Rationale for MASSExtra

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Preamble

This extension package to the classical `MASS` package (Venables & Ripley, of ancient lineage), whose origins go back to nearly 30 years, comes about for a number of reasons.

Firstly, in my teaching I found I was using some of the old functions in the package with consistently different argument settings to the defaults. I was also interested in supplying various convenience extensions that simplified teaching and including various tweaks to improve the interface. Examples follow below.

Secondly, I wanted to provide a few functions that were mainly useful as programming examples. For example, the function `zs` and its allies `zu`, `zq` and `zr` are mainly alternatives to `base::scale`, but they can be used to show how to write functions that can be used in fitting models in such a way that they work as they should when the fitted model object is used for prediction with new data.

Masking `select` from other packages

Finally, there is the perennial `select` problem. When `MASS` is used with other packages, such as `dplyr` the `select` function can easily be masked, causing confusion for users. `MASS::select` is rarely used, but `dplyr::select` is fundamental. There are standard ways of managing this kind of masking, but what we have done in `MASSExtra` is to export the more common functions used from `MASS` along with the extensions, in such a way that users will not need to have `MASS` attached to the search path at all, and hence masking is unlikely.

The remainder of this document will do a walk-through of some of the new functions provided by the package. We begin by setting the computational context:

```
suppressPackageStartupMessages({
  library(visreg)
  library(knitr)
  library(tidyverse)
  library(patchwork)
  library(MASSExtra)
})
options(knitr.kable.NA = "")
theme_set(theme_bw() + theme(plot.title = element_text(hjust = 0.5)))
```

Amble

We now consider some of the extensions that the package offers to the originals. Most of the extensions will have a name that includes an underscore of two somewhere to distinguish it from the V&R original. Note that the original version is *also* exported so that scripts that use it may do so without change, via the new package.

The `box_cox` extensions

This original version, `boxcox` has a fairly rigid display for the plotted output which has been changed to give a more easily appreciated result. The $y-$axis has been changed to give the likelihood-ratio statistic rather

than the log-likelihood, and for the $x-$axis some attempt has been made to focus on the crucial region for the transformation parameter, λ,

The following example shows the old and new plot versions for a simple example.

```
par(mfrow = c(1, 2))
mod0 <- lm(MPG.city ~ Weight, Cars93)
boxcox(mod0)   ## MASS
box_cox(mod0) ## MASSExtra tweak
```

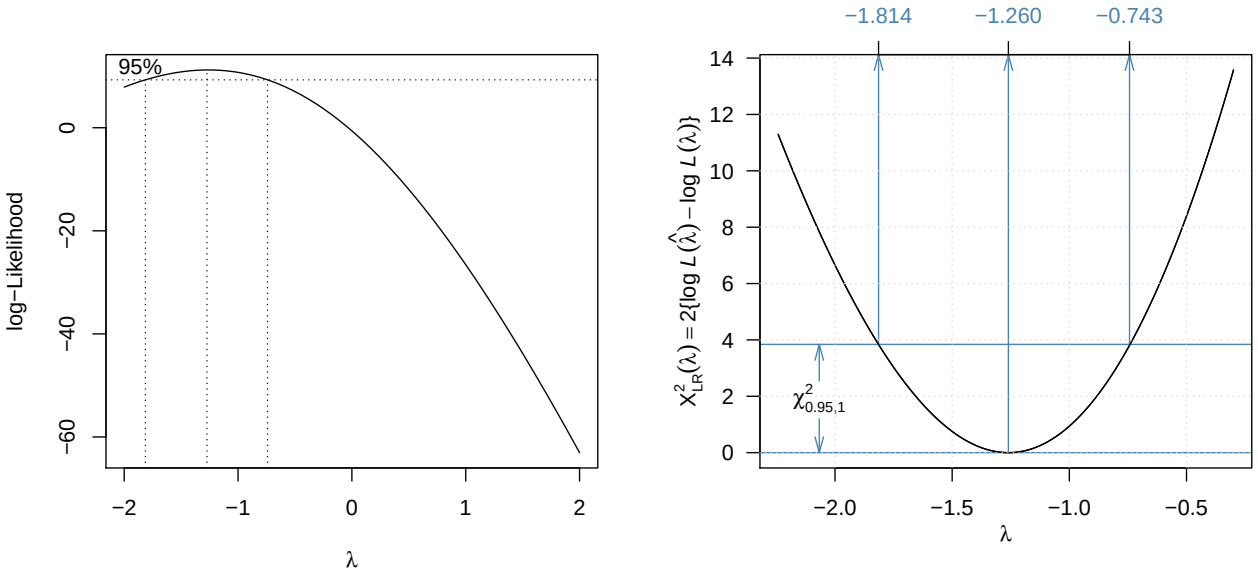


Figure 1: Box-cox, old and new displays

In addition, there are functions `bc` to evaluate the transformation for a given exponent, and a function `lambda` which finds the optimum exponent (not that a precise exponent will usually be needed).

