Solution: Statistics, dimensionality reduction, and clustering

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Demo

The standard normal distribution

pnorm() The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(-5, 5, 0.1)
head(data_quantiles)
```

```
## [1] -5.0 -4.9 -4.8 -4.7 -4.6 -4.5
```

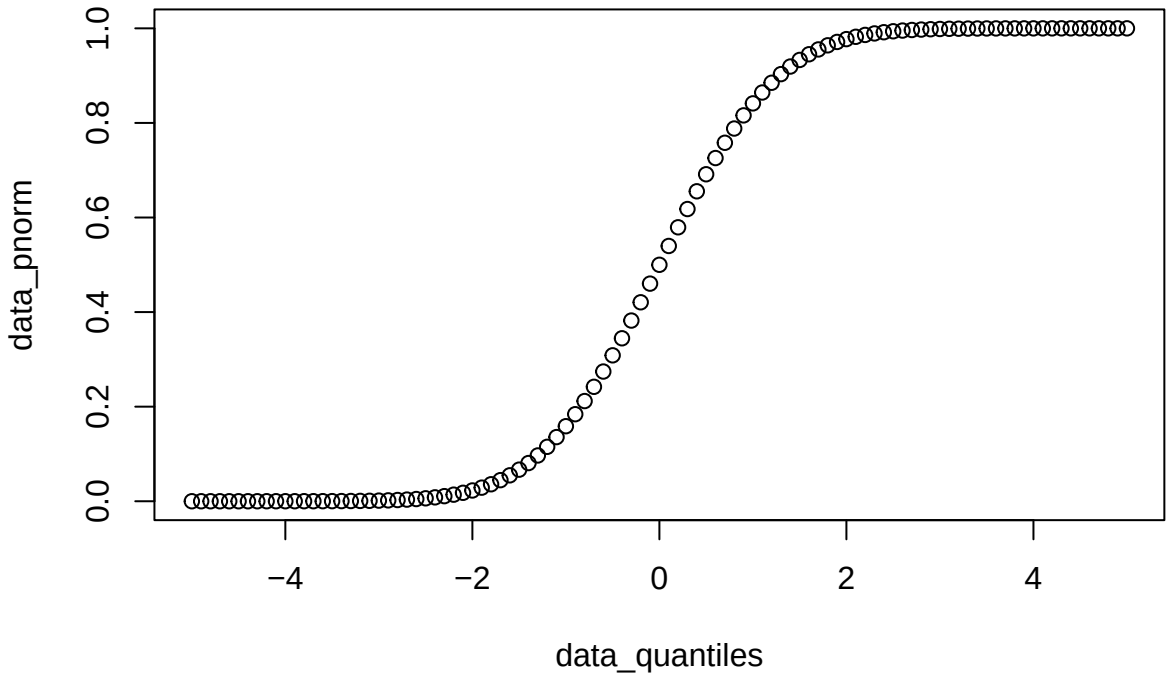
The function `pnorm()` returns the probability of a observing a value less or equal to each quantile given.

```
data_pnorm <- pnorm(q = data_quantiles)
head(data_pnorm)
```

```
## [1] 2.866516e-07 4.791833e-07 7.933282e-07 1.300807e-06 2.112455e-06
## [6] 3.397673e-06
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_pnorm)
```



qnorm() The function `qnorm()` takes as input a vector of probabilities between 0 and 1.

```
data_probabilities <- seq(from = 0, to = 1, by = 0.02)
head(data_probabilities)
```

```
## [1] 0.00 0.02 0.04 0.06 0.08 0.10
```

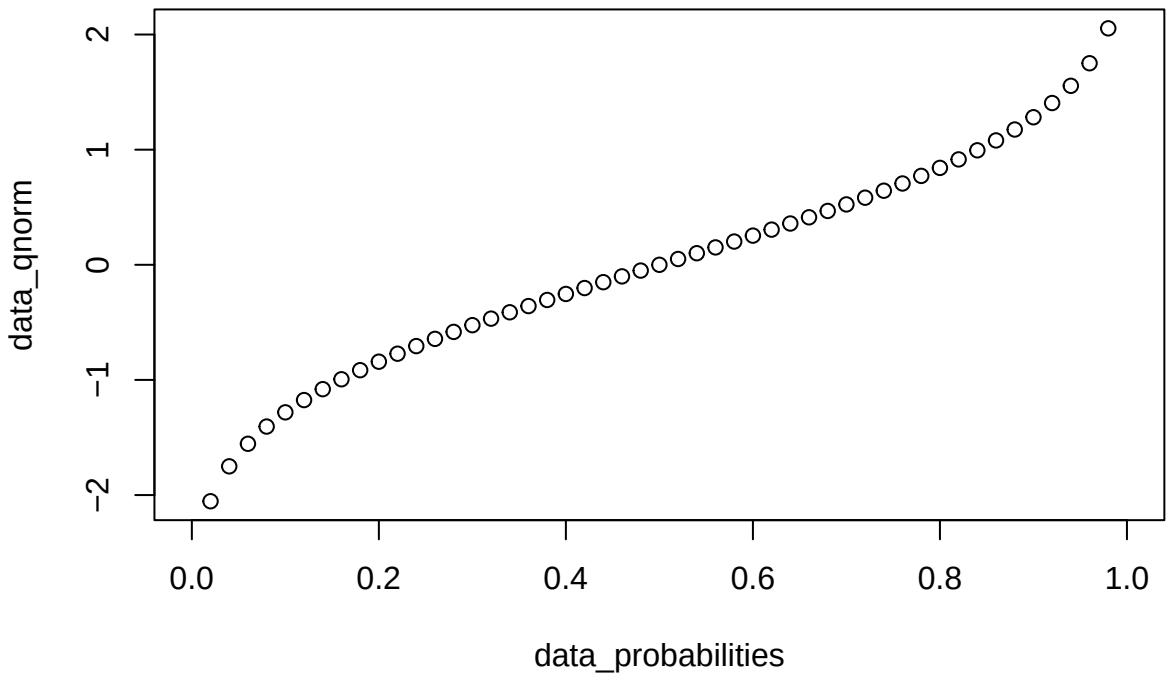
The function `qnorm()` the quantiles (i.e., values) that correspond to those probabilities.

```
data_qnorm <- qnorm(p = data_probabilities)
head(data_qnorm)
```

```
## [1]      -Inf -2.053749 -1.750686 -1.554774 -1.405072 -1.281552
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_probabilities, data_qnorm)
```



dnorm The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(-5, 5, 0.2)
head(data_quantiles)
```

```
## [1] -5.0 -4.8 -4.6 -4.4 -4.2 -4.0
```

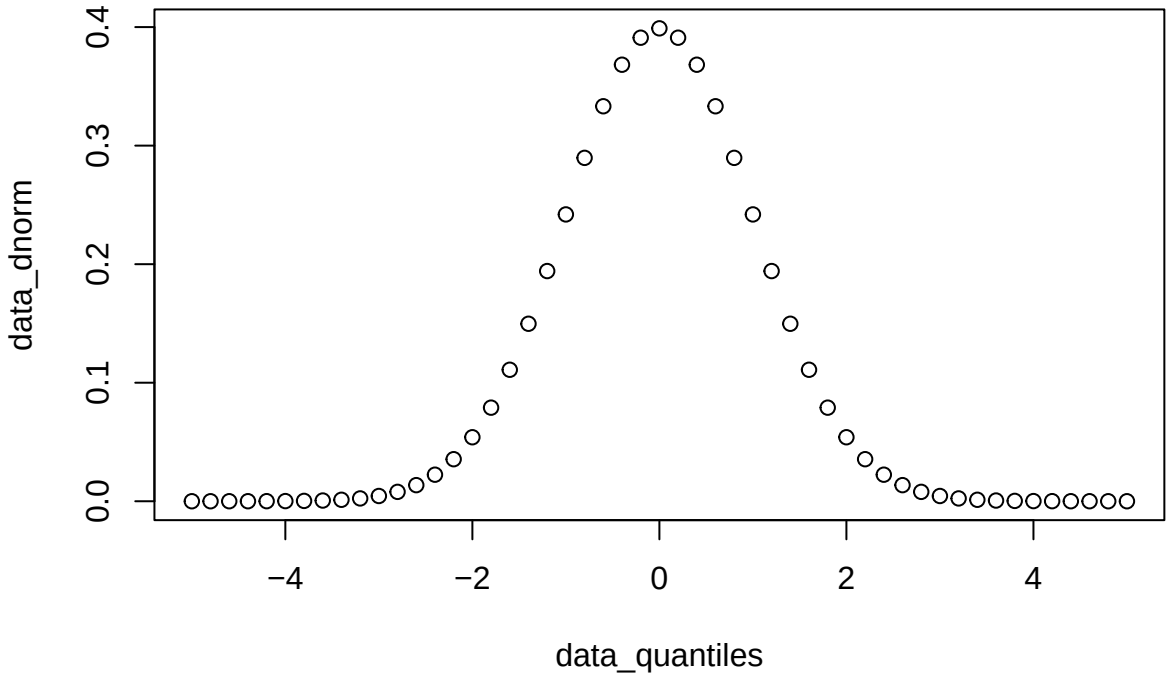
The function `pnorm()` returns the probability of a observing a value less or equal to each quantile given.

```
data_dnorm <- dnorm(x = data_quantiles)
head(data_dnorm)
```

```
## [1] 1.486720e-06 3.961299e-06 1.014085e-05 2.494247e-05 5.894307e-05
## [6] 1.338302e-04
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_dnorm)
```

