Stat 849: Fitting linear models in R

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2010-09-03

Outline

Fitting linear models in R

The `lm` function in `R` provides a formula/data interface for fitting linear models

- The first argument, `formula`, is a two-sided formula with the response on the left hand side and model `terms`, separated by + signs, on the right hand side.
- The second argument, `data`, is the name of a data frame in which to evaluate the formula. It is optional but recommended.
- Most other arguments have default values that are rarely changed

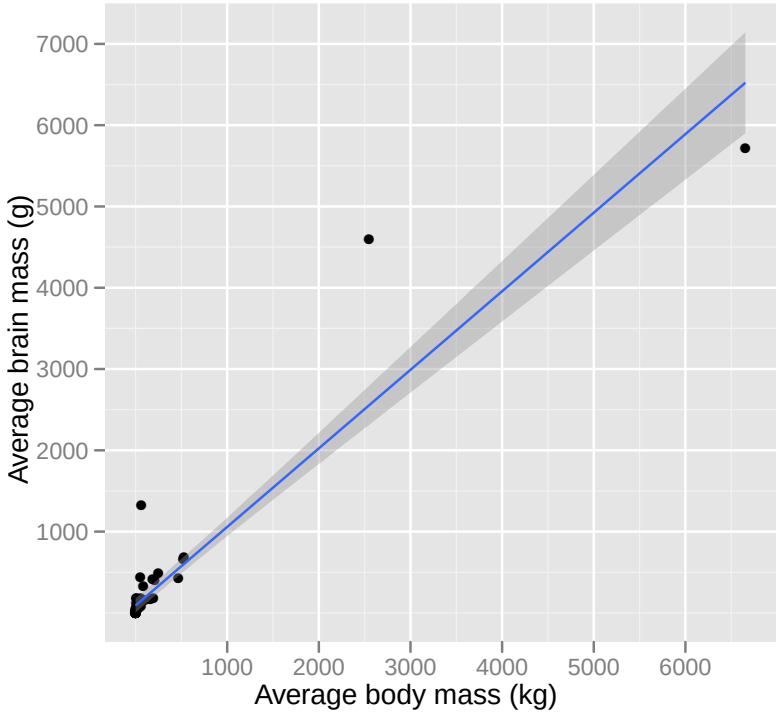
```
1  args(lm)
```

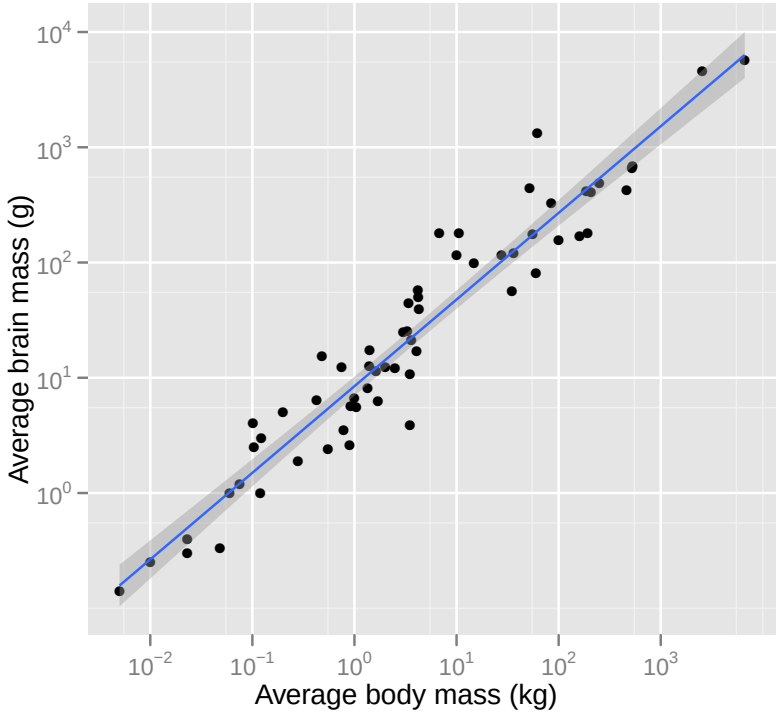
```
function (formula, data, subset, weights, na.action, method = "qr",
    model = TRUE, x = FALSE, y = FALSE, qr = TRUE, singular.ok = TRUE,
    contrasts = NULL, offset, ...)
NULL
```

Brain weight data

Recall the structure of the `brains` data in the `alr3` package

```
'data.frame': 62 obs. of  2 variables:
 $ BrainWt: num  44.5 15.5 8.1 423 119.5 ...
 $ BodyWt : num  3.38 0.48 1.35 464.98 36.33 ...
```





Fitting linear models to the brains data

We fit two linear models, corresponding to the lines on the plots:

- lm1 `BrainWt` as a linear function of `BodyWt`. From the data plots we expect that this will not fit well
- lm2 `log(BrainWt)` as a linear function of `log(BodyWt)`

```
lm1 <- lm(BrainWt ~ BodyWt, brains)
lm2 <- lm(log(BrainWt) ~ log(BodyWt), brains)
```

Notice that we assign the result of fitting a model to a name. The fitted model is a *classed* object

```
class(lm1)
```

```
[1] "lm"
```

to which we can apply several different *extractor* functions, most of which are *methods* for generic functions. It is worthwhile checking the documentation of such methods to see what they do.

