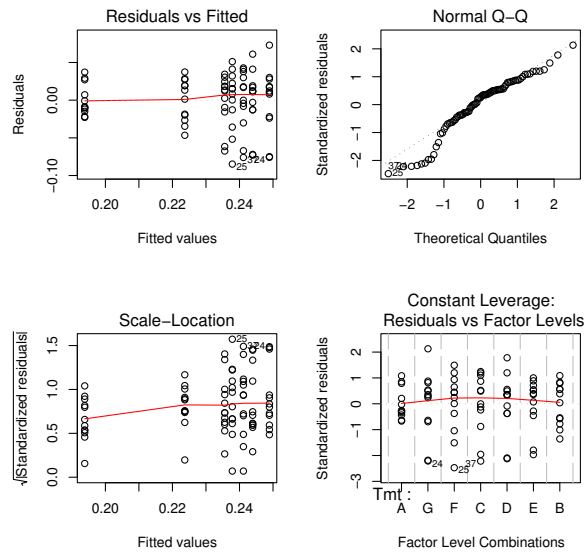
	Estimate	Std. Error	t value	p value	
B - A == 0	0.055083	0.014632	3.765	0.00597	**
C - A == 0	0.044000	0.014632	3.007	0.05256	.
D - A == 0	0.047333	0.014632	3.235	0.02838	*
E - A == 0	0.050083	0.014632	3.423	0.01642	*
F - A == 0	0.041750	0.014632	2.853	0.07792	.
G - A == 0	0.029833	0.014632	2.039	0.39924	
C - B == 0	-0.011083	0.014632	-0.757	0.98819	
D - B == 0	-0.007750	0.014632	-0.530	0.99832	
E - B == 0	-0.005000	0.014632	-0.342	0.99986	
F - B == 0	-0.013333	0.014632	-0.911	0.96971	
G - B == 0	-0.025250	0.014632	-1.726	0.60097	
D - C == 0	0.003333	0.014632	0.228	0.99999	
E - C == 0	0.006083	0.014632	0.416	0.99958	
F - C == 0	-0.002250	0.014632	-0.154	1.00000	
G - C == 0	-0.014167	0.014632	-0.968	0.95931	
E - D == 0	0.002750	0.014632	0.188	1.00000	
F - D == 0	-0.005583	0.014632	-0.382	0.99974	
G - D == 0	-0.017500	0.014632	-1.196	0.89359	
F - E == 0	-0.008333	0.014632	-0.570	0.99748	
G - E == 0	-0.020250	0.014632	-1.384	0.80870	
G - F == 0	-0.011917	0.014632	-0.814	0.98280	

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Adjusted p values reported -- single-step method)

Example 2.10: Multiple Comparison Model Check

Input

```
oldpar <- par(mfrow=c(2,2))
plot(lmres)
par(oldpar)
```



Example 2.11: Diagnostic Using Studentized Residuals

Input

```
library(MASS)
s35$studres <- studres(lmres)
s35[s35$studres < -1,]
```

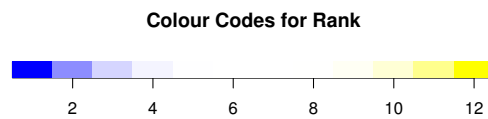
Output

	y	Tmt	Lane	studres
13	0.174	B	1	-2.239390
24	0.173	B	12	-2.271296
25	0.153	C	1	-2.559766
33	0.202	C	9	-1.044865
36	0.186	C	12	-1.523409
37	0.165	D	1	-2.279286
48	0.174	D	12	-1.994858
49	0.171	E	1	-2.175828
60	0.172	E	12	-2.144169
61	0.168	F	1	-2.007887
72	0.174	F	12	-1.821449
73	0.177	G	1	-1.367608
84	0.189	G	12	-1.010381

Example 2.12: Custom Colour Palette

Input

```
oldpar <- par(yaxt="n")
image(x=1:12, z=matrix(1:12,ncol=1),
      col=blueyellow4.colors(12),
      xlab="", main="Colour Codes for Rank")
par(oldpar)
```

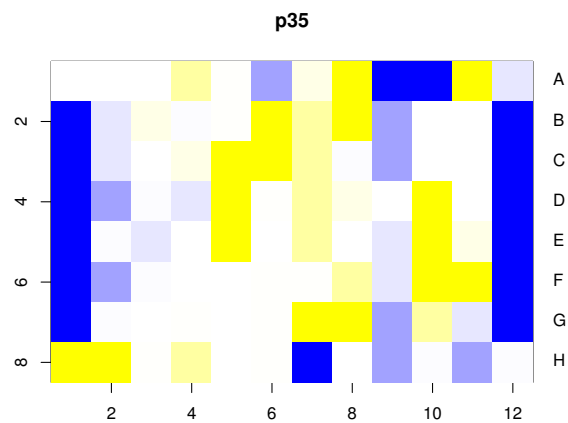


See Colour Figure 2.