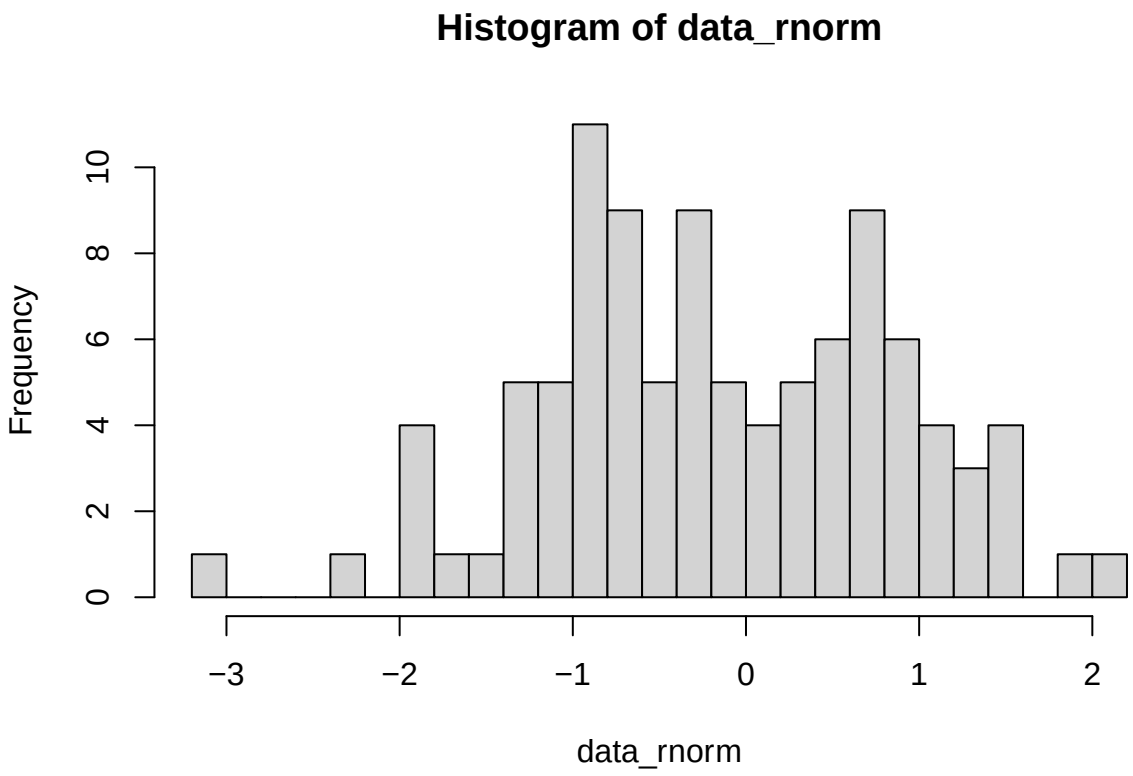



```
data_rnorm <- rnorm(n = 100)
head(data_rnorm)
```

rnorm

```
## [1] -0.552611240 -0.826049910 -0.007565875  0.902770965 -1.181010254
## [6]  1.013859715
```

```
hist(data_rnorm, breaks = 20)
```



Demo

A parameterised normal distribution

pnorm() The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(-500, 500, 50)
head(data_quantiles)
```

```
## [1] -500 -450 -400 -350 -300 -250
```

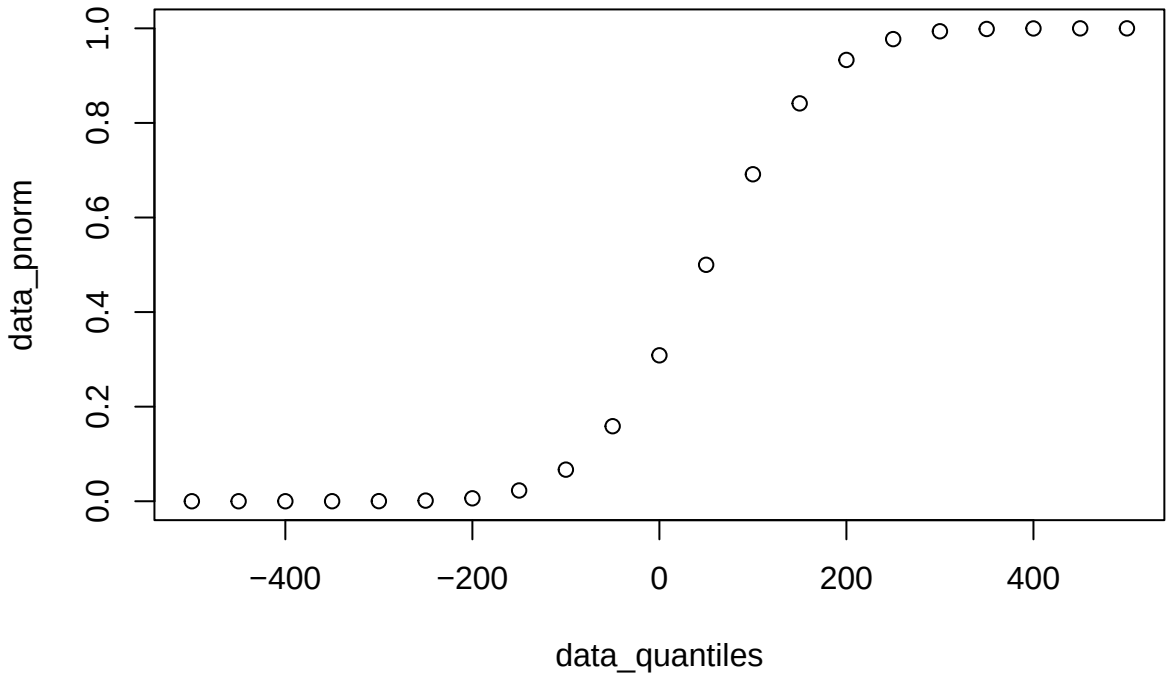
The function `pnorm()` returns the probability of a observing a value less or equal to each quantile given.

```
data_pnorm <- pnorm(q = data_quantiles, mean = 50, sd = 100)
head(data_pnorm)
```

```
## [1] 1.898956e-08 2.866516e-07 3.397673e-06 3.167124e-05 2.326291e-04
## [6] 1.349898e-03
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_pnorm)
```



qnorm() The function `qnorm()` takes as input a vector of probabilities between 0 and 1.

```
data_probabilities <- seq(from = 0, to = 1, by = 0.02)
head(data_probabilities)
```

```
## [1] 0.00 0.02 0.04 0.06 0.08 0.10
```

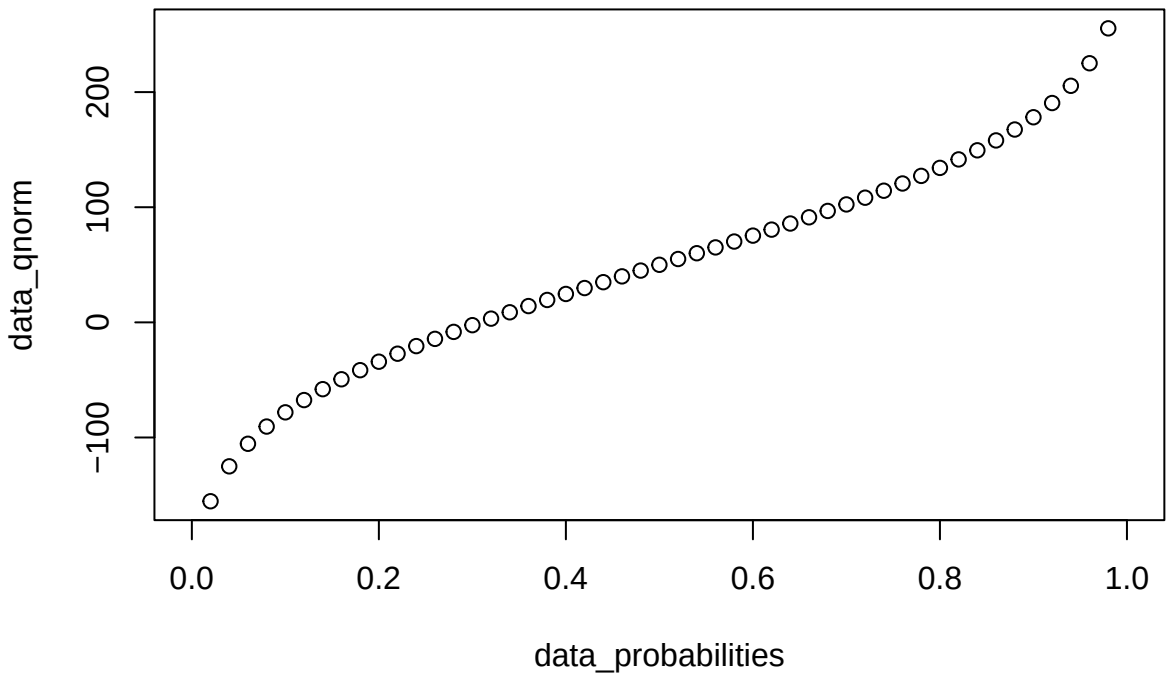
The function `qnorm()` the quantiles (i.e., values) that correspond to those probabilities.

```
data_qnorm <- qnorm(p = data_probabilities, mean = 50, sd = 100)
head(data_qnorm)
```

```
## [1]       -Inf -155.37489 -125.06861 -105.47736  -90.50716  -78.15516
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_probabilities, data_qnorm)
```



dnorm The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(-500, 500, 50)
head(data_quantiles)
```

```
## [1] -500 -450 -400 -350 -300 -250
```

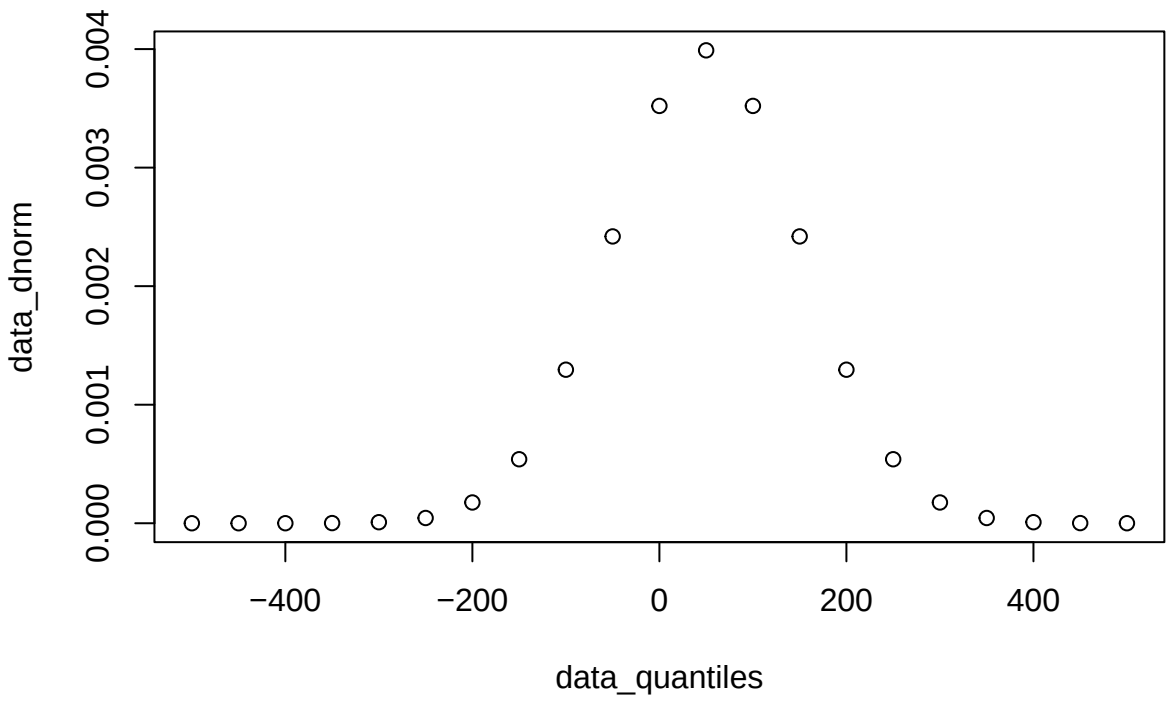
The function `pnorm()` returns the probability of a observing a value less or equal to each quantile given.

```
data_dnorm <- dnorm(x = data_quantiles, mean = 50, sd = 100)
head(data_dnorm)
```

```
## [1] 1.076976e-09 1.486720e-08 1.598374e-07 1.338302e-06 8.726827e-06
## [6] 4.431848e-05
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_dnorm)
```