Listing of the methods for class lm

```
1  methods(class="lm")
```

```
 [1] add1.lm*            alias.lm*           anova.lm
 [4] case.names.lm*      confint.lm*         cooks.distance.lm*
 [7] deviance.lm*        dfbeta.lm*          dfbetas.lm*
[10] drop1.lm*           dummy.coef.lm*      effects.lm*
[13] extractAIC.lm*      family.lm*          formula.lm*
[16] fortify.lm          hatvalues.lm        influence.lm*
[19] kappa.lm            labels.lm*          logLik.lm*
[22] model.frame.lm      model.matrix.lm     plot.lm
[25] predict.lm          print.lm            proj.lm*
[28] residuals.lm        rstandard.lm        rstudent.lm
[31] simulate.lm*        summary.lm          variable.names.lm*
[34] vcov.lm*

   Non-visible functions are asterisked
```

The summary of fitted model lm1

```
1  summary(lm1)
```

```
Call:
lm(formula = BrainWt ~ BodyWt, data = brains)

Residuals:
    Min      1Q  Median      3Q     Max
-810.15  -88.52  -79.65  -13.02 2050.52

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 91.00864   43.55574   2.089   0.0409
BodyWt       0.96646    0.04767  20.276   <2e-16

Residual standard error: 334.7 on 60 degrees of freedom
Multiple R-squared: 0.8726,   Adjusted R-squared: 0.8705
F-statistic: 411.1 on 1 and 60 DF,  p-value: < 2.2e-16
```

The summary of fitted model lm2

```
1  summary(lm2)
```

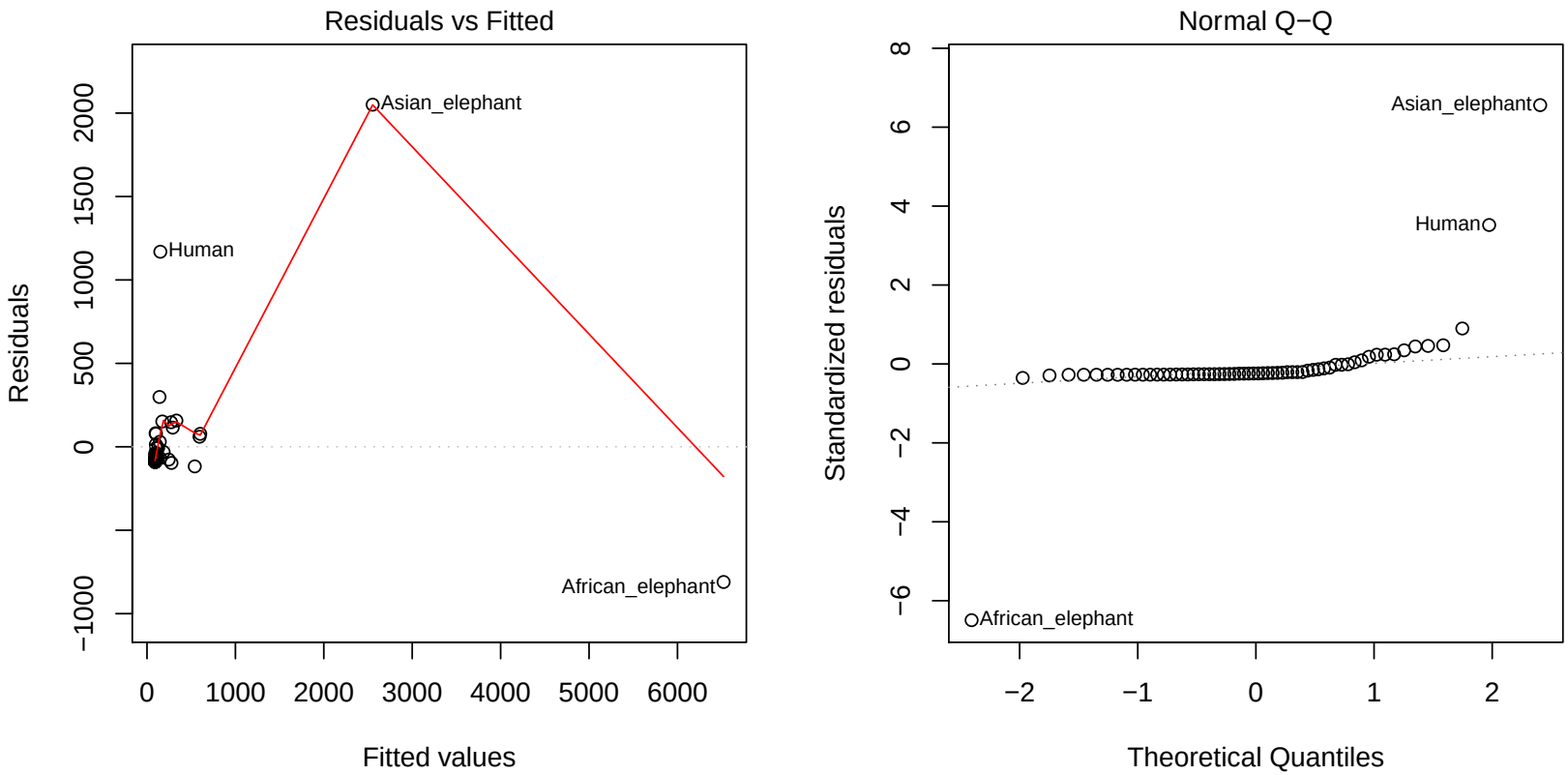
```
Call:
lm(formula = log(BrainWt) ~ log(BodyWt), data = brains)

Residuals:
     Min       1Q   Median       3Q      Max
-1.71550 -0.49228 -0.06162  0.43598  1.94833

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.13479    0.09604   22.23   <2e-16
log(BodyWt)  0.75169    0.02846   26.41   <2e-16

Residual standard error: 0.6943 on 60 degrees of freedom
Multiple R-squared: 0.9208,   Adjusted R-squared: 0.9195
F-statistic: 697.4 on 1 and 60 DF,  p-value: < 2.2e-16
```

