

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

R

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Descriptive statistics

# Descriptive statistics

- R
- 1 Summary statistics for a single group
  - 2 Graphical display of distributions
  - 3 Summary statistics by groups
  - 4 Graphics for grouped data
  - 5 Tables
  - 6 Graphical display of tables
  - 7 Correlation
  - 8 Combinatorics
  - 9 ROC curves

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Descriptive statistics

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

Descriptive statistics describe the main features of a collection of data quantitatively. Descriptive statistics are distinguished from inferential statistics (or inductive statistics), in that descriptive statistics aim to summarize a data set quantitatively without employing a probabilistic formulation, rather than use the data to make inferences about the population that the data are thought to represent.

# Summary statistics for a single group

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

It is easy to calculate simple summary statistics with R.

```
> x <- rnorm(50)
```

```
> mean(x)
```

```
[1] -0.09122392
```

```
> sd(x)
```

```
[1] 1.083760
```

```
> var(x)
```

```
[1] 1.174535
```

```
> median(x)
```

```
[1] -0.1730651
```

# Summary statistics for a single group

R

Empirical quantiles may be obtained with the function `quantile`

```
> quantile(x)
```

	0%	25%	50%	75%
	-2.5543238	-0.7904138	-0.1730651	0.6154567
	100%			
	2.5729806			

What do the quantiles mean?

It is also possible to obtain other quantiles, this is done by adding an argument containing the desired percentage points.

```
> pvec <- seq(0, 1, 0.1)
> quantile(x, pvec)
```

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Summary statistics for a single group

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

	0%	10%	20%	30%
	-2.5543238	-1.4780513	-1.0762851	-0.6074869
	40%	50%	60%	70%
	-0.4221129	-0.1730651	0.1112403	0.4620028
	80%	90%	100%	
	0.9145444	1.1044188	2.5729806	

# Summary statistics for a single group

R

But as you already know there is a function that will calculate most of this summary statistics.

```
> library(ISwR)
> data(juul)
> summary(juul)
```

age	menarche
Min. : 0.170	Min. : 1.000
1st Qu.: 9.053	1st Qu.: 1.000
Median :12.560	Median : 1.000
Mean :15.095	Mean : 1.476
3rd Qu.:16.855	3rd Qu.: 2.000
Max. :83.000	Max. : 2.000
NA's : 5.000	NA's :635.000

sex	igf1
Min. :1.000	Min. : 25.0
1st Qu.:1.000	1st Qu.:202.2
Median :2.000	Median :313.5
Mean :1.534	Mean :340.2
3rd Qu.:2.000	3rd Qu.:462.8
Max. :2.000	Max. :915.0

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Summary statistics for a single group

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

```
NA's :5.000   NA's :321.0
      tanner      testvol
Min.  : 1.000   Min.  : 1.000
1st Qu.: 1.000   1st Qu.: 1.000
Median : 2.000   Median : 3.000
Mean   : 2.640   Mean   : 7.896
3rd Qu.: 5.000   3rd Qu.: 15.000
Max.   : 5.000   Max.   : 30.000
NA's   :240.000  NA's   :859.000
```

Although as you can see, this has a big mistake, since all the variables were interpreted as quantitative, some were qualitative.



# Summary statistics for a single group

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

```
> juul$sex <- factor(juul$sex, labels = c("M",  
+   "F"))  
> juul$menarche <- factor(juul$menarche,  
+   labels = c("No", "Yes"))  
> juul$tanner <- factor(juul$tanner,  
+   labels = c("I", "II", "III", "IV",  
+   "V"))  
> summary(juul)
```

	age	menarche	sex
Min.	: 0.170	No :369	M :621
1st Qu.:	9.053	Yes :335	F :713
Median	:12.560	NA's:635	NA's: 5
Mean	:15.095		
3rd Qu.:	16.855		

# Summary statistics for a single group

R

```
Max.      :83.000
NA's      : 5.000

      igf1      tanner
Min.      : 25.0    I      :515
1st Qu.   :202.2   II     :103
Median    :313.5   III    : 72
Mean      :340.2   IV     : 81
3rd Qu.   :462.8   V      :328
Max.      :915.0   NA's   :240
NA's      :321.0
```

```
      testvol
Min.      : 1.000
1st Qu.   : 1.000
Median    : 3.000
Mean      : 7.896
```

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Summary statistics for a single group

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

```
3rd Qu.: 15.000
Max.    : 30.000
NA's    :859.000
```

# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

You can get a reasonable impression of the shape of a distribution by drawing a histogram, this is, a count of how many observations fall with specified divisions ("bins") if the x-axis

```
> hist(x)
```

# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

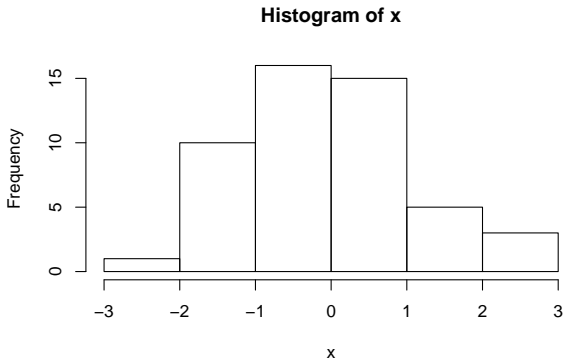
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



By specifying `breaks = n`, you get approximately  $n$  bars in the histogram since the algorithm tries to create pretty cut points.

# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

Although you can have full control of the position of the breaks if you specify a vector rather than a number.

```
> mid.age <- c(2.5, 7.5, 13, 16.5, 17.5,
+             19, 22.5, 44.5, 70.5)
> acc.count <- c(28, 46, 58, 20, 31,
+              64, 149, 316, 103)
> age.acc <- rep(mid.age, acc.count)
> brk <- c(0, 5, 10, 16, 17, 18, 20,
+         25, 60, 80)
> hist(age.acc, breaks = brk)
```

# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

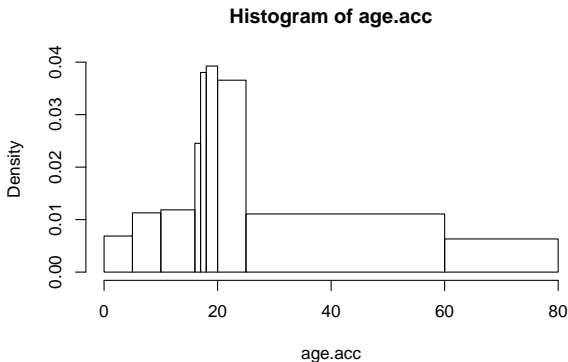
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



Which is the main difference between the histogram with  $n$  breakpoints and the one where we selected specific breaks? Why this is important?

# Empirical cumulative distribution

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

The empirical cumulative distribution function is defined as the fraction of data smaller than or equal to  $x$ .

```
> n <- length(x)
> plot(sort(x), (1:n)/n, type = "s",
+       ylim = c(0, 1))
```



# Empirical cumulative distribution

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

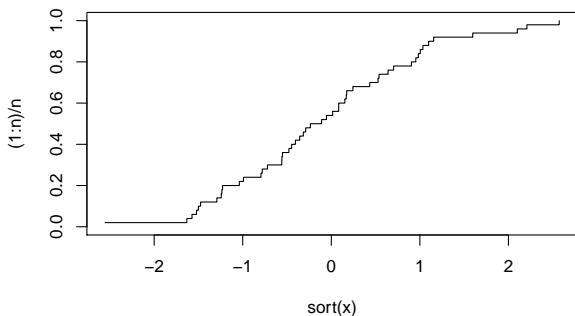
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Q-Q plots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

- One purpose of calculating the empirical cumulative distribution function is to see whether data can be assumed normally distributed.
- For a better assessment, you might plot the  $k$ 'th smallest observation against the expected value of the  $k$ 'th smallest observation out of  $n$  in a standard normal distribution.
- The point is that in this way you would expect to obtain a straight line if the data come from a normal distribution.
- We already know how to compare two data sets using qq plots, but R, has functions to compare data with distributions

> `qqnorm(x)`

# Q-Q plots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

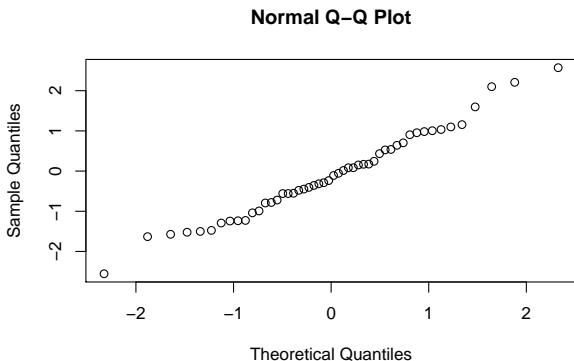
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

A boxplot, or more descriptively a “box-and-whiskers” plot, is a graphical summary of a distribution