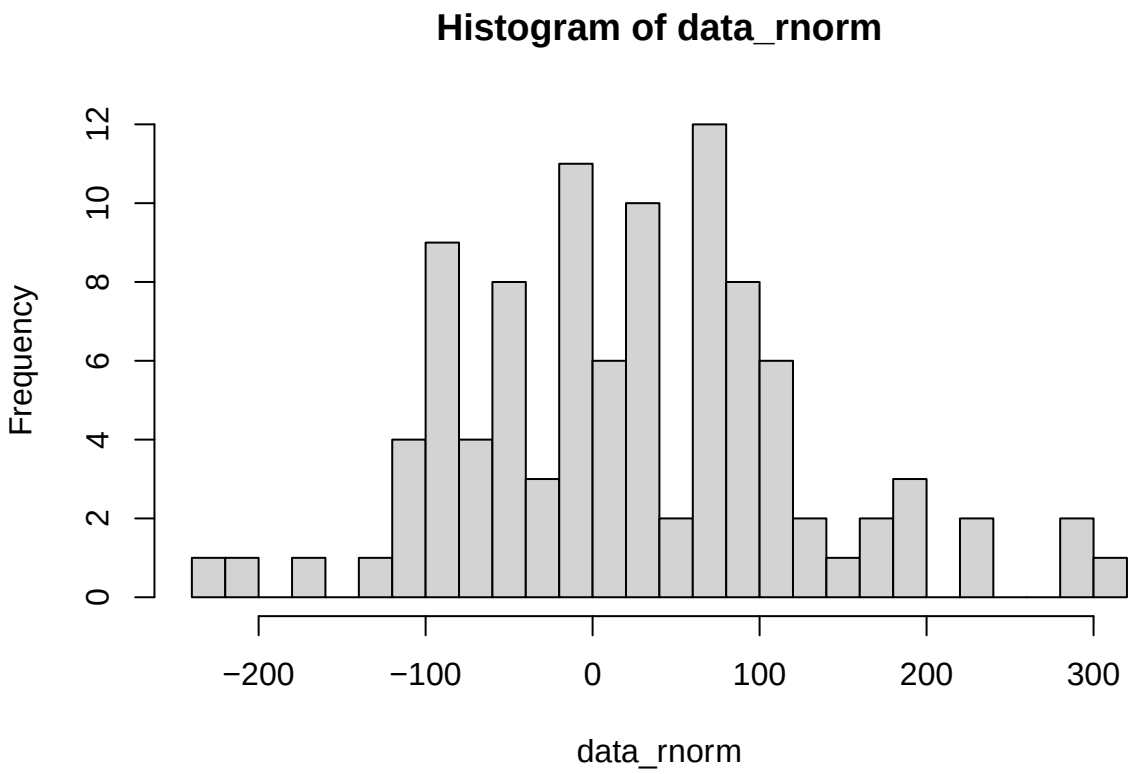



```
data_rnorm <- rnorm(n = 100, mean = 50, sd = 100)
head(data_rnorm)
```

rnorm

```
## [1]  -9.33670  29.76605  95.30812  24.50602 -17.92716  66.45119
```

```
hist(data_rnorm, breaks = 20)
```



Demo

A parameterised binomial distribution

pnorm() The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(0, 50, 1)
head(data_quantiles)
```

```
## [1] 0 1 2 3 4 5
```

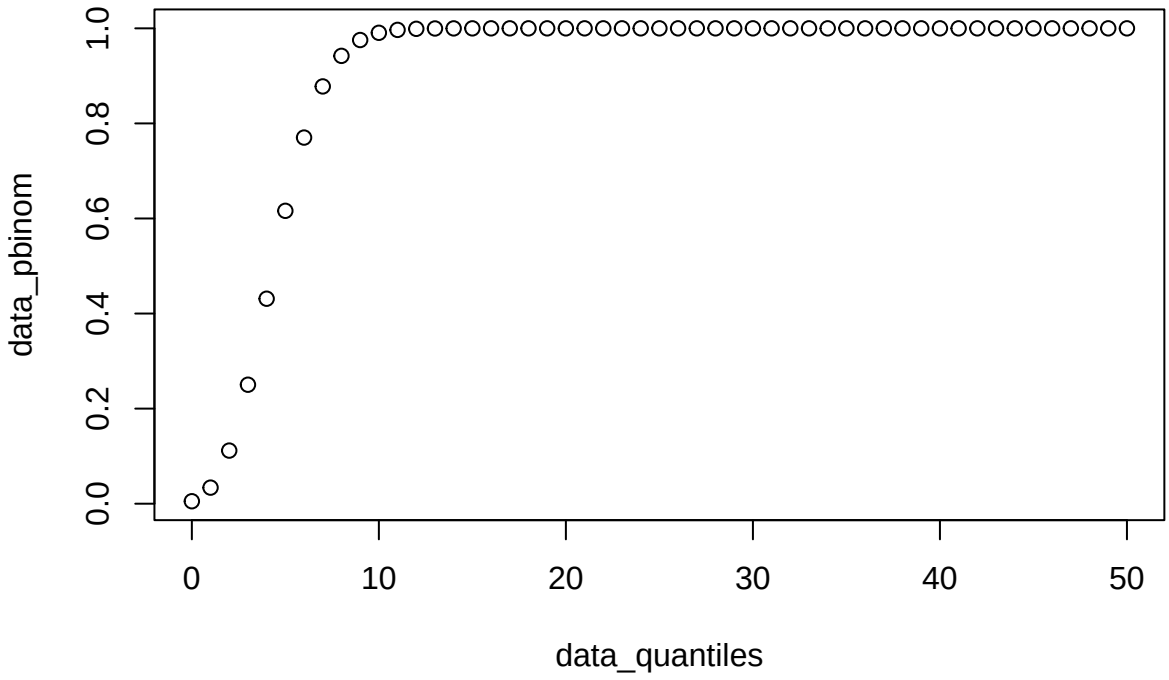
The function `pnorm()` returns the probability of a observing a value less or equal to each quantile given.

```
data_pbinom <- pbinom(q = data_quantiles, size = 50, prob = 0.1)
head(data_pbinom)
```

```
## [1] 0.005153775 0.033785860 0.111728756 0.250293906 0.431198407 0.616123008
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_pbinom)
```



qbinom() The function `qbinom()` takes as input a vector of probabilities between 0 and 1.

```
data_probabilities <- seq(from = 0, to = 1, by = 0.02)
head(data_probabilities)
```

```
## [1] 0.00 0.02 0.04 0.06 0.08 0.10
```

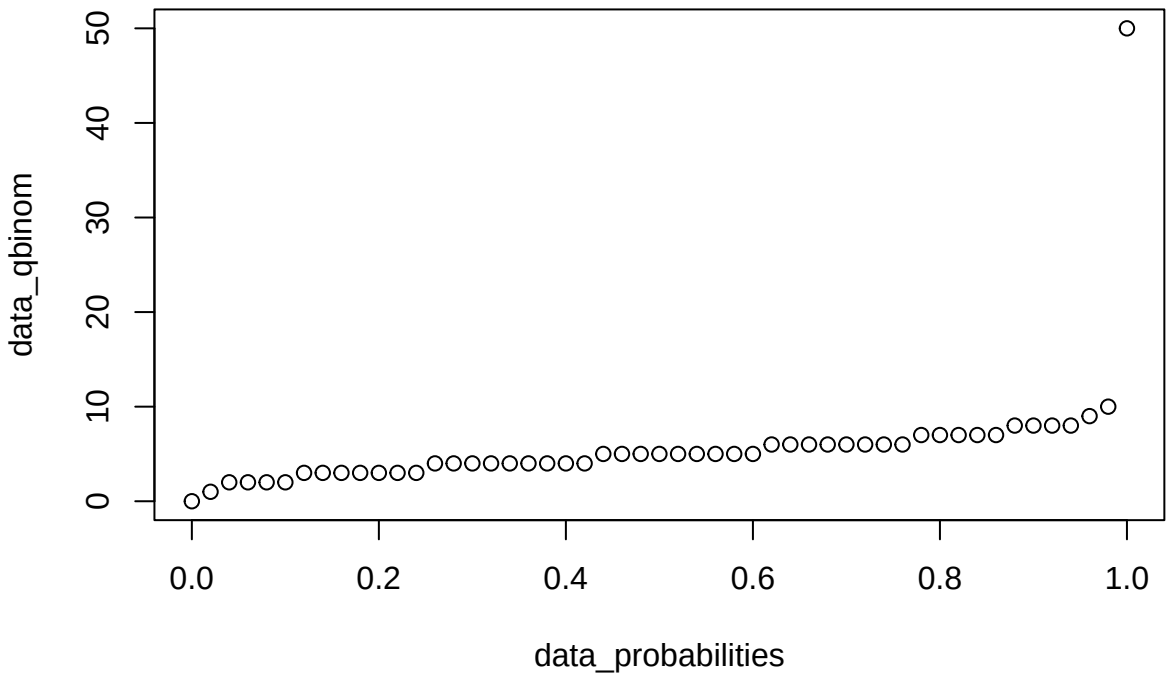
The function `qbinom()` the quantiles (i.e., values) that correspond to those probabilities.

```
data_qbinom <- qbinom(p = data_probabilities, size = 50, prob = 0.1)
head(data_qbinom)
```

```
## [1] 0 1 2 2 2 2
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_probabilities, data_qbinom)
```



dbinom The quantiles represent a set of possible values in the distribution.