Residual plots

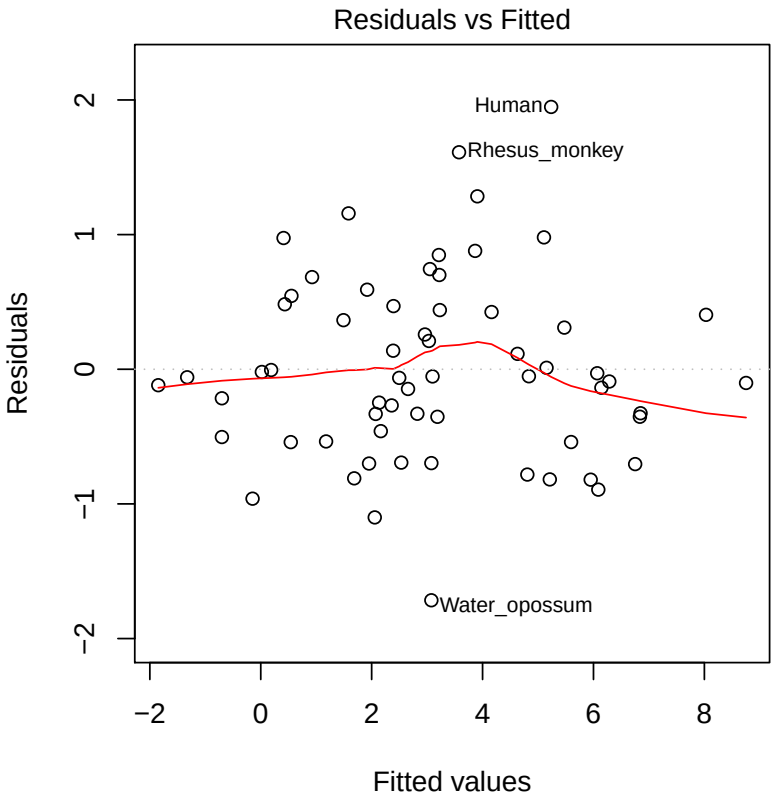
- The base graphics system provides good "canned" residual plots.
- There are 6 possibilities available through the `which` argument to the `plot` method for `lm` objects. See `?plot.lm` for details or experiment for yourself.
- You should always check the first two
- To lay out multiple residual plots in the same figure, set the graphical parameter `mfcol` or `mfrow` using the `par()` function.
- It is a good practice to save the old values of the parameters, which is the value returned by `par()` and restore it after the plot.