It is interesting to see how in this instance the transformation can both straighten the relationship and provide a scale in which the variance is more homogeneous. See Figure 2.

```
p0 <- ggplot(Cars93) + aes(x = Weight) + geom_point(colour = "#2297E6")  + xlab("Weight (lbs)") +
  geom_smooth(se = FALSE, method = "loess", formula = y ~ x, size=0.7, colour = "black")
p1 <- p0 + aes(y = MPG.city) + ylab("Miles per gallon (MPG)") + ggtitle("Untransformed response")
p2 <- p0 + aes(y = bc(MPG.city, lambda(mod0))) + ggtitle("Transformed response") +
  ylab(bquote(bc(MPG, .(round(lambda(mod0), 2)))))
p1 + p2
```

A more natural scale to use, consistent with the Box-Cox suggestion, would be the reciprocal. For example we could use GPM = 100/MPG the "gallons per 100 miles" scale, which would have the added benefit of being more-or-less what the rest of the world uses to gauge fuel efficiency outside the USA. Readers should try this for themselves.

Stepwise model building extensions

The primary `MASS` functions for refining linear models and their allies are `dropterm` and `stepAIC`. The package provides a few extensions to these, but mainly a change of defaults in the argument settings.

1. `drop_term` is a front-end to `MASS::dropterm` with a few tweaks. By default the result is arranged in sorted order, i.e. with `sorted = TRUE`, and also by default with `test = TRUE` (somewhat in defiance of much advice to the contrary given by experienced practitioners: *caveat emptor!*).

   The user may specify the test to use in the normal way, but the default test is decided by an ancillary

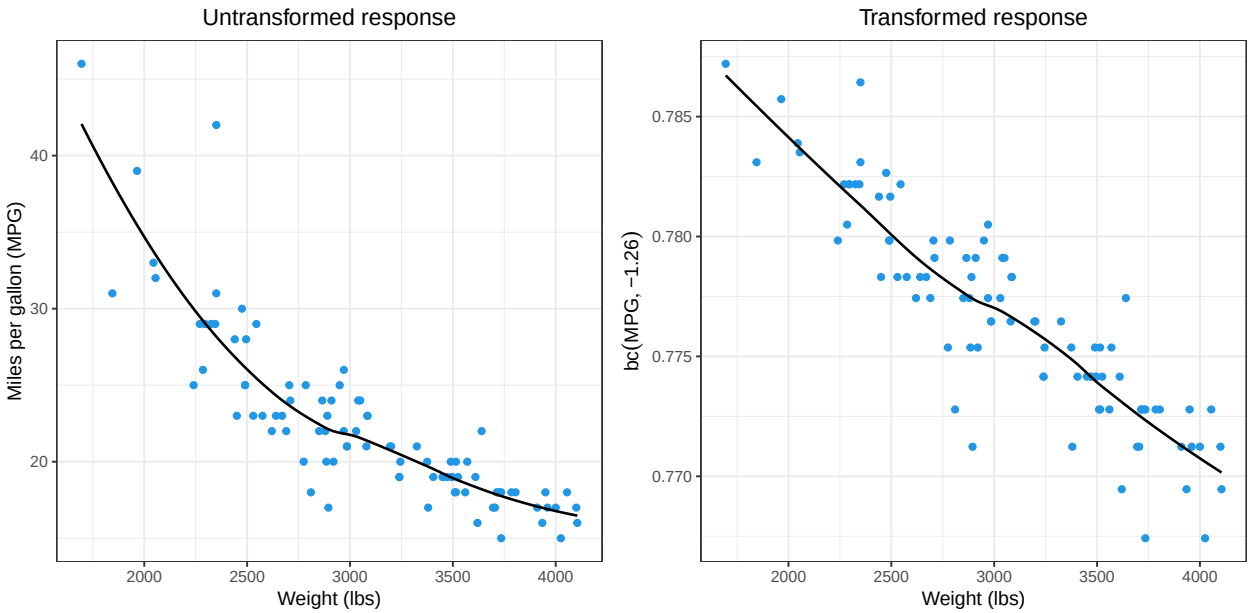


Figure 2: The Box-Cox transformation effect

generic function, `default_test`, which guesses the appropriate test from the object itself. This is an S3 generic and further methods can be supplied for new fitted model objects.

There is also a function `add_term` which provides similar enhancements to those provided by `drop_term`. In this case, of course, the consequences of *adding* individual terms to the model are displayed, rather than of *dropping* them. It follows that using `add_term` you will always need to provide a scope specification, that is, some specification of what extra terms are possible additions.