Example 2.13: Residual Diagnostic

Input

```
a35 <- as.matrix( p35[3:10] )  
a35rk <- apply(a35, 2, rank)  
imagem(t(a35rk), col=blueyellow4.colors(10), main="p35")
```

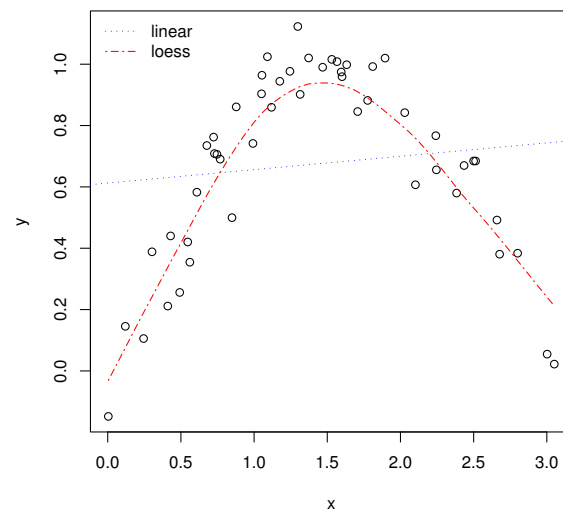


See Colour Figure 2.

Example 2.14: Non-Linear Regression

Input

```
plot(x, y)
abline(lm(y ~ x), lty = 3, col = "blue")
lines(loess.smooth(x, y), lty = 6, col = "red")
legend("topleft",
      legend = c("linear", "loess"),
      lty = c(3, 6), col = c("blue", "red"), bty = "n")
```



Example 2.15: Method Dispatch

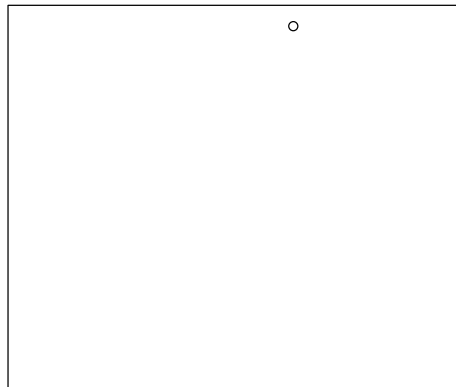
	Input	
	<code>plot</code>	
		Output
		<pre>function (x, y, ...) { if (is.function(x) && is.null(attr(x, "class"))) { if (missing(y)) y <- NULL hasylab <- function(...) !all(is.na(pmatch(names(list(...)), "ylab"))) if (hasylab(...)) plot.function(x, y, ...) else plot.function(x, y, ylab = paste(deparse(substitute(x)), "(x)", ...) } else UseMethod("plot") } <environment: namespace:graphics></pre>

Example 3.1: Interactive Location

Input

```
plot(x = runif(1), y = runif(1),  
     xlim = c(0, 1), ylim = c(0, 1),  
     main = "Please click on the circle",  
     xlab = "", ylab = "",  
     axes = FALSE, frame.plot = TRUE)  
xclick <- locator(1)
```

Please click on the circle



Example 3.2: Click Timing

Input

```
click1 <- function(){
  x <- runif(1); y <- runif(1)
  plot(x = x, y = y, xlim = c(0, 1), ylim = c(0, 1),
       main = "Please click on the circle",
       xlab = "", ylab = "",
       axes = FALSE, frame.plot = TRUE)
  clicktime <- system.time(xyclick <- locator(1))
  list(timestamp = Sys.time(),
       x = x, y = y,
       xclick = xyclick$x, yclick = xyclick$y,
       tclick = clicktime[3])
}
```

Example 3.3: Sequential Recording

Input

```
dx <- as.data.frame(click1())  
dx <- rbind(dx, data.frame(click1()))  
dx
```