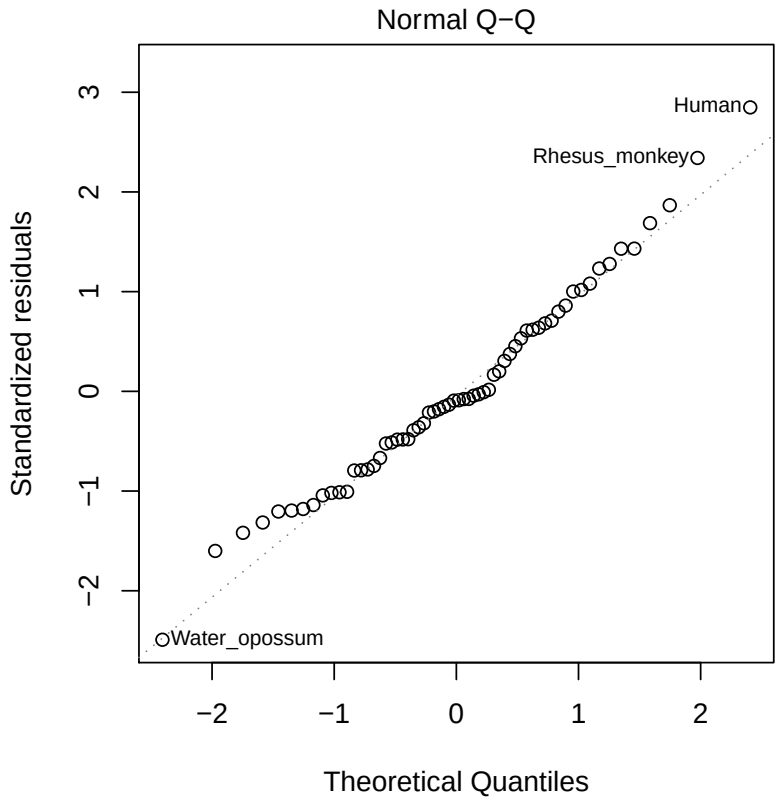
Residuals vs fitted and normal Q-Q plot, model `lm1`

```
1  opar <- par(mfcol=c(1,2))
2  plot(lm1, which=1:2)
3  par(opar)
```



Residuals vs fitted and normal Q-Q plot, model `lm2`





Analysis of variance table

For a simple linear regression, the anova table is not too interesting but, for other models, it will be.

```
1  anova(lm2)
```

```
Analysis of Variance Table

Response: log(BrainWt)
             Df Sum Sq Mean Sq F value    Pr(>F)
log(BodyWt)   1 336.19  336.19  697.42 < 2.2e-16
Residuals    60  28.92    0.48
```

- This anova table is based on the **sequential** sums of squares. We will discuss later what that means.
- The anova generic can take as arguments several fitted models, in which case it provides the analysis of variance for comparing nested models.

The coefficients table

A little-known extractor

```
coef(summary(lm2))
```

```
             Estimate Std. Error  t value     Pr(>|t|)
(Intercept) 2.1347883 0.09604321 22.22737 1.183103e-30
log(BodyWt) 0.7516861 0.02846349 26.40878 9.834309e-35
```

provides the coefficients table. To print the table as it is shown in the summary output, use

```
printCoefmat(coef(summary(lm2)))
```

```
            Estimate Std. Error t value  Pr(>|t|)
(Intercept) 2.134788   0.096043  22.227 < 2.2e-16
log(BodyWt) 0.751686   0.028463  26.409 < 2.2e-16
```

Incorporating tables in LaTeX documents

The `xtable` package provides a LaTeX table for pretty-printing. Options for captions, labels, special environments, etc. are available.

```
1 library(xtable)
2 xtable(lm2)
```

	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	2.1348	0.0960	22.23	0.0000
log(BodyWt)	0.7517	0.0285	26.41	0.0000

```
1 xtable(anova(lm2))
```

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
log(BodyWt)	1	336.19	336.19	697.42	0.0000
Residuals	60	28.92	0.48		

Extractor methods for $\hat{\beta}$, RSS, etc.

```
1  deviance(lm2) # residual sum of squares
```

```
[1] 28.92261
```

```
1  coef(lm2)      # coefficient estimates
```

```
(Intercept) log(BodyWt)
  2.1347883   0.7516861
```

```
1  vcov(lm2)      # variance-covariance of coef est.
```

```
             (Intercept)   log(BodyWt)
(Intercept)  0.009224299 -0.0010836348
log(BodyWt) -0.001083635  0.0008101703
```

```
1  logLik(lm2)    # log-likelihood
```

```
'log Lik.' -64.33635 (df=3)
```

Confidence intervals, model matrix

```
confint(lm2)  # confidence intervals on coefficients
```

```
                2.5 %    97.5 %
(Intercept) 1.9426733 2.3269033
log(BodyWt) 0.6947507 0.8086216
```

```
kappa(lm2)     # condition number of the X matrix
```

```
[1] 3.967229
```

```
str(model.matrix(lm2)) # the X matrix itself
```

```
 num [1:62, 1:2] 1 1 1 1 1 1 1 1 1 1 ...
 - attr(*, "dimnames")=List of 2
  ..$ : chr [1:62] "Arctic_fox" "Owl_monkey" "Beaver" "Cow" ...
  ..$ : chr [1:2] "(Intercept)" "log(BodyWt)"
 - attr(*, "assign")= int [1:2] 0 1
```