In addition `drop_term` and `add_term` return an object which retains information on the criterion used, `AIC`, `BIC`, `GIC` (see below) or some specific penalty value `k`. The object also has a class `"drop_term"` for which a `plot` method is provided. Both the `plot` and `print` methods display the criterion. See the example below for how this is done.

2. `step_AIC` is a front-end to `MASS::stepAIC` with the default argument `trace = FALSE` set. This may of course be over-ruled, but it seems the most frequent choice by users, anyway. In addition the actual criterion used, by dafault `k = 2`, i.e. AIC, is retained with the result and passed on to methods in much the same say as for `drop_term` above.

   Since the (default) criterion name is encoded in the function name, two further versions are supplied, namely `step_BIC` and `step_GIC` (again, see below), which use a different, and obvious, default criterion.

   In any of `step_AIC`, `step_BIC` or `step_GIC` a different value of `k` may be specified in which case that value of `k` is retained with the object and displayed as appropriate in further methods.

   Finally in any of these functions `k` may be specified either as a numeric penalty, such as `k = 4` for example, or by character string `k = "AIC"` or `k = "BIC"` with an obvious meaning in either case.

3. Criteria. The **Akaike Information Criterion**, AIC, corresponds to a penalty `k = 2` and the **Bayesian Information Criterion**, BIC, corresponds to `k = log(n)` where `n` is the sample size. In addition to these two the present functions offer an intermediate default penalty `k = (2 + log(n))/2` which is "not too strong and not too weak", making it the **Goldilocks Information Criterion**, GIC. There is also a standalone function `GIC` to evaluate this `k` if need be.

   This suggestion appears to be original, but *no particular claim is made for it* other than with intermediate to largish data sets it has proved useful for exploratory purposes in our experience.

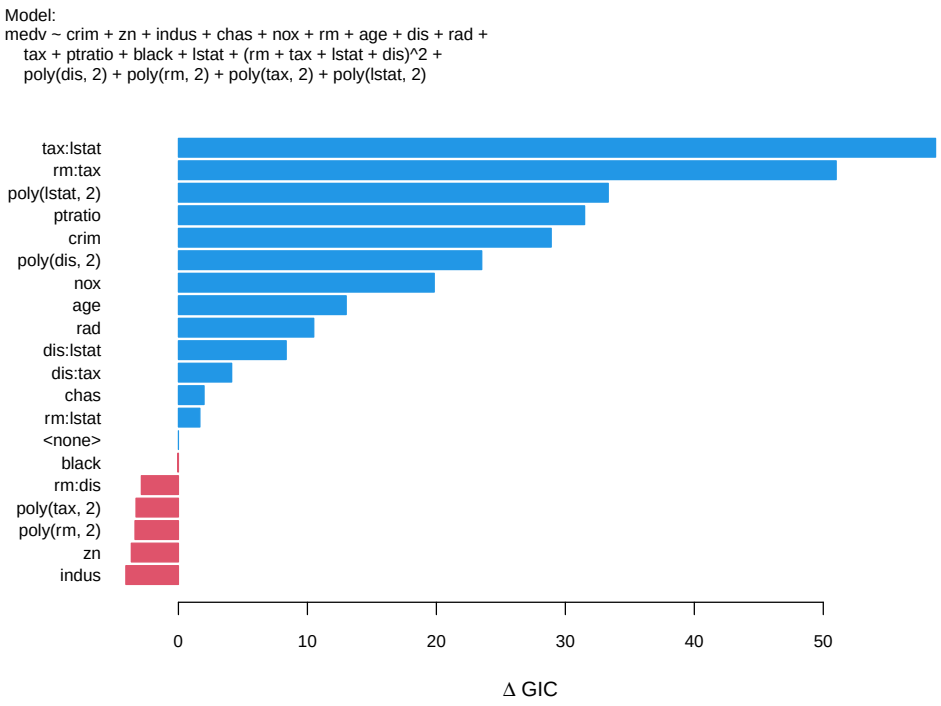
   Our strong advice is that these tools should ***only*** be used for exploratory purposes in any case, and should ***never*** be used in isolation. They have a well-deserved very negative reputation when misused, as they

commonly are.

