xtable package in R
Simulation studies

Lecture 13
Oct. 6, 2010

Kate Cowles
374 SH, 335-0727
kcowles@stat.uiowa.edu
Create Export Tables

Description:

Function converting an R object to an 'xtable' object, which can then be printed as a LaTeX or HTML table.

Usage:

```r
xtable(x, caption=NULL, label=NULL, align=NULL, digits=NULL, display=NULL, ...)
```

Arguments:

- `x`: An R object of class found among 'methods(xtable)'. See below on how to write additional method functions for 'xtable'.

- `caption`: Character vector of length 1 containing the table's caption or title. Set to 'NULL' to suppress the caption. Default value is 'NULL'.

- `label`: Character vector of length 1 containing the LaTeX label or HTML anchor. Set to 'NULL' to suppress the label. Default value is 'NULL'.

- `align`: Character vector of length equal to the number of columns of the resulting table indicating the alignment of the corresponding columns. Also, '|' may be used to produce vertical lines between columns in LaTeX tables, but these are effectively ignored when considering the required length of the supplied vector. If a character vector of length one is supplied, it is split as 'strsplit(align,"")[[1]]' before processing. Since the row names are printed in the first column, the length of 'align' is one greater than 'ncol(x)' if 'x' is a 'data.frame'. Use '"l"', '"r"', and '"c"' to denote left, right, and center alignment, respectively. Use '"p{3cm}"' etc for a LaTeX column of the specified width. For HTML output the '"p"' alignment is interpreted as '"l"', ignoring the width request. Default depends on the class of 'x'.
digits: Numeric vector of length equal to one (in which case it will be replicated as necessary) or to the number of columns of the resulting table *or* matrix of the same size as the resulting table indicating the number of digits to display in the corresponding columns. Since the row names are printed in the first column, the length of the vector 'digits' or the number of columns of the matrix 'digits' is one greater than 'ncol(x)' if 'x' is a 'data.frame'. Default depends of class of 'x'. If values of 'digits' are negative, the corresponding values of 'x' are displayed in scientific format with 'abs(digits)' digits.

display: Character vector of length equal to the number of columns of the resulting table indicating the format for the corresponding columns. Since the row names are printed in the first column, the length of 'display' is one greater than 'ncol(x)' if 'x' is a 'data.frame'. These values are passed to the 'formatC' function. Use "d" (for integers), "f", "e", "E", "g", "G", "fg" (for reals), or "s" (for strings). "f" gives numbers in the usual 'xxx.xxx' format; "e" and "E" give 'n.ddde+nn' or 'n.dddE+nn' (scientific format); "g" and "G" put 'x[i]' into scientific format only if it saves space to do so. "fg" uses fixed format as "f", but 'digits' as number of _significant_ digits. Note that this can lead to quite long result strings. Default depends on the class of 'x'.

...: Additional arguments. (Currently ignored.)
Details:

This function extracts tabular information from 'x' and returns an object of class "xtable". The nature of the table generated depends on the class of 'x'. For example, 'aov' objects produce ANOVA tables while 'data.frame' objects produce a table of the entire data.frame. One can optionally provide a caption (called a title in HTML) or label (called an anchor in HTML), as well as formatting specifications. Default values for 'align', 'digits', and 'display' are class dependent.

The available method functions for 'xtable' are given by 'methods(xtable)'. Users can extend the list of available classes by writing methods for the generic function 'xtable'. These methods functions should have 'x' as their first argument with additional arguments to specify 'caption', 'label', 'align', 'digits', and 'display'. Optionally, other arguments may be present to specify how the object 'x' should be manipulated. All method functions should return an object whose class if given by 'c("xtable","data.frame")'. The resulting object can have attributes 'caption' and 'label', but must have attributes 'align', 'digits', and 'display'. It is strongly recommended that you set these attributes through the provided replacement functions as they perform validity checks.

Value:

An object of class "xtable" which inherits the 'data.frame' class and contains several additional attributes specifying the table formatting options.