- The box in the middle indicates “hinges” and median.
- The lines (“whiskers”) show the largest/smallest observation that falls within a distance of 1.5 times the box size from the nearest hinge.
- If any observation fall farther away, the additional points are considered “extreme” values and are shown separately

```
> data(IgM)
> par(mfrow = c(1, 2))
> boxplot(IgM)
> boxplot(log(IgM))
> par(mfrow = c(1, 1))
```

# Boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

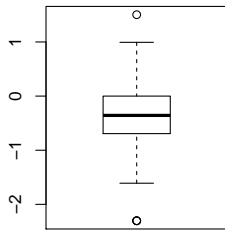
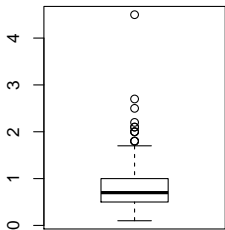
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Summary statistics by groups

R

When dealing with grouped data, you will often want to have various summary statistics computed within groups.

```
> data(red.cell.folate)
> tapply(red.cell.folate$folate, red.cell.folate$vent
+       mean)
```

N20+02,24h	N20+02,op	02,24h
316.6250	256.4444	278.0000

```
> tapply(red.cell.folate$folate, red.cell.folate$vent
+       sd)
```

N20+02,24h	N20+02,op	02,24h
58.71709	37.12180	33.75648

```
> tapply(red.cell.folate$folate, red.cell.folate$vent
+       length)
```

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Summary statistics by groups

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

N20+02, 24h	N20+02, op	02, 24h
8	9	5

# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

In dealing with grouped data it is important to be able not only to create plots for each group but also to be able to compare the plots between groups.

```
> data(energy)
> expend.lean <- energy$expend[energy$stature ==
+   "lean"]
> expend.obese <- energy$expend[energy$stature ==
+   "obese"]
> par(mfrow = c(2, 1))
> hist(expend.lean, breaks = 10, xlim = c(5,
+   13), ylim = c(0, 4), col = "white")
> hist(expend.obese, breaks = 10, xlim = c(5,
+   13), ylim = c(0, 4), col = "grey")
> par(mfrow = c(1, 1))
```



# Histograms

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

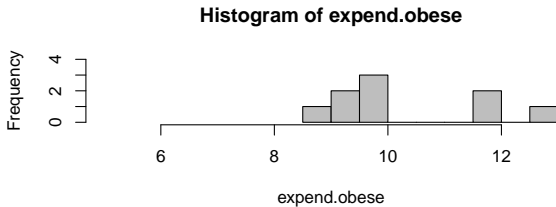
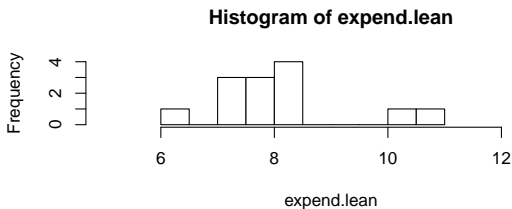
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Parallel boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

You might want a set of boxplots from several groups in the same frame. `boxplot` can handle this, both when data are given in the form of separate vectors from each group and when data are in one long vector and a is classified with a factor.

```
> boxplot(energy$expend ~ energy$stature)
```

# Parallel boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

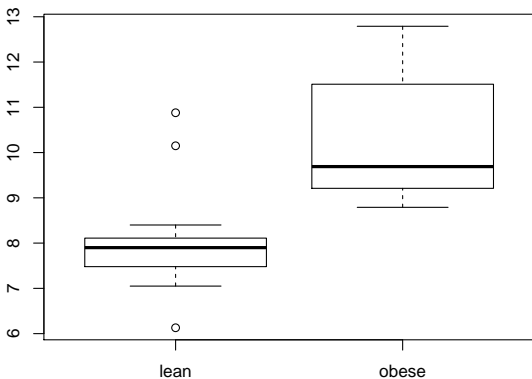
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Parallel boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

```
> boxplot(expend.lean, expend.obese)
```

# Parallel boxplots

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

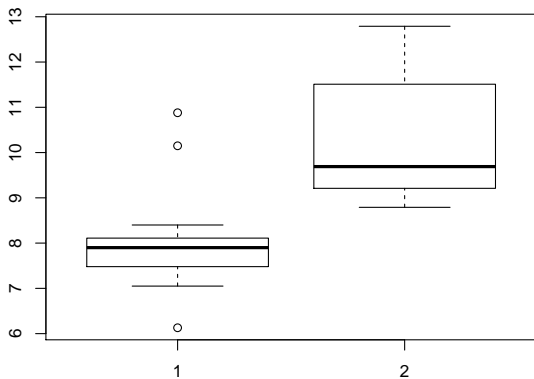
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Stripcharts

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

On the pervious boxplot you can see that since the interquartile range is quiet a bit larger in one group than in the other one of the boxplots looks fatter.