```
data_quantiles <- seq(0, 50, 1)
head(data_quantiles)
```

```
## [1] 0 1 2 3 4 5
```

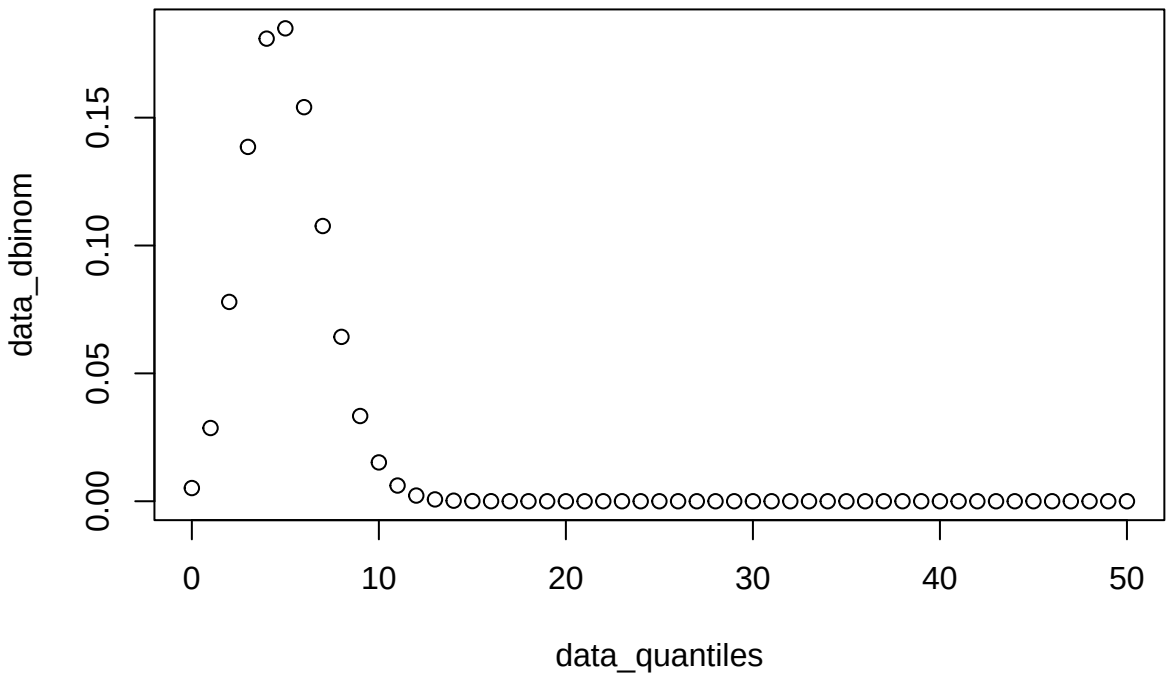
The function `pbinom()` returns the probability of a observing a value less or equal to each quantile given.

```
data_dbinom <- dbinom(x = data_quantiles, size = 50, prob = 0.1)
head(data_dbinom)
```

```
## [1] 0.005153775 0.028632084 0.077942897 0.138565150 0.180904501 0.184924601
```

The base R `plot()` function can be used to quickly plot each quantile and its probability.

```
plot(data_quantiles, data_dbinom)
```

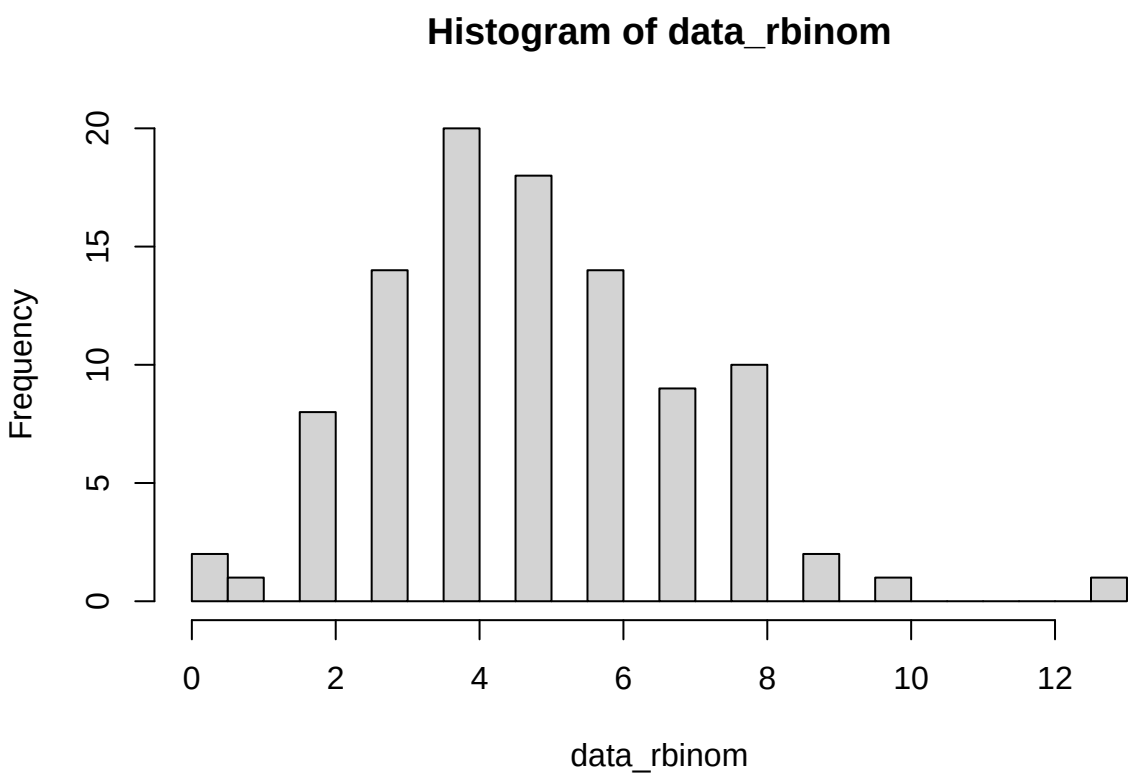



```
data_rbinom <- rbinom(n = 100, size = 50, prob = 0.1)
head(data_rbinom)
```

rbinom

```
## [1] 5 8 4 5 8 7
```

```
hist(data_rbinom, breaks = 20)
```



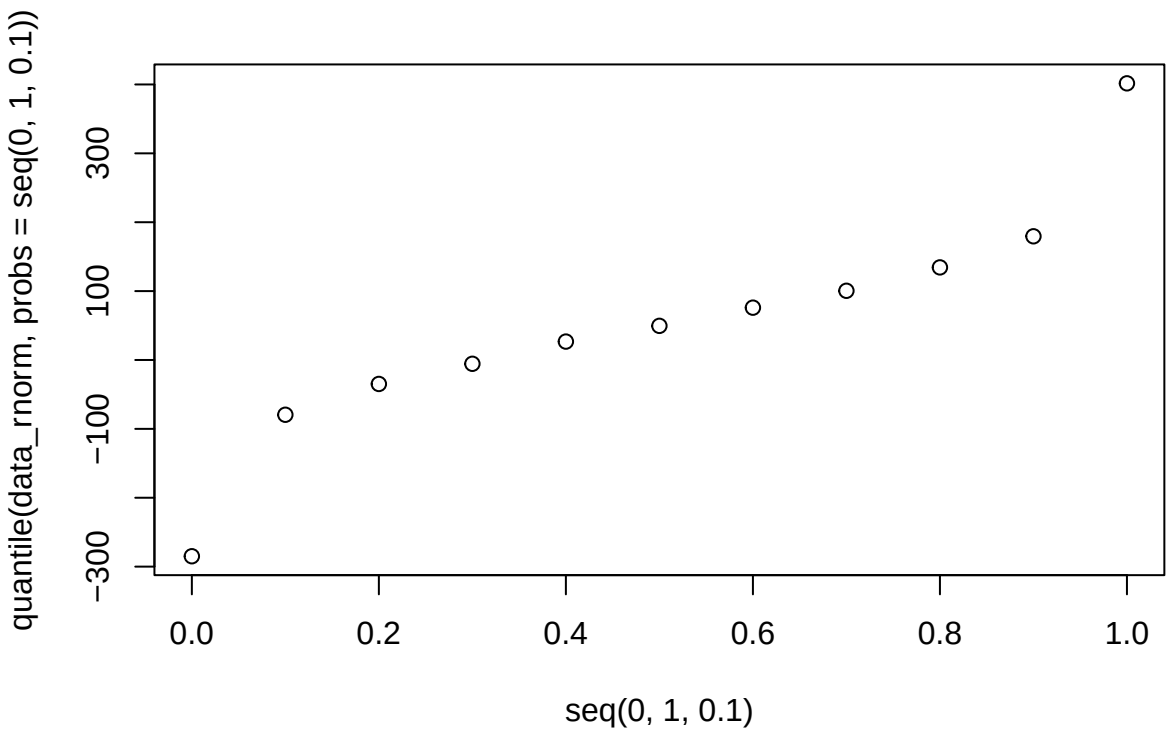
Demo

Quantiles

```
data_rnorm <- rnorm(n = 1000, mean = 50, sd = 100)
quantile(data_rnorm, probs = seq(0, 1, 0.1))
```

```
##          0%         10%         20%         30%         40%         50%
## -284.916968  -79.516288  -34.814888   -5.535373   26.716152   49.533217
##         60%         70%         80%         90%        100%
##   75.960882  100.474771  134.407947  179.566700  401.595599
```

```
plot(
  seq(0, 1, 0.1),
  quantile(data_rnorm, probs = seq(0, 1, 0.1))
)
```



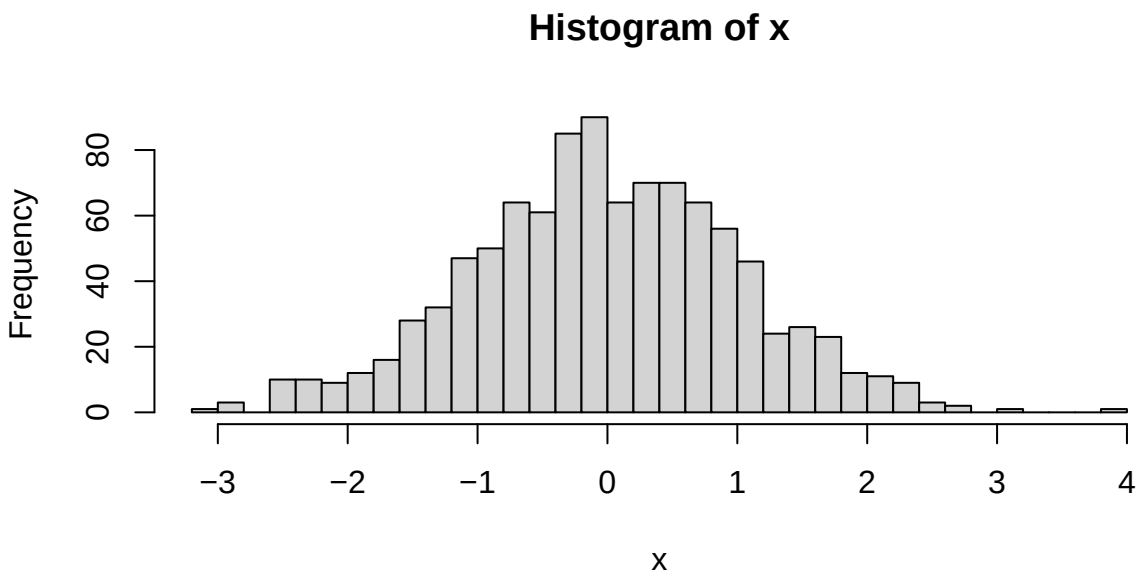
Demo

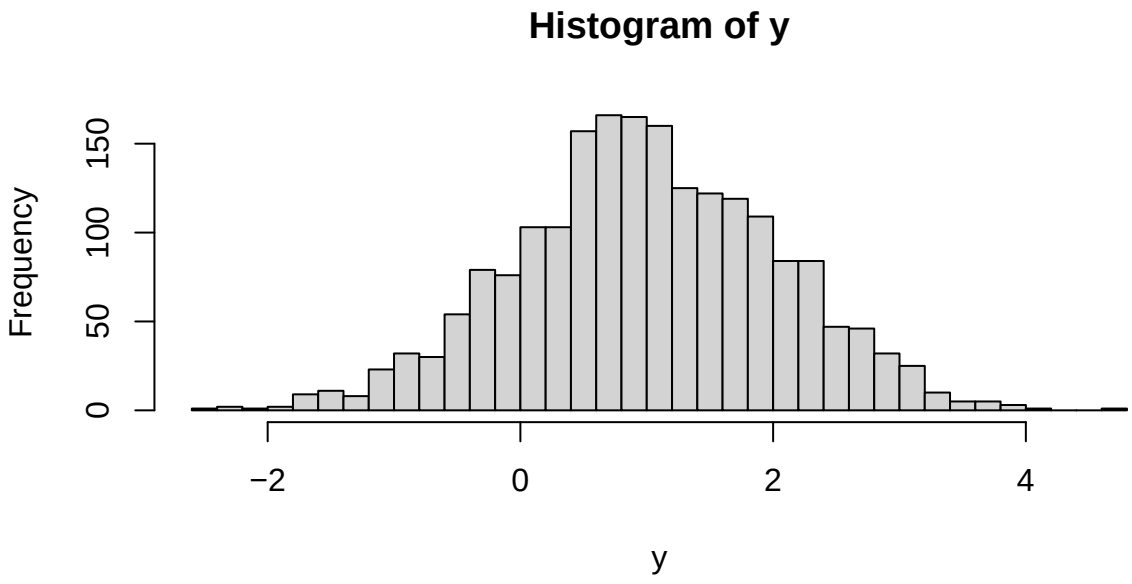
Parametric t-test