Author(s):

David Dahl dahl@stat.tamu.edu with contributions and suggestions from many others (see source code).

See Also:

'print.xtable', 'caption', 'label', 'align', 'digits', 'display', 'formatC', 'methods'
• very handy if you are producing results in R and writing them up in \LaTeX

• can be used with different kinds of objects produced by R, including
  – matrices
  – regression output

• examples with data frame created from \texttt{Davis}
dataset on course web page
  – when input object is data frame, \texttt{xtable} always puts row names in the first column of output table
> Davis[1:5,]

<table>
<thead>
<tr>
<th></th>
<th>sex</th>
<th>weight</th>
<th>height</th>
<th>repwt</th>
<th>repht</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M</td>
<td>77</td>
<td>182</td>
<td>77</td>
<td>180</td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>58</td>
<td>161</td>
<td>51</td>
<td>159</td>
</tr>
<tr>
<td>3</td>
<td>F</td>
<td>53</td>
<td>161</td>
<td>54</td>
<td>158</td>
</tr>
<tr>
<td>4</td>
<td>M</td>
<td>68</td>
<td>177</td>
<td>70</td>
<td>175</td>
</tr>
<tr>
<td>5</td>
<td>F</td>
<td>59</td>
<td>157</td>
<td>59</td>
<td>155</td>
</tr>
</tbody>
</table>

> xDavis <- xtable(Davis[1:5,], align="rcrrrr", caption="Example of xtable for matrix or data frame")

> xDavis

\begin{table}[ht]
\begin{center}
\begin{tabular}{rcrrrr}
\hline
& sex & weight & height & repwt & repht \\
1 & M & 77 & 182 & 77 & 180 \\
2 & F & 58 & 161 & 51 & 159 \\
3 & F & 53 & 161 & 54 & 158 \\
4 & M & 68 & 177 & 70 & 175 \\
5 & F & 59 & 157 & 59 & 155 \\
\hline
\end{tabular}
\caption{Example of xtable for matrix or data frame}
\end{center}
\end{table}
<table>
<thead>
<tr>
<th>sex</th>
<th>weight</th>
<th>height</th>
<th>repwt</th>
<th>repht</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>M</td>
<td>77</td>
<td>182</td>
<td>77</td>
</tr>
<tr>
<td>2</td>
<td>F</td>
<td>58</td>
<td>161</td>
<td>51</td>
</tr>
<tr>
<td>3</td>
<td>F</td>
<td>53</td>
<td>161</td>
<td>54</td>
</tr>
<tr>
<td>4</td>
<td>M</td>
<td>68</td>
<td>177</td>
<td>70</td>
</tr>
<tr>
<td>5</td>
<td>F</td>
<td>59</td>
<td>157</td>
<td>59</td>
</tr>
</tbody>
</table>

Table 1: Example of xtable for matrix or data frame
> lmout <- lm( weight ~ repwt + sex, data = Davis)
> summary(lmout)

Call:
lm(formula = weight ~ repwt + sex, data = Davis)

Residuals:
     Min       1Q   Median       3Q      Max
-7.59200 -1.79128 -0.75769  0.63995 108.41060

Coefficients:
                               Estimate Std. Error   t value  Pr(>|t|)
(Intercept)                    3.47433    3.78632    0.918   0.3605
repwt                          0.96634    0.06507  14.8504  <2e-16 ***
sexM                            -1.48263    1.79775   -0.825   0.4112
---
Signif. codes:  *** 0.001 ** 0.01 * 0.05 . 0.1  1