Model frame

- Some of the processing of the formula and of arguments like `subset`, `offset` and `na.action` takes place in the formation of the `model.frame` before the creation of the `model.matrix`.
- The model frame contains many attributes that are useful for extractors like anova.
- It contains only the data actually used to fit the model.

```
1  str(model.frame(lm2))
```

```
'data.frame': 62 obs. of  2 variables:
 $ log(BrainWt): num  3.8 2.74 2.09 6.05 4.78 ...
 $ log(BodyWt) : num  1.219 -0.734 0.3 6.142 3.593 ...
 - attr(*, "terms")=Classes 'terms', 'formula' length 3 log(Bra..
  .. ..- attr(*, "variables")= language list(log(BrainWt), log(..
  .. ..- attr(*, "factors")= int [1:2, 1] 0 1
  .. .. ..- attr(*, "dimnames")=List of 2
  .. .. .. ..$ : chr [1:2] "log(BrainWt)" "log(BodyWt)"
  .. .. .. ..$ : chr "log(BodyWt)"
  .. ..- attr(*, "term.labels")= chr "log(BodyWt)"
  .. ..- attr(*, "order")= int 1
  .. ..- attr(*, "intercept")= int 1
```

Simulation

- The list of methods includes `simulate.lm`, which simulates a matrix of responses from the parameter estimates of the model.
- Furthermore, you can generate all the information on the fitted models for these responses with a single call to `lm` or to `lm.fit`, which does the calculations within `lm`.
- This is orders of magnitude faster than calling `lm` inside a loop.
- To fit model `lm2` to 10000 simulated responses takes a couple of seconds

```
1 system.time({Ymat <- data.matrix(simulate(lm2,10000))
2      lm2Sim <- lm(Ymat ~ log(BodyWt), brains)})
```

```
   user  system elapsed
  3.450   0.060   3.514
```

Extracting the results of the simulation

All of the extractor functions for an `lm` model apply to `lm2Sim`.
Extractors that return scalars now return a vector

```
str(deviance(lm2Sim))
```

```
Named num [1:10000] 29.3 36.6 25.2 34.2 27.2 ...
- attr(*, "names")= chr [1:10000] "sim_1" "sim_2" "sim_3" "sim..
```

Extractors that return a vector now return a matrix

```
str(coef(lm2Sim))
```

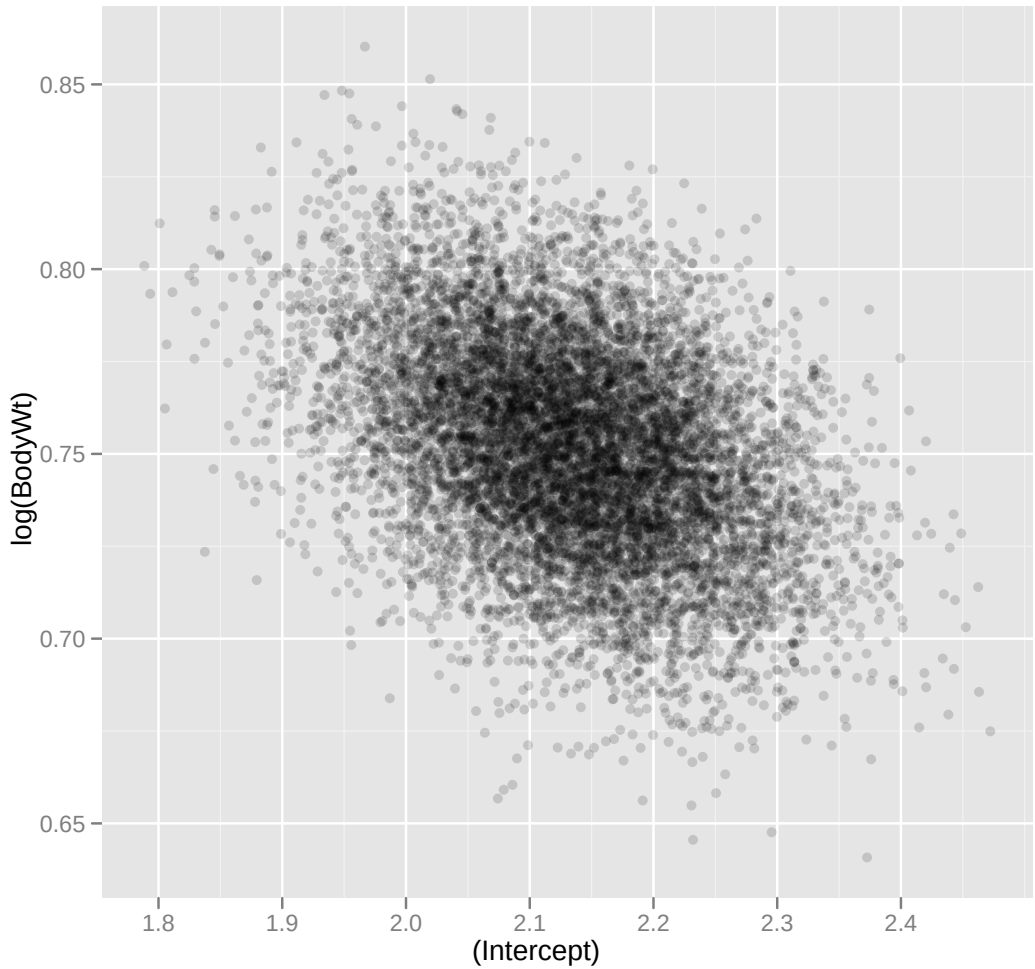
```
num [1:2, 1:10000] 1.906 0.726 1.992 0.801 2.09 ...
- attr(*, "dimnames")=List of 2
 ..$ : chr [1:2] "(Intercept)" "log(BodyWt)"
 ..$ : chr [1:10000] "sim_1" "sim_2" "sim_3" "sim_4" ...
```