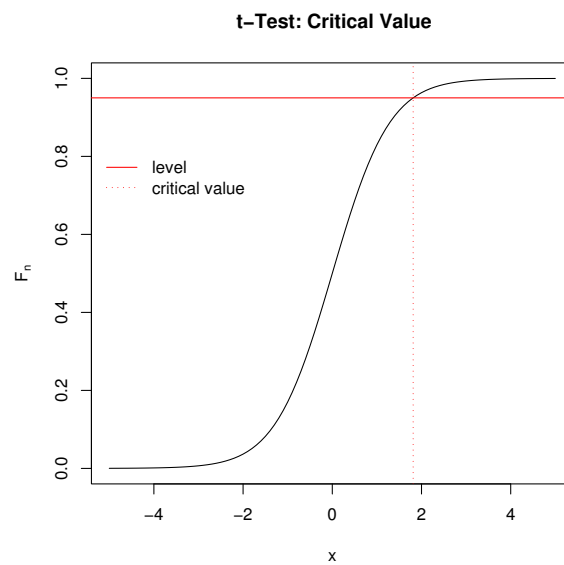
Output

	timestamp	x	y	xclick	yclick	tclick
elapsed	2008-12-12 15:14:26	0.7034	0.6072	0.7044	0.6070	1.899
elapsed1	2008-12-12 15:14:28	0.6948	0.9285	0.7003	0.9352	1.855

Example 3.4: Test Construction

Input

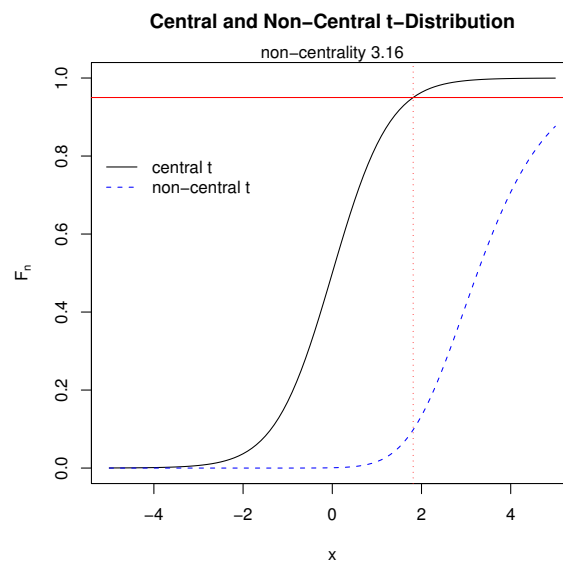
```
n1<- 6; n2 <- 6
df <-  n1 + n2 -2
alpha <- 0.05
curve(pt(x,df=df),from=-5, to=5, ylab= expression(F[n]),
      main="t-Test: Critical Value")
abline(h=1-alpha, col="red")      # cut at upper quantile
abline(v=qt(1-alpha, df=df), lty=3, col="red") # get critical value
legend("topleft", legend=c("level","critical value"),
      lty=c(1,3),col="red",
      bty="n", inset=c(0,0.2))
```



Example 3.5: Power (Fixed Non-Centrality)

Input

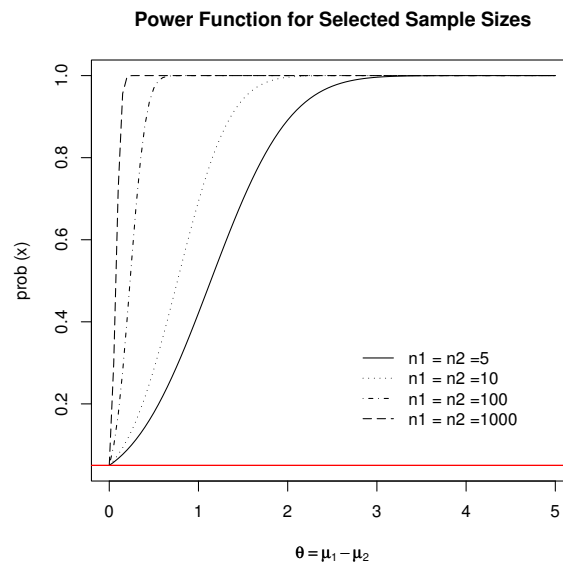
```
n1<- 6; n2 <- 6
df <-  n1 + n2 -2
alpha <- 0.05
curve(pt(x,df=df),from=-5, to=5, ylab= expression(F[n]),
      main="Central and Non-Central t-Distribution")
abline(h=1-alpha, col="red")      # cut at upper quantile
abline(v=qt(1-alpha, df=df), lty=3, col="red") # get critical value
n1 <- 5
n2 <- 5
n <- n1+n2
theta <- 2
ncp <- theta * sqrt(n1 * n2/(n1+n2))
mtext(paste("non-centrality",round(ncp,2)))
curve(pt(x,df=df, ncp=ncp), lty=2, add=TRUE, col="blue")
legend("topleft", legend=c("central t","non-central t"),
      lty=c(1,2), col=c("black","blue"),
      bty="n", inset=c(0,0.2))
```