Residual standard error: 8.426 on 180 degrees of freedom
(17 observations deleted due to missingness)
Multiple R-squared:  0.6998, Adjusted R-squared:  0.6964
F-statistic: 209.8 on 2 and 180 DF,  p-value: < 2.2e-16
> lmout.table <- xtable(lmout, caption='xtable for regression output')
> lmout.table
% latex table generated in R 2.9.1 by xtable 1.5-4 package
% Fri Nov 20 13:34:00 2009
\begin{table}[ht]
\begin{center}
\begin{tabular}{rrrrr}
\hline
& Estimate & Std. Error & t value & Pr(>|t|) \\
\hline
(Intercept) & 3.4743 & 3.7863 & 0.92 & 0.3601 \\
repwt & 0.9663 & 0.0651 & 14.85 & 0.0000 \\
sexM & -1.4826 & 1.7977 & -0.82 & 0.4106 \\
\hline
\end{tabular}
\caption{xtable for regression output}
\end{center}
\end{table}
|         | Estimate | Std. Error | t value | Pr(>|t|) |
|---------|----------|------------|---------|---------|
| (Intercept) | 3.4743   | 3.7863     | 0.92    | 0.3601  |
| repwt   | 0.9663   | 0.0651     | 14.85   | 0.0000  |
| sexM    | -1.4826  | 1.7977     | -0.82   | 0.4106  |

Table 2: xtable for regression output
Statistical inference (review)

• statistical inference: drawing conclusions about an entire *population* based on information contained in a *sample* drawn from the population
  
  – *parameter*: a numeric quantity that describes an entire population
    
    * we can never know the exact value of a parameter unless we can measure every member of the population
  
  – *statistic*: a numeric quantity that describes a sample
  
  – inference about parameter usually uses the corresponding statistic calculated for a sample drawn from the population of interest
How do we know whether statistical procedures work as advertised?

- e.g. “95% confidence interval” means that applying this procedure will produce an interval that traps the true parameter value in 95% of all possible simple random samples from a population.

- e.g. a hypothesis testing procedure claims to give us a significance level of .05 (only .05 risk of rejecting the null hypothesis when it’s true).

- since we never know the true values of population parameters, how can we verify that these claims are true?

- can’t do it by testing methods on real data.

- sometimes we can mathematically prove properties of statistical procedures by using probability.
  - often this is possible to do if we can assume that sample sizes are arbitrarily large (asymptotic theory).
  - but we usually need to know how the procedures work for small or moderate sample sizes.
Simulation studies

• enable us to test statistical procedures because we create the populations and therefore we know the true parameter values

• simulation studies are experiments

• we decide under what conditions we want to test a procedure
  – what kind of population(s)
    * often characterized by different probability distributions
  – what parameter values
  – what size(s) of samples drawn from those populations
  – perhaps other characteristics that are important to the performance of the particular procedure we are interested in

• then we use a computer to draw many, many simple random samples from the population with the distribution and parameter values we have chosen (this is “simulation”)

• we apply the statistical procedure to each of the samples we have simulated
• we can use the results to assess how well the procedure works
Example: procedure to calculate 95% confidence intervals for a population variance

Perhaps we are interested in estimating the variance $\sigma^2$ of heights in the population of U.S. undergraduate males.

• we can’t possibly measure every single undergraduate male in the U.S., so we plan to take a simple random sample of 35 guys and measure their heights in inches

• we know how to calculate the sample variance $s^2$ given a set of values
  – $s^2$ will be our point estimate of $\sigma^2$

• we find online a formula for calculating confidence intervals for variances, but it looks weird and we’d like to know whether it works before applying it to our data

http://sixsigmatutorial.com/Six-Sigma/Six-Sigma-t-Confidence-Interval-Variance.aspx
Our plan

• we are interested in testing this confidence intervals procedure in two kinds of populations
  – normal distribution (note: it’s actually possible to prove mathematically that it works in this case)
  – a skewed population that isn’t normal (we’ll use the gamma distribution)

• We’ll pick values of the population mean $\mu$ and the population variance $\sigma^2$.