We often want a data frame of the transpose

```
coefSim <- data.frame(t(coef(lm2Sim)), check.names=FALSE)
```

Scatter plot of coefficient estimates

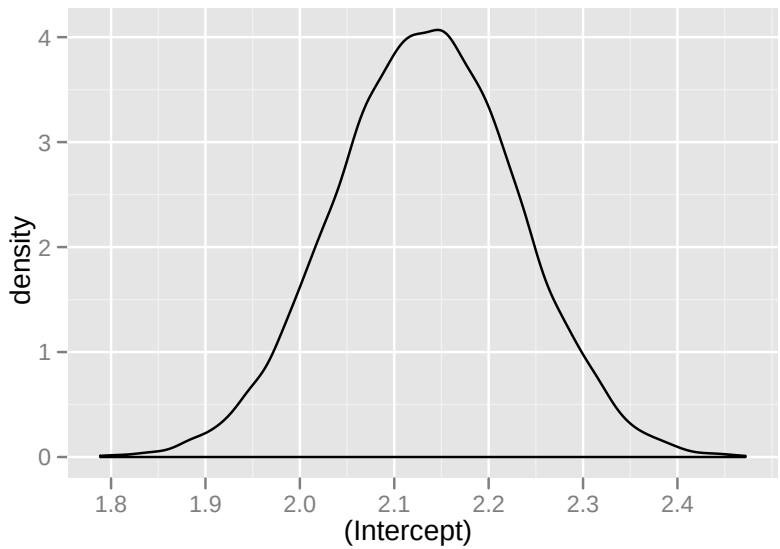
```
qplot(`(Intercept)`, `log(BodyWt)`, data=coefSim,
      alpha="0.15")
```