```
set.seed(1)
x <- rnorm(n = 1000, mean = 0, sd = 1)
y <- rnorm(n = 2000, mean = 1, sd = 1)
```

In base R, `par(mfrow=c(i, j))` can be used to display plots in a grid of `i` rows and `j` columns.

```
par(mfrow = c(2, 1))
hist(x, breaks = 30)
hist(y, breaks = 30)
```






```
par(mfrow = c(1, 1 ))
```

```
t.test(x, y)
```

```
##
##  Welch Two Sample t-test
##
## data:  x and y
## t = -25.223, df = 1999, p-value < 2.2e-16
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  -1.089791 -0.932552
```

```
## sample estimates:
##   mean of x   mean of y
## -0.01164814  0.99952356
```

```
t.test(y, x)
```

```
##
##  Welch Two Sample t-test
##
## data:  y and x
## t = 25.223, df = 1999, p-value < 2.2e-16
## alternative hypothesis: true difference in means is not equal to 0
## 95 percent confidence interval:
##  0.932552 1.089791
## sample estimates:
##   mean of x   mean of y
##  0.99952356 -0.01164814
```

Demo

Paired test

Simulate a vector of values `x`. Then simulate values `y` that are systematically 2 units greater than their `x` counterpart, with a bit of noise (normally distributed).

```
set.seed(1)
n_sample <- 10
x <- runif(n = n_sample, min = 10, max = 20)
y <- x + 2 + rnorm(n = n_sample, mean = 0, sd = 1)
```

The average difference between `y` and `x` values is approximately 2, as intended.

```
mean(y - x)
```

```
## [1] 2.086629
```

```
t.test(x, y, paired = TRUE)
```

```
##
##  Paired t-test
##
## data:  x and y
## t = -6.0238, df = 9, p-value = 0.0001967
## alternative hypothesis: true mean difference is not equal to 0
## 95 percent confidence interval:
##  -2.870241 -1.303017
## sample estimates:
## mean difference
##       -2.086629
```

Demo

Non-parametric tests

```
set.seed(1)
x <- runif(n = 10, min = 1, max = 11)
y <- runif(n = 5, min = 3, max = 13)
```

```r
wilcox.test(x, y)
```

```
##
##  Wilcoxon rank sum exact test
##
## data:  x and y
## W = 20, p-value = 0.5941
## alternative hypothesis: true location shift is not equal to 0
```

```r
wilcox.test(x, y, alternative = "less")
```

```
##
##  Wilcoxon rank sum exact test
##
## data:  x and y
## W = 20, p-value = 0.297
## alternative hypothesis: true location shift is less than 0
```

Demo

Analysis of Variance (ANOVA)

```r
set.seed(1)
n_sample <- 1000
x1 <- rnorm(n = n_sample, mean = 10, sd = 2)
x2 <- x1 + 5 + rnorm(n = n_sample, mean = 0, sd = 1)
x3 <- x2 + 0 + rnorm(n = n_sample, mean = 0, sd = 0.5)
data_aov <- data.frame(
  value = c(x1, x2, x3),
  group = c(
    rep("x1", length(x1)),
    rep("x2", length(x2)),
    rep("x3", length(x3))
  )
)
head(data_aov)
```

```
##       value group
## 1  8.747092    x1
## 2 10.367287    x1
## 3  8.328743    x1
## 4 13.190562    x1
## 5 10.659016    x1
## 6  8.359063    x1
```

```r
aov_result <- aov(value ~ group, data_aov)
aov_result
```

```
## Call:
##    aov(formula = value ~ group, data = data_aov)
##
## Terms:
##                     group Residuals
## Sum of Squares  16583.9   15450.7
## Deg. of Freedom       2      2997
##
```

```
## Residual standard error: 2.270548
## Estimated effects may be unbalanced
```

```
summary(aov_result)
```

```
##               Df Sum Sq Mean Sq F value Pr(>F)
## group          2  16584    8292    1608 <2e-16 ***
## Residuals   2997  15451       5
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Demo

Fisher's Exact Test

```
data_fisher <- matrix(
  data = c(12, 4, 3, 23),
  nrow = 2, ncol = 2,
  dimnames = list(
    c("DE", "Not DE"),
    c("In pathway", "Not in pathway")
  )
)
data_fisher
```

```
##        In pathway Not in pathway
## DE             12              3
## Not DE          4             23
```

```
fisher.test(data_fisher)
```

```
##
##  Fisher's Exact Test for Count Data
##
## data:  data_fisher
## p-value = 4.983e-05
## alternative hypothesis: true odds ratio is not equal to 1
## 95 percent confidence interval:
##    3.592731 170.706615
## sample estimates:
## odds ratio
##   20.56889
```

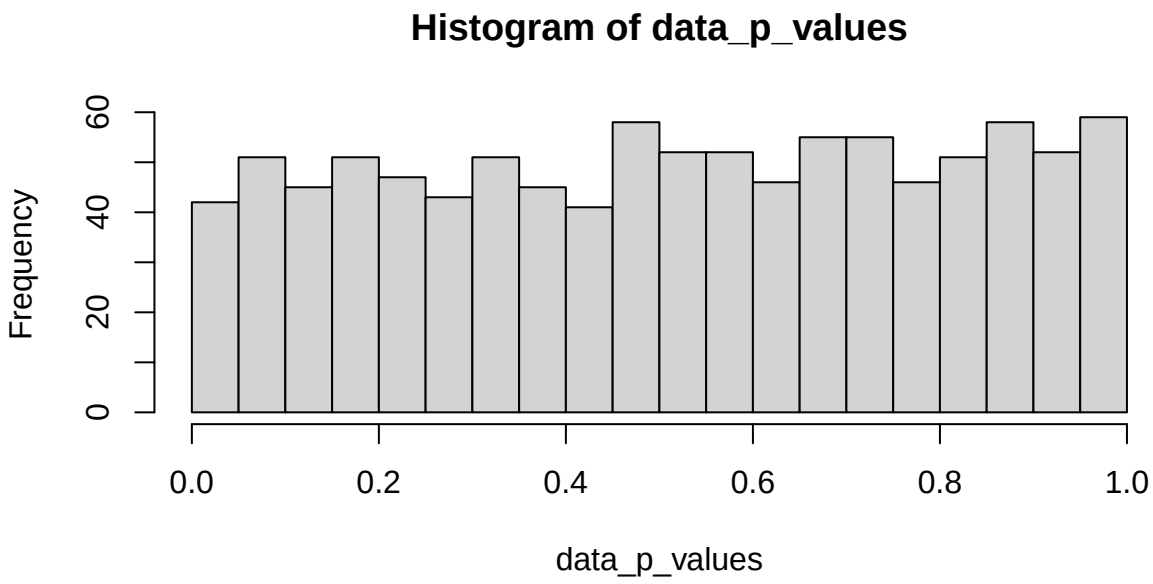
Demo

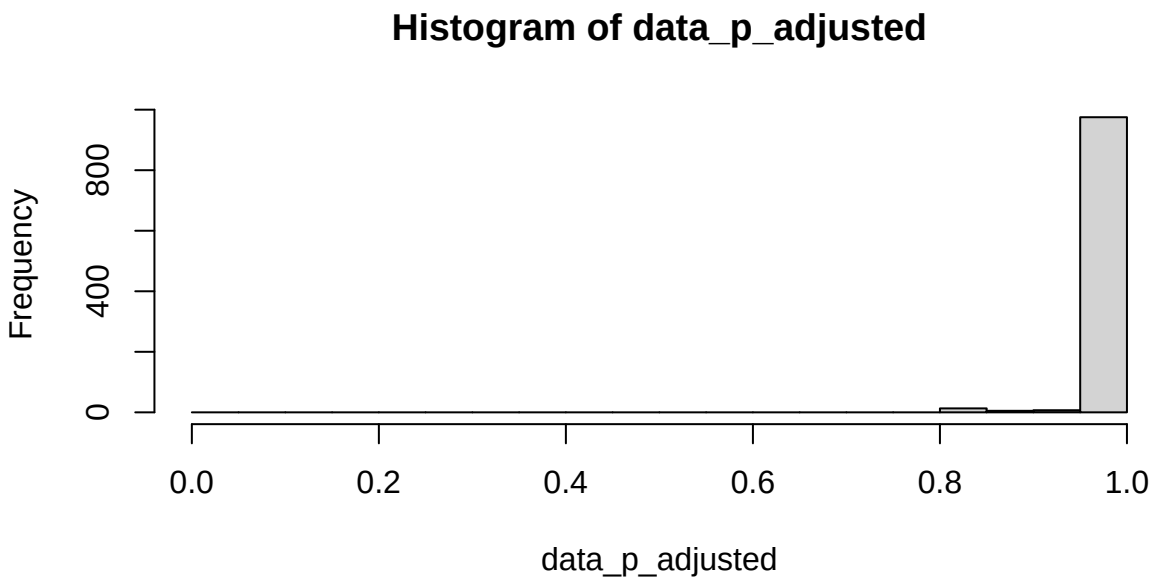
Multiple-testing correction

```
data_p_values <- runif(1E3, min = 0, max = 1)
data_p_adjusted <- p.adjust(data_p_values, method = "BH")
head(sort(data_p_adjusted))
```

```
## [1] 0.8215773 0.8215773 0.8215773 0.8215773 0.8215773 0.8215773
```

```
par(mfrow = c(2, 1))
hist(data_p_values, xlim = c(0, 1), breaks = seq(0, 1, 0.05))
hist(data_p_adjusted, xlim = c(0, 1), breaks = seq(0, 1, 0.05))
```






```
par(mfrow = c(1, 1))
```