• We’ll choose the confidence level that we want to test the procedure for (let’s use 95%)

• We’ll use the computer (R!) to simulate 1000 samples of size 35 from a normal distribution with $\mu$ and $\sigma^2$ we chose

• We’ll apply the confidence interval calculating procedure to each of the 1000 samples, producing 1000 confidence intervals
• We’ll count how many of these 1000 intervals contain the true value of $\sigma^2$, and use this to calculate the proportion

\[
\frac{\text{number of intervals containing } \sigma^2}{\text{total number of datasets}}
\]

This is our simulation-based estimate of the true “coverage probability” of the procedure. Due to random variability, it probably won’t be exactly equal to the confidence level. But if the procedure works well, it should be very close.

• We will repeat all the steps from the preceding page for the non-normal population.
R for the confidence interval procedure for variances

# Get the Chisquare values needed to compute confidence intervals

> chisqs <- qchisq(c(0.025, 0.975), 34 )
> chisqs
[1] 19.80625 51.96600

# Simulate 1000 datasets of size 35 from a normal distribution with
#   mean 0 and variance 2
#   Put them in a table; each row is one dataset

> normals <- matrix( rnorm( 35000, mean=0, sd = sqrt(2) ), nrow=1000 )

# Here’s what the first row (dataset) looks like:

> normals[1,]
[7] -1.438510 0.764424 -1.560179 1.578609 0.539696 -1.822125
[13] 2.301967 -1.634460 0.545252 0.779276 2.608455 0.127560
[19] -0.216069 -2.425004 0.935366 0.772572 2.157019 0.792212
[25] -0.554624 0.578819 -0.115696 0.357321 1.929322 1.195243
[31] -0.392629 0.403475 1.460448 0.298659 -2.413320

# And here are the sample mean and sample variance of the first dataset:

> mean(normals[1,])
[1] 0.5352847
> var(normals[1,])
[1] 2.322497

# Calculate the sample variance s² of each of the 1000 rows;
# R lets you do this with 1 line of code!

```r
> ssq <- apply( normals, 1, var )
```

# Now ssq is a vector of 1000 numbers, each the sample variance of one of
# the datasets

```r
> length(ssq)
[1] 1000

> ssq[1:20]
[1] 2.3224967 2.6569998 2.7430414 1.3453956 2.7515834 2.7217364 1.4419119
[8] 2.1723866 1.2222191 0.9203172 1.7110501 1.7675063 1.8160497 1.6341400
[15] 2.6805865 1.9869705 2.1378744 1.9456557 2.0919452 1.0685756
```
# Now use the formula to calculate the left endpoint and the right endpoint for a confidence interval based on each dataset

```r
> leftend <- 34 * ssq / chisqs[2]
> rightend <- 34 * ssq / chisqs[1]
```

# Here are the first 20 confidence intervals:

```r
cbind( leftend, rightend)[1:10,]
```

```
leftend rightend
[1,] 1.5195493 3.986867
[2,] 1.7384059 4.561084
[3,] 1.7947007 4.708786
[4,] 0.8802573 2.309546
[5,] 1.8002895 4.723450
[6,] 1.7807614 4.672213
[7,] 0.9434055 2.475229
[8,] 1.4213361 3.729183
[9,] 0.7996662 2.098098
[10,] 0.6021396 1.579844
```

# Now we can use R to determine whether each of the confidence intervals we calculated contains 2, that is, is 2 greater than the left endpoint and smaller than right

```r
> contains2 <- 2 > leftend & 2 < rightend
> contains2
```

```
[1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE FALSE TRUE TRUE
[13] TRUE TRUE TRUE TRUE TRUE TRUE TRUE FALSE TRUE TRUE TRUE TRUE
[25] TRUE TRUE TRUE TRUE TRUE TRUE TRUE FALSE TRUE TRUE TRUE TRUE
[37] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
[49] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
```
# convert the logical values TRUE and FALSE to numeric
> contains2 <- as.numeric(contains2)
> as.numeric(contains2)
   [1]  1  1  1  1  1  1  1  1  0  1  1  1  1  1  1  1  0  1  1  1  1  1  1  1  0  1  1  1  1
   [38] 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  0  1  1  1  1  1