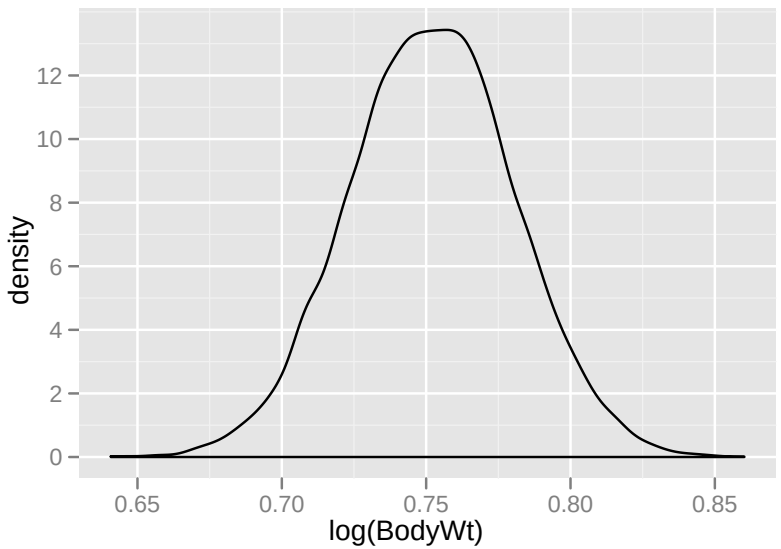


Distribution of parameter estimates

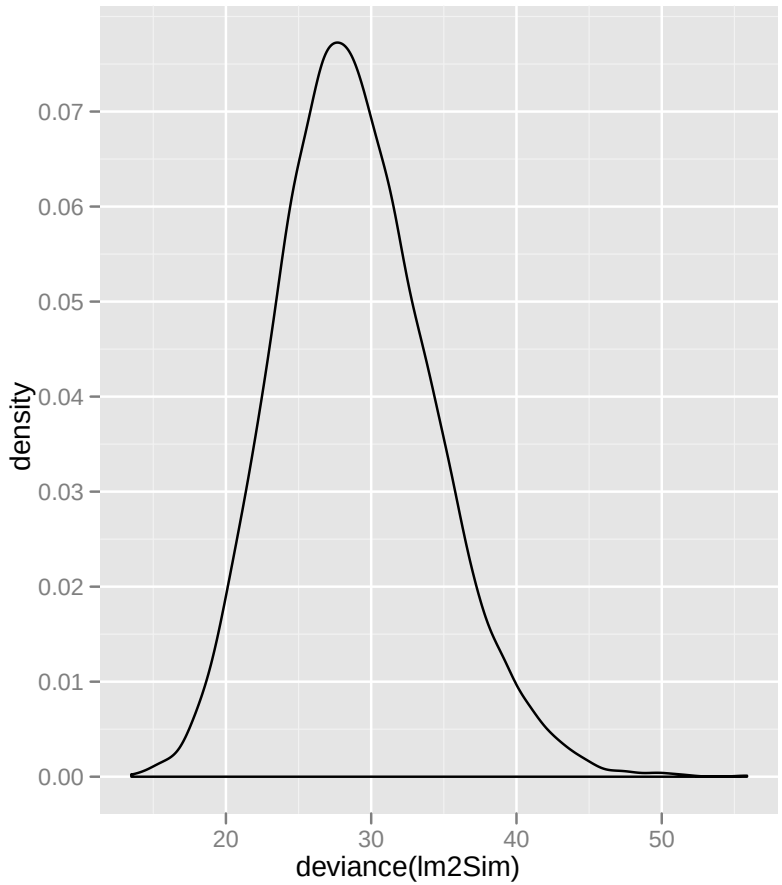
```
cbind(coef(summary(lm2))[,1:2],
      simMn=sapply(coefSim, mean),
      simSd=sapply(coefSim, sd))
```

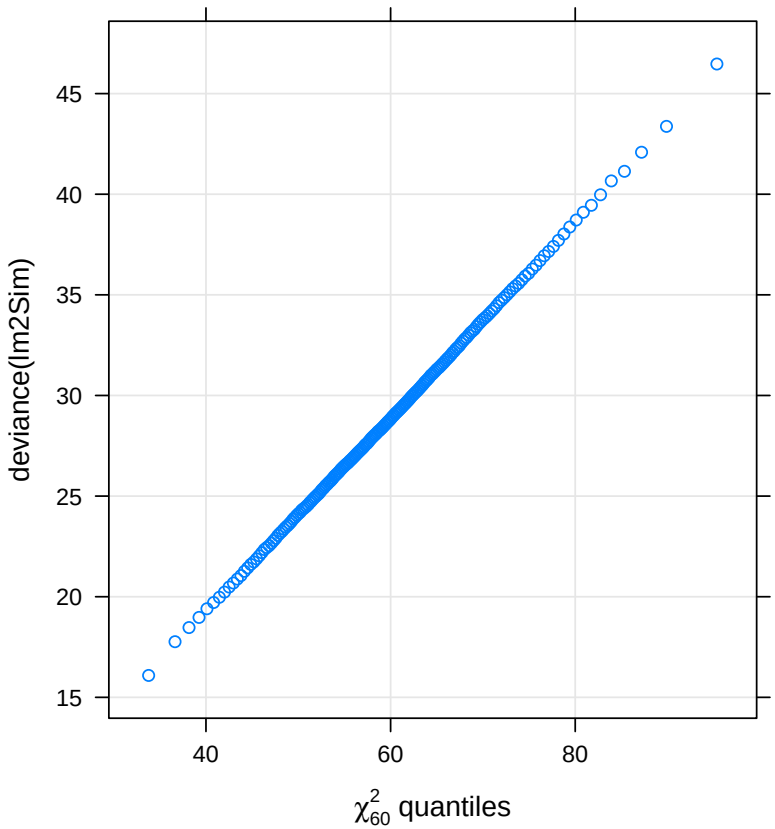
	Estimate	Std. Error	simMn	simSd
(Intercept)	2.1347883	0.09604321	2.1337564	0.09615131
log(BodyWt)	0.7516861	0.02846349	0.7519274	0.02852459





Distribution of the residual sum of squares





Diagnostic measures

- Many of the methods for `lm` objects, such as `fitted`, `residuals`, `rstandard`, `rstudent`, `cooks.distance`, `hatvalues`, `dffit`, and `dfbetas` provide information used in diagnostics. We will discuss these later.
- See also the results of the `influence` method and the `lm.influence` function.
- ggplot2 provides a convenience method `fortify` that extracts the model frame and augments it with diagnostic measures.

```
1  head(fortify(lm2), 3)
```

```
            log(BrainWt) log(BodyWt)     .hat .sigma  .cooksd
Arctic_fox         3.795      1.2194 0.01615 0.6933 0.009584
Owl_monkey         2.741     -0.7340 0.02334 0.6833 0.034018
Beaver             2.092      0.3001 0.01794 0.6993 0.001391
            .fitted  .resid .stdresid
Arctic_fox    3.051  0.7441    1.0805
Owl_monkey    1.583  1.1577    1.6873
Beaver        2.360 -0.2685   -0.3903
```