Exercise

Setup

- Import the `iris` data set.

```
data(iris)
head(iris)
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
```

```
## 1          5.1         3.5          1.4         0.2  setosa
## 2          4.9         3.0          1.4         0.2  setosa
## 3          4.7         3.2          1.3         0.2  setosa
## 4          4.6         3.1          1.5         0.2  setosa
## 5          5.0         3.6          1.4         0.2  setosa
## 6          5.4         3.9          1.7         0.4  setosa
```

- Separate the matrix of measurements in a new object named `iris_features`.

```
iris_features <- iris[, 1:4]
head(iris_features)
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width
## 1          5.1         3.5          1.4         0.2
## 2          4.9         3.0          1.4         0.2
## 3          4.7         3.2          1.3         0.2
## 4          4.6         3.1          1.5         0.2
## 5          5.0         3.6          1.4         0.2
## 6          5.4         3.9          1.7         0.4
```

Exercise

Apply Principal Components Analysis (PCA)

The `prcomp()` function allows you to standardise the data as part of the principal components analysis itself.

- Apply PCA, centering and scaling the matrix of features. Assign the result to an object called `pca_iris`.

```
pca_iris <- prcomp(iris_features, center = TRUE, scale. = TRUE )
pca_iris
```

```
## Standard deviations (1, .., p=4):
## [1] 1.7083611 0.9560494 0.3830886 0.1439265
##
## Rotation (n x k) = (4 x 4):
##                     PC1         PC2        PC3        PC4
## Sepal.Length  0.5210659 -0.37741762  0.7195664  0.2612863
## Sepal.Width  -0.2693474 -0.92329566 -0.2443818 -0.1235096
## Petal.Length  0.5804131 -0.02449161 -0.1421264 -0.8014492
## Petal.Width   0.5648565 -0.06694199 -0.6342727  0.5235971
```

- Examine the object `pca_iris`. Display the loading of each feature on each principal component.

```
pca_iris
```

```
## Standard deviations (1, .., p=4):
## [1] 1.7083611 0.9560494 0.3830886 0.1439265
##
## Rotation (n x k) = (4 x 4):
##                     PC1         PC2        PC3        PC4
## Sepal.Length  0.5210659 -0.37741762  0.7195664  0.2612863
## Sepal.Width  -0.2693474 -0.92329566 -0.2443818 -0.1235096
## Petal.Length  0.5804131 -0.02449161 -0.1421264 -0.8014492
## Petal.Width   0.5648565 -0.06694199 -0.6342727  0.5235971
```

```
summary(pca_iris)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4
```

```
## Standard deviation     1.7084 0.9560 0.38309 0.14393
## Proportion of Variance 0.7296 0.2285 0.03669 0.00518
## Cumulative Proportion  0.7296 0.9581 0.99482 1.00000
```

```
pca_iris$rotation[1:4, ]
```

```
##                     PC1         PC2        PC3        PC4
## Sepal.Length  0.5210659 -0.37741762  0.7195664  0.2612863
## Sepal.Width  -0.2693474 -0.92329566 -0.2443818 -0.1235096
## Petal.Length  0.5804131 -0.02449161 -0.1421264 -0.8014492
## Petal.Width   0.5648565 -0.06694199 -0.6342727  0.5235971
```

```
pca_iris$x
```

```
##                PC1          PC2          PC3          PC4
##   [1,] -2.25714118 -0.478423832  0.127279624  0.024087508
##   [2,] -2.07401302  0.671882687  0.233825517  0.102662845
##   [3,] -2.35633511  0.340766425 -0.044053900  0.028282305
##   [4,] -2.29170679  0.595399863 -0.090985297 -0.065735340
##   [5,] -2.38186270 -0.644675659 -0.015685647 -0.035802870
##   [6,] -2.06870061 -1.484205297 -0.026878250  0.006586116
##   [7,] -2.43586845 -0.047485118 -0.334350297 -0.036652767
##   [8,] -2.22539189 -0.222403002  0.088399352 -0.024529919
##   [9,] -2.32684533  1.111603700 -0.144592465 -0.026769540
##  [10,] -2.17703491  0.467447569  0.252918268 -0.039766068
##  [11,] -2.15907699 -1.040205867  0.267784001  0.016675503
##  [12,] -2.31836413 -0.132633999 -0.093446191 -0.133037725
##  [13,] -2.21104370  0.726243183  0.230140246  0.002416941
##  [14,] -2.62430902  0.958296347 -0.180192423 -0.019151375
##  [15,] -2.19139921 -1.853846555  0.471322025  0.194081578
##  [16,] -2.25466121 -2.677315230 -0.030424684  0.050365010
##  [17,] -2.20021676 -1.478655729  0.005326251  0.188186988
##  [18,] -2.18303613 -0.487206131  0.044067686  0.092779618
##  [19,] -1.89223284 -1.400327567  0.373093377  0.060891973
##  [20,] -2.33554476 -1.124083597 -0.132187626 -0.037630354
##  [21,] -1.90793125 -0.407490576  0.419885937  0.010884821
##  [22,] -2.19964383 -0.921035871 -0.159331502  0.059398340
##  [23,] -2.76508142 -0.456813301 -0.331069982  0.019582826
##  [24,] -1.81259716 -0.085272854 -0.034373442  0.150636353
##  [25,] -2.21972701 -0.136796175 -0.117599566 -0.269238379
##  [26,] -1.94532930  0.623529705  0.304620475  0.043416203
##  [27,] -2.04430277 -0.241354991 -0.086075649  0.067454082
##  [28,] -2.16133650 -0.525389422  0.206125707  0.010241084
##  [29,] -2.13241965 -0.312172005  0.270244895  0.083977887
##  [30,] -2.25769799  0.336604248 -0.068207276 -0.107918349
##  [31,] -2.13297647  0.502856075  0.074757996 -0.048027970
##  [32,] -1.82547925 -0.422280389  0.269564311  0.239069476
##  [33,] -2.60621687 -1.787587272 -0.047070727 -0.228470534
##  [34,] -2.43800983 -2.143546796  0.082392024 -0.048053409
##  [35,] -2.10292986  0.458665270  0.169706329  0.028926042
##  [36,] -2.20043723  0.205419224  0.224688852  0.168343905
##  [37,] -2.03831765 -0.659349230  0.482919584  0.195702902
##  [38,] -2.51889339 -0.590315163 -0.019370918 -0.136048774
##  [39,] -2.42152026  0.901161067 -0.192609402 -0.009705907
##  [40,] -2.16246625 -0.267981199  0.175296561  0.007023875
```