For small data set it is recommended to plot the raw data on a dot diagram.

```
> stripchart(energy$expend ~ energy$stature)
```

# Stripcharts

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

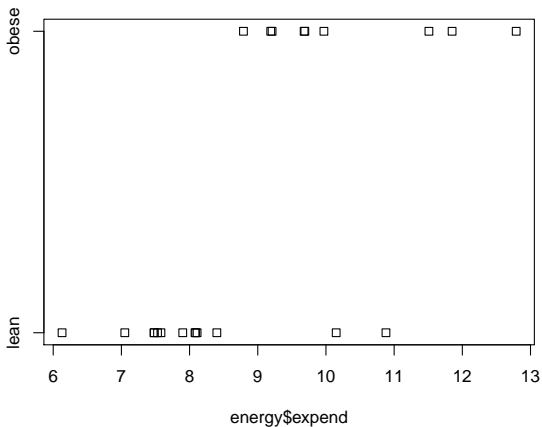
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves



# Generating Tables

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

The common case is that you have a data-frame with different variables, in this case you can obtain a table out from the data using the commands `table()`, `xtable()` and `ftable()`. The `table()` function is the basic one.

```
> table(juul$sex)
```

```
  M   F
621 713
```

```
> table(juul$sex, juul$menarche)
```

```
      No Yes
M      0   0
F    369 335
```

```
> table(juul$menarche, juul$tanner)
```



# Generating Tables

R

	I	II	III	IV	V
No	221	43	32	14	2
Yes	1	1	5	26	202

```
> table(juul$menarche, juul$tanner,  
+       juul$sex)  
  
, , = M
```

	I	II	III	IV	V
No	0	0	0	0	0
Yes	0	0	0	0	0

```
, , = F
```

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Generating Tables

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

	I	II	III	IV	V
No	221	43	32	14	2
Yes	1	1	5	26	202

# Marginal Tables and relative frequency

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

The common case is that you have a data-frame with different variables, in this case you can obtain a table out from the data using the commands `table()`, `xtable()` and `ftable()`. The `table()` function is the basic one.

```
> tanner.sex <- table(juul$tanner, juul$sex)
> margin.table(tanner.sex, 1)
```

	I	II	III	IV	V
515	103	72	81	328	

```
> margin.table(tanner.sex, 2)
```

	M	F
545	554	

Relative frequencies in a table are generally expressed as proportions of the row or column totals.

# Marginal Tables and relative frequency

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

```
> prop.table(tanner.sex, 1)
```

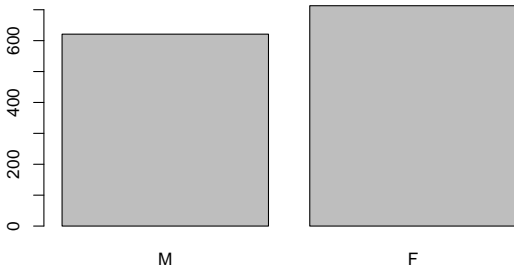
	M	F
I	0.5650485	0.4349515
II	0.5339806	0.4660194
III	0.4722222	0.5277778
IV	0.5061728	0.4938272
V	0.3780488	0.6219512

# Bar plots

R

Tables can be the input of the `barplot()` function we already know.

```
> barplot(table(juul$sex))
```



Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

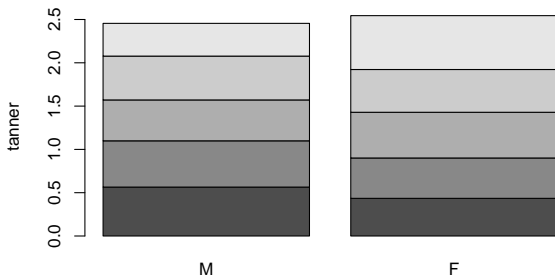
Combinatorics

ROC curves

# Bar plots

R

```
> barplot(prop.table(tanner.sex, 1),  
+         ylab = "tanner")
```



Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Pie charts

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

- Pie charts are traditionally scored upon statistics because they are often used to make trivial data look impressive and are difficult to decode for the human mind.
- They very rarely contain information that couldn't better be displayed as a bar plot.
- Even though R can draw pretty pie charts.

```
> pie(table(juul$sex))
```