Example 3.6: Power Function

Input

```
tpower <- function(n1, n2, alpha,...){  
  df <- n1 + n2 -2  
  tlim <- qt(1-alpha,df=df)  
  prob <- function(theta){  
    pt(tlim, df = df,  
       ncp = theta * sqrt(n1 * n2/(n1+n2)),  
       lower.tail=FALSE)}  
  curve(prob, 0, 5, xlab=expression(theta==mu[1]-mu[2]), ...)  
  abline(h=alpha, col="red")  
}  
  
tpower(5, 5, 0.05, main="Power Function for Selected Sample Sizes")  
tpower(10, 10, 0.05, add =TRUE, lty = 3)  
tpower(100,100, 0.05, add =TRUE, lty = 4)  
tpower(1000, 1000, 0.05, add =TRUE, lty = 5)  
legend("bottomright",  
      lty=c(1,3,4,5),  
      legend=c("n1 = n2 =5", "n1 = n2 =10", "n1 = n2 =100", "n1 = n2 =1000"),  
      inset=0.1, bty="n")
```



Example 3.7: Sample Size Determination

Input

```
power.t.test(delta=2,  
  power=0.8,  
  sig.level=0.01,  
  type="two.sample",  
  alternative="one.sided")
```

Output

Two-sample t test power calculation

```
      n = 6.553292  
delta = 2  
  sd = 1  
sig.level = 0.01  
  power = 0.8  
alternative = one.sided
```

NOTE: n is number in *each* group

Example 3.8: Violation of Assumptions (log-normal)

Input

```
nsimul <- 500
n1<- 10; n2 <- 10
alpha <- 0.01 #nominal level
x <- 0
for (i in 1:nsimul) {
  if (t.test(exp(rnorm(n1)),exp(rnorm(n2)),
    alternative="less",
    var.equal = TRUE)$p.value < alpha){
    x <- x+1}
}
p <- x/nsimul
cat("estimated level p", p)
```

Output

```
estimated level p 0.006
```

Example 3.9: Binomial Confidence Set

Input

```
prop.test(n=nsimul, x=x)
```

Output

```
1-sample proportions test with continuity correction
```

```
data:  x out of nsimul, null probability 0.5
X-squared = 486.098, df = 1, p-value < 2.2e-16
alternative hypothesis: true p is not equal to 0.5
95 percent confidence interval:
 0.001550854 0.018951807
sample estimates:
      p
0.006
```

Example 3.10:

Input

```
nsimul <- 500
n1<- 10; n2 <-10
alpha <- 0.01
x<-0
for (i in 1:nsimul) {
  if (t.test(exp(rnorm(n1)),exp(rnorm(n2, mean = 1)),
    alternative="less",
    var.equal = TRUE)$p.value < alpha){
    x <- x+1}
}
p <- x/nsimul
cat("estim p", p)
```

Output

```
estim p 0.188
```

Input

```
prop.test(n = nsimul, x = x)
```

Output

1-sample proportions test with continuity correction

```
data:  x out of nsimul, null probability 0.5
X-squared = 193.442, df = 1, p-value < 2.2e-16
alternative hypothesis: true p is not equal to 0.5
95 percent confidence interval:
 0.1552568 0.2256388
sample estimates:
      p
0.188
```

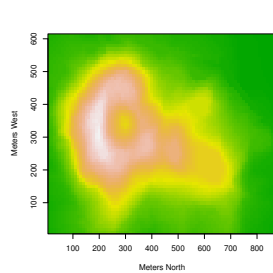
Example 4.1: 3d Surface Displays Using Base Graphics