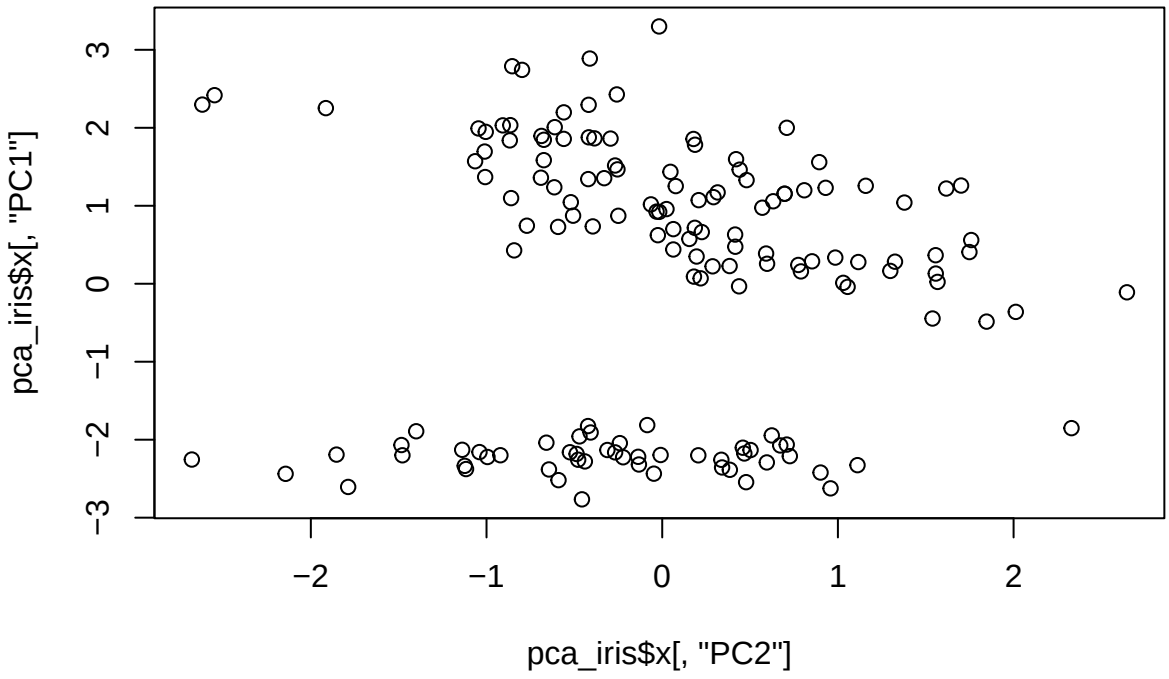
```
##  [41,] -2.27884081 -0.440240541 -0.034778398  0.106626042
##  [42,] -1.85191836  2.329610745  0.203552303  0.288896090
##  [43,] -2.54511203  0.477501017 -0.304745527 -0.066379077
##  [44,] -1.95788857 -0.470749613 -0.308567588  0.176501717
##  [45,] -2.12992356 -1.138415464 -0.247604064 -0.150539117
##  [46,] -2.06283361  0.708678586  0.063716370  0.139801160
##  [47,] -2.37677076 -1.116688691 -0.057026813 -0.151722682
##  [48,] -2.38638171  0.384957230 -0.139002234 -0.048671707
##  [49,] -2.22200263 -0.994627669  0.180886792 -0.014878291
##  [50,] -2.19647504 -0.009185585  0.152518539  0.049206884
##  [51,]  1.09810244 -0.860091033  0.682300393  0.034717469
##  [52,]  0.72889556 -0.592629362  0.093807452  0.004887251
##  [53,]  1.23683580 -0.614239894  0.552157058  0.009391933
##  [54,]  0.40612251  1.748546197  0.023024633  0.065549239
##  [55,]  1.07188379  0.207725147  0.396925784  0.104387166
##  [56,]  0.38738955  0.591302717 -0.123776885 -0.240027187
##  [57,]  0.74403715 -0.770438272 -0.148472007 -0.077111455
##  [58,] -0.48569562  1.846243998 -0.248432992 -0.040384912
##  [59,]  0.92480346 -0.032118478  0.594178807 -0.029779844
##  [60,]  0.01138804  1.030565784 -0.537100055 -0.028366154
##  [61,] -0.10982834  2.645211115  0.046634215  0.013714785
##  [62,]  0.43922201  0.063083852 -0.204389093  0.039992104
##  [63,]  0.56023148  1.758832129  0.763214554  0.045578465
##  [64,]  0.71715934  0.185602819  0.068429700 -0.164256922
##  [65,] -0.03324333  0.437537419 -0.194282030  0.108684396
##  [66,]  0.87248429 -0.507364239  0.501830204  0.104593326
##  [67,]  0.34908221  0.195656268 -0.489234095 -0.190869932
##  [68,]  0.15827980  0.789451008  0.301028700 -0.204612265
##  [69,]  1.22100316  1.616827281  0.480693656  0.225145511
##  [70,]  0.16436725  1.298259939  0.172260719 -0.051554138
##  [71,]  0.73521959 -0.395247446 -0.614467782 -0.083006045
##  [72,]  0.47469691  0.415926887  0.264067576  0.113189079
##  [73,]  1.23005729  0.930209441  0.367182178 -0.009911322
##  [74,]  0.63074514  0.414997441  0.290921638 -0.273304557
##  [75,]  0.70031506  0.063200094  0.444537765  0.043313222
##  [76,]  0.87135454 -0.249956017  0.471001057  0.101376117
##  [77,]  1.25231375  0.076998069  0.724727099  0.039556002
##  [78,]  1.35386953 -0.330205463  0.259955701  0.066604931
##  [79,]  0.66258066  0.225173502 -0.085577197 -0.036318171
##  [80,] -0.04012419  1.055183583  0.318506304  0.064571834
##  [81,]  0.13035846  1.557055553  0.149482697 -0.009371129
##  [82,]  0.02337438  1.567225244  0.240745761 -0.032663020
##  [83,]  0.24073180  0.774661195  0.150707074  0.023572390
##  [84,]  1.05755171  0.631726901 -0.104959762 -0.183354200
##  [85,]  0.22323093  0.286812663 -0.663028512 -0.253977520
##  [86,]  0.42770626 -0.842758920 -0.449129446 -0.109308985
##  [87,]  1.04522645 -0.520308714  0.394464890  0.037084781
##  [88,]  1.04104379  1.378371048  0.685997804  0.136378719
##  [89,]  0.06935597  0.218770433 -0.290605718 -0.146653279
##  [90,]  0.28253073  1.324886147 -0.089111491  0.008876070
##  [91,]  0.27814596  1.116288852 -0.094172116 -0.269753497
##  [92,]  0.62248441 -0.024839814  0.020412763 -0.147193289
##  [93,]  0.33540673  0.985103828  0.198724011  0.006508757
##  [94,] -0.36097409  2.012495825 -0.105467721  0.019505467
```

```
##  [95,]  0.28762268  0.852873116 -0.130452657 -0.107043742
##  [96,]  0.09105561  0.180587142 -0.128547696 -0.229191812
##  [97,]  0.22695654  0.383634868 -0.155691572 -0.132163118
##  [98,]  0.57446378  0.154356489  0.270743347 -0.019794366
##  [99,] -0.44617230  1.538637456 -0.189765199  0.199278855
## [100,]  0.25587339  0.596852285 -0.091572385 -0.058426315
## [101,]  1.83841002 -0.867515056 -1.002044077 -0.049085303
## [102,]  1.15401555  0.696536401 -0.528389994 -0.040385459
## [103,]  2.19790361 -0.560133976  0.202236658  0.058986583
## [104,]  1.43534213  0.046830701 -0.163083761 -0.234982858
## [105,]  1.86157577 -0.294059697 -0.394307408 -0.016243853
## [106,]  2.74268509 -0.797736709  0.580364827 -0.101045973
## [107,]  0.36579225  1.556289178 -0.983598122 -0.132679346
## [108,]  2.29475181 -0.418663020  0.649530452 -0.237246445
## [109,]  1.99998633  0.709063226  0.392675073 -0.086221779
## [110,]  2.25223216 -1.914596301 -0.396224508  0.104488870
## [111,]  1.35962064 -0.690443405 -0.283661780  0.107500284
## [112,]  1.59732747  0.420292431 -0.023108991  0.058136869
## [113,]  1.87761053 -0.417849815 -0.026250468  0.145926073
## [114,]  1.25590769  1.158379741 -0.578311891  0.098826244
## [115,]  1.46274487  0.440794883 -1.000517746  0.274738504
## [116,]  1.58476820 -0.673986887 -0.636297054  0.191222383
## [117,]  1.46651849 -0.254768327 -0.037306280 -0.154811637
## [118,]  2.41822770 -2.548124795  0.127454475 -0.272892966
## [119,]  3.29964148 -0.017721580  0.700957033  0.045037725
## [120,]  1.25954707  1.701046715  0.266643612 -0.064963167
## [121,]  2.03091256 -0.907427443 -0.234015510  0.167390481
## [122,]  0.97471535  0.569855257 -0.825362161  0.027662914
## [123,]  2.88797650 -0.412259950  0.854558973 -0.126911337
## [124,]  1.32878064  0.480202496  0.005410239  0.139491837
## [125,]  1.69505530 -1.010536476 -0.297454114 -0.061437911
## [126,]  1.94780139 -1.004412720  0.418582432 -0.217609339
## [127,]  1.17118007  0.315338060 -0.129503907  0.125001677
## [128,]  1.01754169 -0.064131184 -0.336588365 -0.008625505
## [129,]  1.78237879  0.186735633 -0.269754304  0.030983849
## [130,]  1.85742501 -0.560413289  0.713244682 -0.207519953
## [131,]  2.42782030 -0.258418706  0.725386035 -0.017863520
## [132,]  2.29723178 -2.617554417  0.491826144 -0.210968943
## [133,]  1.85648383  0.177953334 -0.352966242  0.099675959
## [134,]  1.11042770  0.291944582  0.182875741 -0.185721512
## [135,]  1.19845835  0.808606364  0.164173760 -0.487849130
## [136,]  2.78942561 -0.853942542  0.541093785  0.294893130
## [137,]  1.57099294 -1.065013214 -0.942695700  0.035486875
## [138,]  1.34179696 -0.421020154 -0.180271551 -0.214702016
## [139,]  0.92173701 -0.017165594 -0.415434449  0.005220919
## [140,]  1.84586124 -0.673870645  0.012629804  0.194543500
## [141,]  2.00808316 -0.611835930 -0.426902678  0.246711805
## [142,]  1.89543421 -0.687273065 -0.129640697  0.468128374
## [143,]  1.15401555  0.696536401 -0.528389994 -0.040385459
## [144,]  2.03374499 -0.864624030 -0.337014969  0.045036251
## [145,]  1.99147547 -1.045665670 -0.630301866  0.213330527
## [146,]  1.86425786 -0.385674038 -0.255418178  0.387957152
## [147,]  1.55935649  0.893692855  0.026283300  0.219456899
## [148,]  1.51609145 -0.268170747 -0.179576781  0.118773236
```

```
## [149,]  1.36820418 -1.007877934 -0.930278721  0.026041407
## [150,]  0.95744849  0.024250427 -0.526485033 -0.162533529
```

- Visualise the PCA projection using `plot()`.

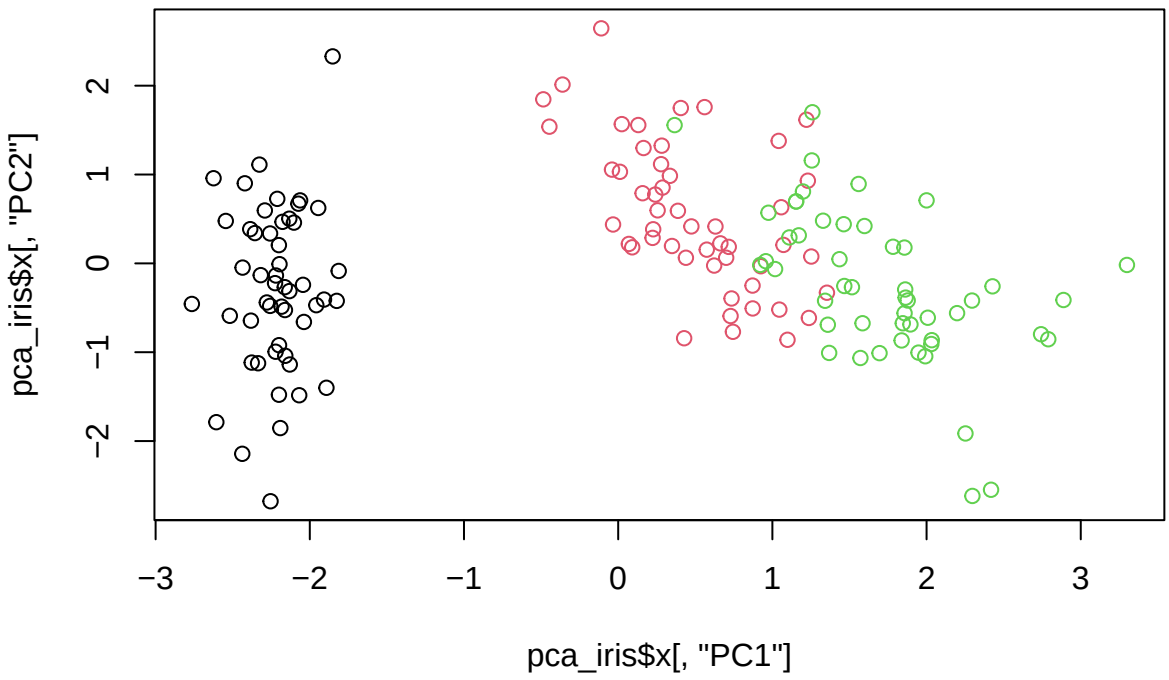
```
plot(x = pca_iris$x[,"PC2"], y = pca_iris$x[,"PC1"]  )
```



Bonus point

- Edit the plot above, coloring data points according to their class label.

```
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col = iris$Species )
```