# Pie charts

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

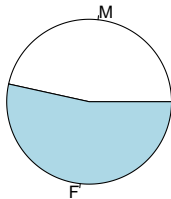
Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves





# Person correlation

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

- In R to obtain the pearson soeficient correaltion between two variables is easy.

```
> data(thuesen)
> cor(thuesen$blood.glucose, thuesen$short.velocity,
+      use = "complete.obs")

[1] 0.4167546
```

# Arrangements

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

an arrangement is a list of elements in a specific order

- Sampling with replacement Imagine we want to sample the 4 nucleotides for creating an oligonucleotide of length 7, so we can get any of the 4 nucleotides at each position

```
> n <- 4
```

```
> n * n
```

```
[1] 16
```

```
> n^7
```

```
[1] 16384
```

So we can get 16384 different oligonucleotides of length 7

# Arrangements

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

- Permutation of the elements of a set: the factorial Imagine we want to have all the oligonucleotides of size 4 that contain all the four nucleotides: ATCG, TACG,ACGT, etc ...

Intuitively, the generating process is quite simple: we will enumerate all the possible ways to rank the  $x$  elements of a set ( $x = 4$ ). For this, we will first select a single element in the set, and place it on the top of the ordered list. For this first step, there are  $x$  possible choices (each letter of the considered alphabet). As soon as the first element has been drawn, it is excluded from the set (since we want no more than one occurrence of each nucleotide).

$$> n * (n - 1) * (n - 2) * (n - 3)$$

[1] 24

# Arrangements

R

```
> factorial(n)
```

```
[1] 24
```

- Ordered selections without replacement The 6,000 genes of a genome were sorted according to their level of expression, as measured with a microarray. The 15 top genes were selected. How many possible selections are there, if we consider that the order of the selection matters?

In a set of size  $n$ , there are  $n$  possible choices for the first element,  $n-1$  choices left for the second element, . . . , and  $n-14$  choices for the 15th element. Thus, for a selection of  $x = 15$  elements among  $n = 6000$  genes, the number of possibilities is  $N = 6000 \cdot 5999 \cdot 5998 \cdot \dots \cdot (6000 - 14) = 4,62E56$ .

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

# Arrangements

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

$$A_n^x = \frac{n!}{(n-x)!} \quad (1)$$

Orderless selections without replacement (combinations) The 6,000 genes of a genome were sorted according to their level of expression, measured with an oligonucleotide microarray. The 15 top genes were selected. How many distinct sets would be possible, if one does not take into account the order of the selection?

$$C_n^x = \frac{n!}{x!(n-x)!} \quad (2)$$

```
> choose(6000, 15)
```

```
[1] 3.533156e+44
```

# ROC curves

R

Summary statistics for a single group

Graphical display of distributions

Summary statistics by groups

Graphics for grouped data

Tables

Graphical display of tables

Correlation

Combinatorics

ROC curves

- The real-valued output of scoring classifiers is turned into a binary class decision by choosing a cutoff.
- As no cutoff is optimal according to all possible performance criteria, cutoff choice involves a trade-off among different measures.
- Typically a trade-off between a pair of criteria (eg. sensitivity versus specificity) is visualized as a cutoff-parametrized curve.
- Receiver operating characteristic (ROC) curves are one of the most popular graphs
- A variety of libraries are available for these tasks: ROCR, ROC, nonbinROC. Remember you can always create your own functions. if needed.
- We are going to explore only the ROCR package.

- First we have to install and load the package

```
> install.packages("ROCR")
> library(ROCR)
```
- The data for today comes from a 10-fold cross-validation set of predictions and corresponding class labels from a study on predicting HIV coreceptor usage from the sequence of the viral envelope protein.

```
gdata: read.xls support for 'XLS'
gdata: (Excel 97-2004) files ENABLED.
```

```
gdata: Unable to load perl libraries
gdata: needed by read.xls()
gdata: to support 'XLSX' (Excel 2007+)
gdata: files.
```

```
gdata: Run the function
gdata: 'installXLSXsupport()'
gdata: to automatically download and
gdata: install the perl
gdata: libraries needed to support Excel
gdata: XLS and XLSX formats.
```

```
> data(ROCR.hiv)
```

- Then we are going to create a prediction data structure, so for one experiment we will take our values for the predictions and the labels of classification.

```
> pred <- prediction(ROCR.hiv$hiv.svm$predictions
+   ROCR.hiv$hiv.svm$labels)
```



- What we actually want now is to measure the performance of the method of classification,  

```
> perf <- performance(pred, "tpr", "fpr")
```

```
> plot(perf, avg = "threshold", colorize = TRUE)
```

# ROCR

R

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