Input

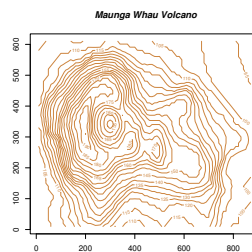
```
x <- 10*(1:nrow(volcano))
y <- 10*(1:ncol(volcano))
image(x, y, volcano, col = terrain.colors(100),
      axes = FALSE, xlab = "Meters North", ylab = "Meters West")
axis(1, at = seq(100, 800, by = 100))
axis(2, at = seq(100, 600, by = 100))
box()
title(main = "Maunga Whau Volcano", font.main = 4)

contour(x, y, volcano, levels = seq(90, 200, by = 5),
        col = "peru", main = "Maunga Whau Volcano", font.main = 4,
        xlab = "Meters North", ylab = "Meters West")
z <- 2 * volcano      # Exaggerate the relief
x <- 10 * (1:nrow(z)) # 10 meter spacing (S to N)
y <- 10 * (1:ncol(z)) # 10 meter spacing (E to W)

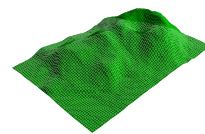
## Don't draw the grid lines : border = NA
persp(x, y, z, theta = 135, phi = 30, col = "green3", scale = FALSE,
      ltheta = -120, shade = 0.75, border = NA, box = FALSE)
```



`image()`



`contour()`
See Colour Figure 3.

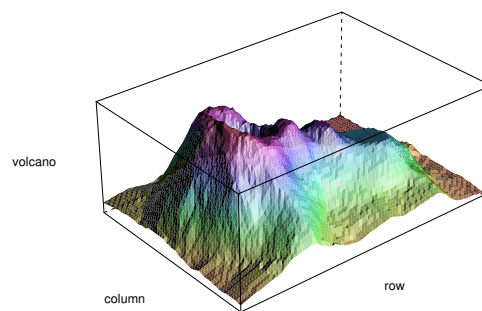


`persp()`

Example 4.2: 3d Surface Display Using Lattice Graphics

Input

```
library(lattice)
print(wireframe(volcano, shade = TRUE,
  aspect = c(61/87, 0.4),    ## volcano ## 87 x 61 matrix
  par.settings = list(axis.line = list(col = "transparent")),
  light.source = c(10,0,10)))
```



See Colour Figure 4.

Example 4.3: Scatterplot Matrix for Diabetes Data

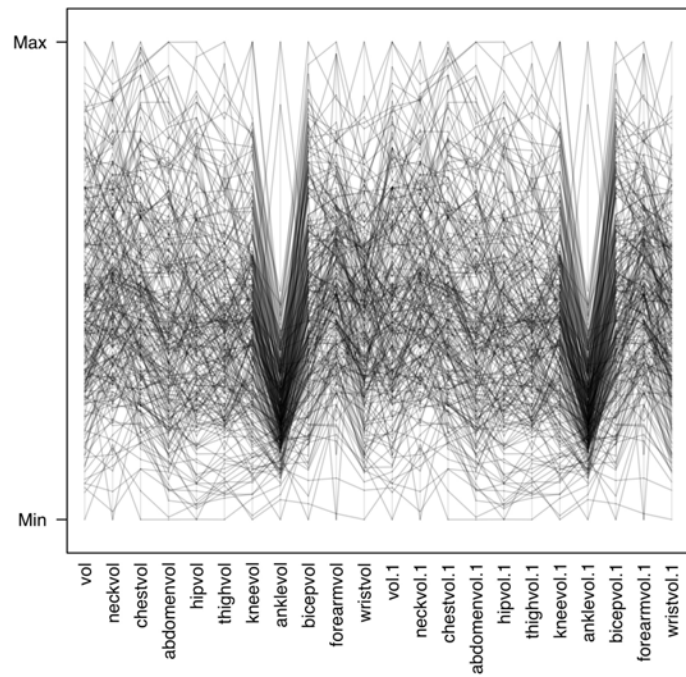
Input

```
pairs(~fpg + ga + ina + sspg, data = chemdiab,      pch = 21,
      main = "Diabetes-data",
      bg = c("magenta", "green3", "cyan")[unclass(chemdiab$cc)],
      oma = c(8, 8, 8, 8))
mtext(c("Colour codes:", levels(chemdiab$cc)),
      col = c("black", "magenta", "green3", "cyan"),
      at = c(0.1, 0.4, 0.6, 0.8), side = 1, line = 2)
```

Output: see Figure 4.1.

Example 4.4: Parallel Plots

```
print(parallel(fat[ -c(39, 41, 216), c(19:29,19:29)],  
             horizontal.axis = FALSE, scales = list(x = list(rot = 90)),  
             col = rgb(red=0, blue=0, green=0, alpha=0.2))  
)
```



Input

Input