Exercise

Variance explained

- Compute the variance explained by principal components, using information present in the return value of the `prcomp()` function.

```
pca_iris$sdev
```

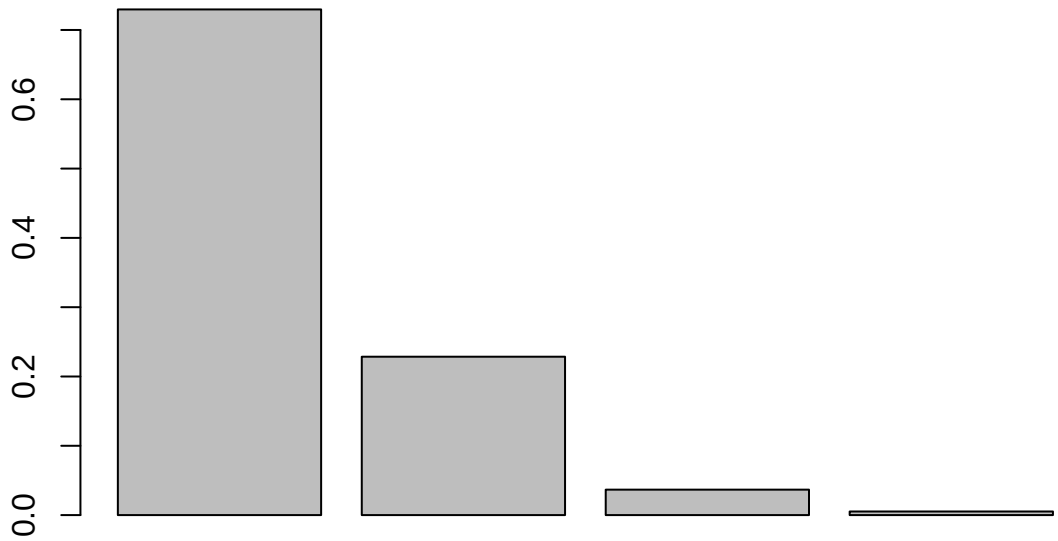
```
## [1] 1.7083611 0.9560494 0.3830886 0.1439265
```

```
explained_variance_ratio <- (pca_iris$sdev^2)/ sum(pca_iris$sdev^2)
explained_variance_ratio
```

```
## [1] 0.729624454 0.228507618 0.036689219 0.005178709
```

- Visualise the variance explained by each principal component using `barplot()`.

```
barplot(explained_variance_ratio )
```



Exercise

Hierarchical clustering

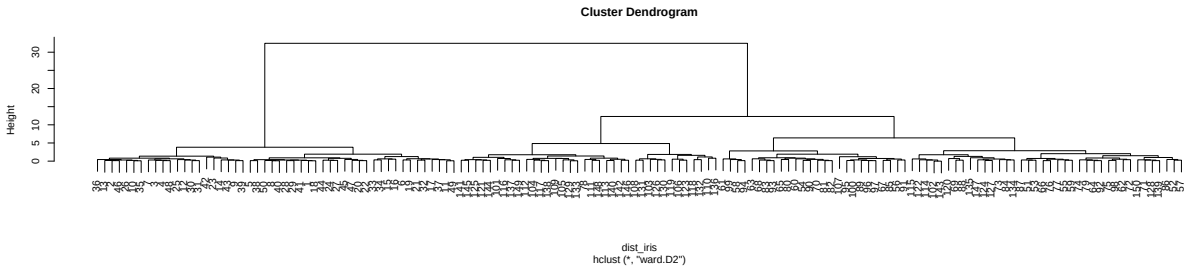
- Perform hierarchical clustering on the `iris_features` data set, using the `euclidean` distance and method `ward.D2`. Use the functions `dist()` and `hclust()`.

```
dist_iris <- dist(iris_features, method = "euclidean", diag = FALSE, upper=FALSE, p=2)
hclust_iris_ward <- hclust(dist_iris, "ward.D2", members = NULL )
hclust_iris_ward
```

```
##
## Call:
## hclust(d = dist_iris, method = "ward.D2", members = NULL)
##
## Cluster method   : ward.D2
## Distance         : euclidean
## Number of objects: 150
```

- Plot the clustering tree using `plot()`.

```
plot(hclust_iris_ward, labels = NULL, hang =0.1, check = TRUE, axes = TRUE, frame.plot=FALSE, ann=TRUE,
```



How many clusters would you call from a visual inspection of the tree?

Answer:

- Cut the tree in 3 clusters and extract the cluster label for each flower. Use the function `cutree()`.

```
iris_hclust_ward_labels <- cutree(hclust_iris_ward, k = 3 )
iris_hclust_ward_labels
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
##  [75] 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 2 3 3 3 3 2 3 3 3 3
## [112] 3 3 2 2 3 3 3 3 2 3 2 3 2 3 3 2 2 3 3 3 3 3 2 2 3 3 3 2 3 3 3 2 3 3 3 2 3
## [149] 3 2
```

- Repeat clustering using 3 other agglomeration methods:
  - `complete`
  - `average`
  - `single`

```
# complete
hclust_iris_complete <- hclust(dist_iris, "complete", members = NULL )
iris_hclust_complete_labels <- cutree(hclust_iris_complete, k =3 )
iris_hclust_complete_labels
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 3 2 3 2 3 2 3 3 3 3 2 3 2 3 3 2 3 2 3 2 2
##  [75] 2 2 2 2 2 3 3 3 3 2 3 2 2 2 3 3 3 2 3 3 3 3 2 3 3 2 2 2 2 2 2 3 2 2 2 2
## [112] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
## [149] 2 2
```

```
# average
hclust_iris_average <- hclust(dist_iris, "average", members = NULL  )
iris_hclust_average_labels <- cutree(hclust_iris_average, k =3 )
iris_hclust_average_labels
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
##  [75] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 2 3 3 3 3 2 3 3 3 3
## [112] 3 3 2 2 3 3 3 3 2 3 2 3 2 3 3 2 2 3 3 3 3 3 2 3 3 3 2 3 3 3 2 3 3 3 2 3
## [149] 3 2
```

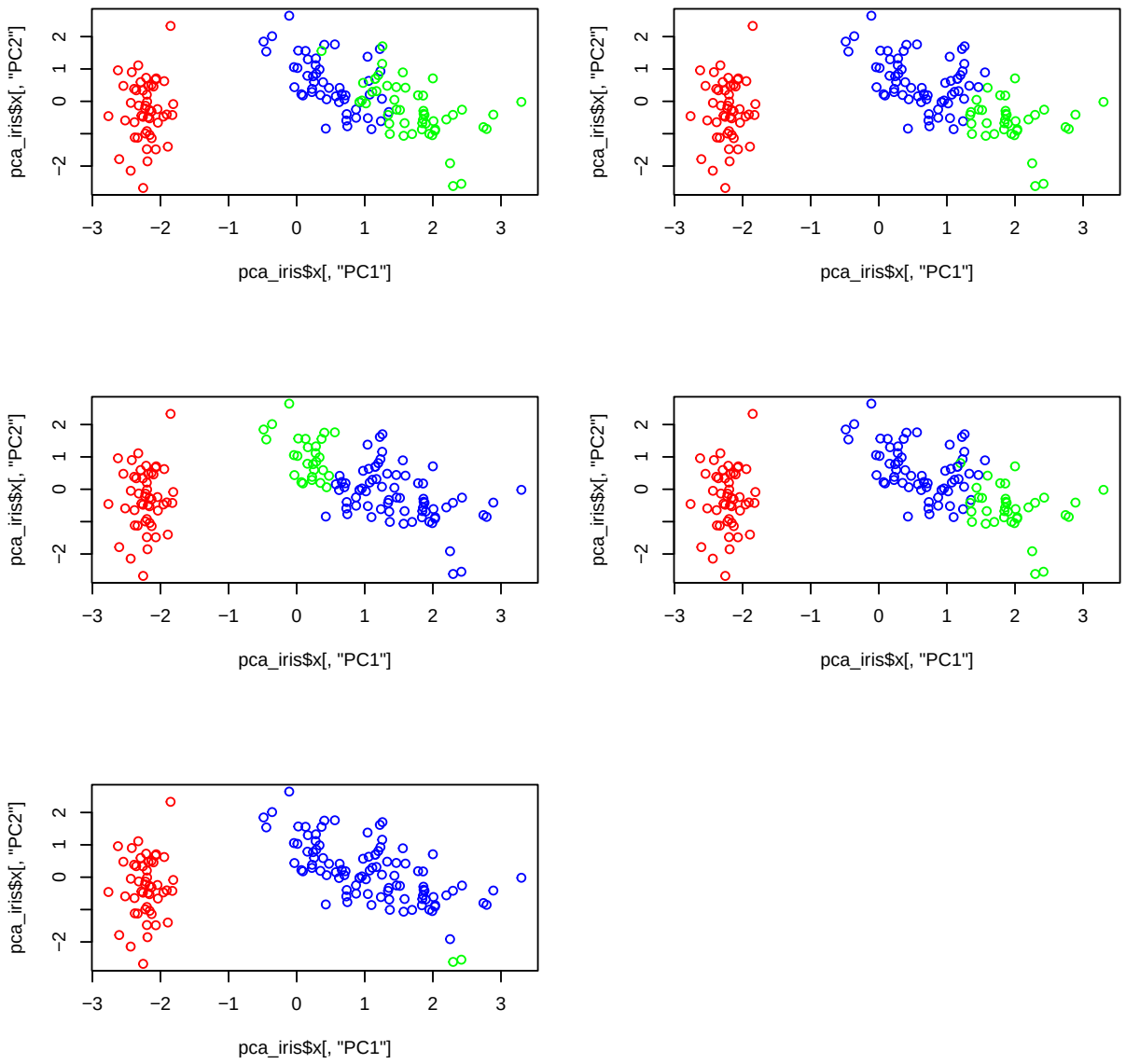
```
# single
hclust_iris_single <- hclust(dist_iris, "single", members = NULL   )
iris_hclust_single_labels <- cutree(hclust_iris_single, k=3 )
iris_hclust_single_labels
```

```
##   [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
##  [38] 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

```
##  [75] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
## [112] 2 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
## [149] 2 2
```

- Compare clustering results on scatter plots of the data using `plot()`.

```
par(mfrow = c(3, 2))
palette(c("red", "blue", "green"))
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col =iris$Species)
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col =iris_hclust_ward_labels )
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col =iris_hclust_complete_labels)
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col =iris_hclust_average_labels )
plot(x = pca_iris$x[,"PC1"], y = pca_iris$x[,"PC2"] , col =iris_hclust_single_labels  )
par(mfrow = c(1, 1))
```



```r
table(iris_hclust_ward_labels, iris$Species)
```

```
##
## iris_hclust_ward_labels setosa versicolor virginica
##                       1     50          0         0
##                       2      0         49        15
##                       3      0          1        35
```