> sum( contains2 ) / length(contains2)
[1] 0.951
Now let’s do it for a non-normal population

# Simulate 1000 datasets of size 35 from a gamma distribution with
# mean sqrt(2) and variance 2
# Put them in a table; each row is one dataset

> gammas <- matrix( rgamma(35000, 1, 1/sqrt(2)), nrow=1000)

# The gamma density with parameters 1 and 1/sqrt(2) is NOT symmetric!
> ssqgammas <- apply( gammas, 1, var)
> ssqgammas[1:20]
[1] 1.3470058 1.8985875 2.3153270 5.1593305 1.3587234 1.4856546 1.9841449
[8] 1.9489576 1.3338598 1.0878279 0.5044098 2.3987975 1.8152692 1.5331041
[15] 1.5600314 2.0573240 1.8465979 0.9101784 3.1174721 1.9953191

> leftendgammas <- 34 * ssqgammas / chisqs[2]
> rightendgammas <- 34 * ssqgammas / chisqs[1]
> cbind( leftendgammas, rightendgammas)[1:10,]

    leftendgammas rightendgammas
[1,]    0.8813109    2.312310
[2,]    1.2421964    3.259171
[3,]    1.5148583    3.974559
[4,]    3.3756159    8.856660
[5,]    0.8889774    2.332425
[6,]    0.9720252    2.550319
[7,]    1.2981744    3.406042
[8,]    1.2751523    3.345638
[9,]    0.8727098    2.289743
[10,]   0.7117375    1.867398

> contains2gammas <- 2 > leftendgammas & 2 < rightendgammas
> contains2gammas <- as.numeric(contains2gammas)
> sum(contains2gammas) / length(contains2gammas)

[1] 0.705

# Uh-oh. This procedure doesn’t seem to work very well for this non-normal population!

# When we analyze real data, we’d better check whether the sample is likely to have come from a normal population before using this confidence interval method.
Figure 1: Gamma density plot
Properties of point estimation procedures that we can evaluate with simulation studies

• bias
  – the average value of the estimator minus the true parameter value
  – tells you whether the estimation procedure gives results that are systematically too high or too low

• mean squared error
  – the average squared difference between the estimator and the true parameter value
  – assesses how variable the estimator is and how far off on average (regardless of direction)
Assessing bias and MSE in our variance problem

# bias in normal case

> ssq <- apply( normals, 1, var)
> mean(ssq) - 2
[1] -0.007934868

# mean squared error in normal case

> mean( (ssq - 2)^2 )
[1] 0.2300223

# bias in skewed case

> mean(ssqgammas) - 2
[1] -0.02777675

# mean squared error in skewed case

> mean( (ssqgammas - 2)^2 )
[1] 0.8638287
Using simulation studies to evaluate properties of hypothesis tests

- significance level $\alpha$
- power
Types of error in hypothesis testing

\[ H_0 : \mu = \mu_0 \]
\[ H_a : \mu \neq \mu_0 \]

True state of the world

<table>
<thead>
<tr>
<th>Reject ( H_0 )</th>
<th>( H_0 ) is false</th>
<th>( H_0 ) is true</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correct!</td>
<td>Type I error</td>
<td></td>
</tr>
</tbody>
</table>

| Do not reject \( H_0 \) | Type II error | Correct! |

\( \alpha = P(\text{reject } H_0 \mid H_0 \text{ is true}) \)
\( \beta = P(\text{fail to reject } H_0 \mid H_0 \text{ is false}) \)

or, put another way

\( \alpha = \) probability of making Type I error
\( \beta = \) probability of making Type II error
\( \text{power} = 1 - \beta = \) probability of correctly rejecting \( H_0 \) when it is false
Reproducible research and simulation studies

• research should be conducted in such an organized way, and documented well enough, that a different researcher could figure out how to repeat it and get the same (or similar) results

• pseudorandom number generation

• setting random number seeds and keeping track of which ones were used in any pseudorandom operations is necessary for simulation studies that will be formally presented or submitted for publication