QR decomposition of the model matrix

- Most formulas you have seen for regression and analysis of variance results (e.g. $\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\boldsymbol{X}'\boldsymbol{y}$) bear no resemblance to the way things are actually calculated.
- Virtually all the numerical work for linear models in R uses the QR decomposition, $\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{R} = \boldsymbol{Q}_1\boldsymbol{R}_1$, where $\boldsymbol{Q}$ is orthogonal (i.e. $\boldsymbol{Q}'\boldsymbol{Q} = \boldsymbol{Q}\boldsymbol{Q}' = \boldsymbol{I}_n$) and $\boldsymbol{R}$ is zero below the main diagonal. Sometimes we write $\boldsymbol{R}_1$ for the first p rows of $\boldsymbol{R}$ and $\boldsymbol{Q}_1$ for the first p columns of $\boldsymbol{Q}$.
- From version 2.12.0 (Oct., 2010) R will provide a qr extractor for lm objects. For now you need to use $qr

```
1  str(lm2$qr)
```

```
List of 5
 $ qr   : num [1:62, 1:2] -7.874 0.127 0.127 0.127 0.127 ...
  ..- attr(*, "dimnames")=List of 2
  .. ..$ : chr [1:62] "Arctic_fox" "Owl_monkey" "Beaver" "Cow" ..
  .. ..$ : chr [1:2] "(Intercept)" "log(BodyWt)"
  ..- attr(*, "assign")= int [1:2] 0 1
 $ qraux: num [1:2] 1.13 1.08
```

Relationship to the Cholesky decomposition

```
qr.R(lm2$qr)     # R matrix from the QR
```

```
           (Intercept) log(BodyWt)
Arctic_fox   -7.874008   -10.53180
Owl_monkey    0.000000    24.39242
```

```
X <- model.matrix(lm2)
chol(XtX <- crossprod(X)) # Cholesky of X'X
```

```
            (Intercept) log(BodyWt)
(Intercept)    7.874008    10.53180
log(BodyWt)    0.000000    24.39242
```

```
XtX
```

```
            (Intercept) log(BodyWt)
(Intercept)    62.00000    82.92745
log(BodyWt)    82.92745   705.90906
```

The effects vector

```
1  head(effects(lm2), 5)
```

```
 (Intercept)  log(BodyWt)
-24.72594592  18.33544667  -0.39394094  -0.59250661  -0.04375128
```

- This curious vector is $\boldsymbol{Q}'\boldsymbol{y}$. Not only is it used to calculate $\hat{\boldsymbol{\beta}}$ as the solution to $\boldsymbol{R}_1\hat{\boldsymbol{\beta}} = \boldsymbol{Q}_1'\boldsymbol{y}$ but also the anova sums of squares are calculated from it.
- Compare sum of squares for `log(BodyWt)` to the `log(BodyWt)` component of

```
1  head(effects(lm2)^2, 5)
```

```
 (Intercept)  log(BodyWt)
6.113724e+02 3.361886e+02 1.551895e-01 3.510641e-01 1.914174e-03
```

Is that really the analysis of variance calculation?

Yes, Virginia, it is. Consider an example of a two-factor anova with interactions. We simulate the data

```
set.seed(1234321)
dat <- data.frame(f1=gl(4,6,labels=LETTERS[1:4]),
                  f2=gl(3,2,labels=letters[1:3]),
                  y=8+rnorm(24, sd=0.1))
xtabs(~ f2 + f1, dat)
```

```
   f1
f2  A B C D
  a 2 2 2 2
  b 2 2 2 2
  c 2 2 2 2
```

and fit the model

```
lm3 <- lm(y ~ f1 * f2, dat)
```

Fitting the anova model with interactions

```
anova(lm3)
```

```
Analysis of Variance Table

Response: y
          Df   Sum Sq   Mean Sq F value Pr(>F)
f1         3 0.018342 0.0061139  0.4656 0.7116
f2         2 0.036907 0.0184535  1.4053 0.2829
f1:f2      6 0.096525 0.0160876  1.2251 0.3588
Residuals 12 0.157575 0.0131313
```

Compare the sums of squares to the results of summing elements of `effects(am1)^2` according to

```
(asgn <- attr(model.matrix(lm3), "assign"))
```

```
 [1] 0 1 1 1 2 2 3 3 3 3 3 3
```

```
tapply(effects(lm3)[1:12]^2, asgn, sum)
```

```
           0            1            2            3
1.552090e+03 1.834185e-02 3.690692e-02 9.652533e-02
```