Examples

We consider the well-known (and much maligned) Boston house price data. See `?Boston`. We begin by fitting a model that has more terms in it than the usual model, as it contains a few extra quadratic terms, including some key linear by linear interactions.

```
big_model <- lm(medv ~ . + (rm + tax + lstat + dis)^2 + poly(dis, 2) + poly(rm, 2) +
                  poly(tax, 2) + poly(lstat, 2), Boston)
big_model %>% drop_term(k = "GIC") %>% plot() %>% kable(booktabs=TRUE, digits=3)
```



	Df	Sum of Sq	RSS	delta_GIC	F Value	Pr(F)
tax:lstat	1	728.695	6241.320	58.707	63.714	0.000
rm:tax	1	634.356	6146.981	51.000	55.465	0.000
poly(lstat, 2)	1	423.361	5935.985	33.327	37.017	0.000
ptratio	1	401.916	5914.540	31.495	35.142	0.000
crim	1	371.709	5884.334	28.905	32.501	0.000
poly(dis, 2)	1	309.410	5822.034	23.519	27.053	0.000
nox	1	267.160	5779.784	19.833	23.359	0.000
age	1	189.742	5702.366	13.010	16.590	0.000
rad	1	161.441	5674.065	10.492	14.116	0.000
dis:lstat	1	137.523	5650.148	8.355	12.024	0.001
dis:tax	1	90.529	5603.153	4.129	7.915	0.005
chas	1	66.861	5579.485	1.987	5.846	0.016
rm:lstat	1	63.305	5575.929	1.664	5.535	0.019
			5512.624	0.000		
black	1	44.479	5557.103	-0.047	3.889	0.049
rm:dis	1	13.525	5526.149	-2.873	1.183	0.277
poly(tax, 2)	1	9.012	5521.636	-3.287	0.788	0.375
poly(rm, 2)	1	8.130	5520.755	-3.368	0.711	0.400
zn	1	5.035	5517.659	-3.651	0.440	0.507
indus	1	0.405	5513.029	-4.076	0.035	0.851

Unlike `MASS::dropterm`, the table shows the terms beginning with the most important ones, that is those which, if dropped, would *increase* the criterion and ending with those of least looking importance, that is those whose removal would most *decrease* the criterion. And also note that here we are using the `GIC`, which is displayed in the output.

Note particularly that rather than give the *value* of the criterion by default the table and plot show *change* in the criterion which would result if the term is removed from the model at that point. This is a more meaningful quantity, and invariant with respect to the way in which the log-likelihood is defined.

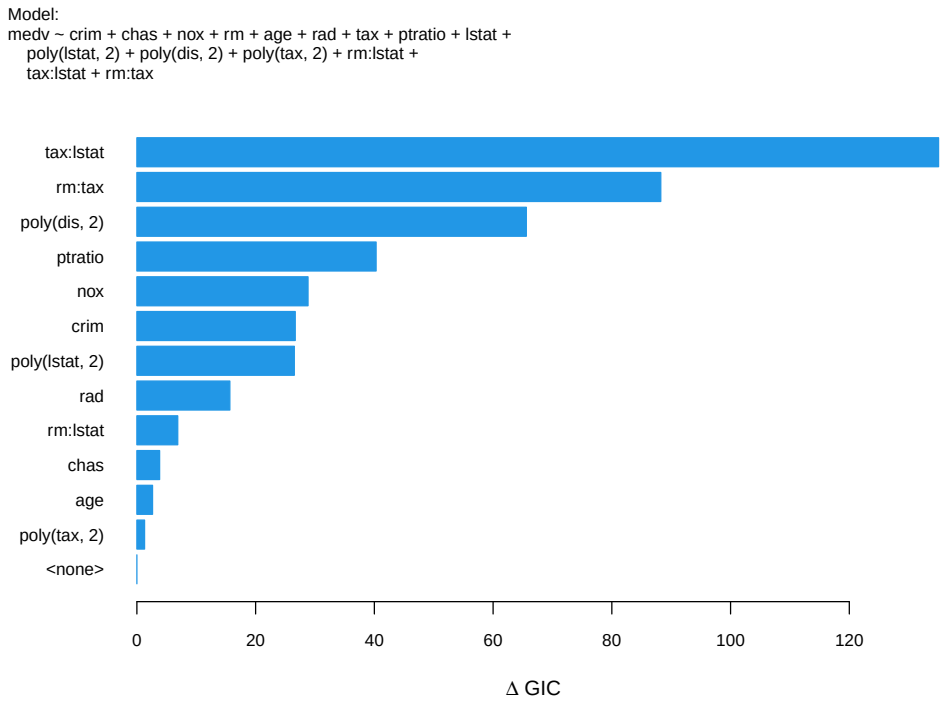
The `plot` method gives a graphical view of the same key bits of information, in the same vertical order as given in the table. Terms whose removal would (at this point) improve the model are shown in *red* and those which would not, and hence should (again, at this point) be retained are shown in *blue*.

With all stepwise methods it is critically important to notice that the whole picture can change once any change is made to the current model. This terms which appear "promising" at this stage may not seem so once any variable is removed from the model or some other variable brought into it. This is a notoriously tricky area for the inexperienced.

Notice that the `plot` method returns the original object, which can then be passed on via a pipe to more operations. (`kable` does not, so this pipe sequence cannot be changed.)

We now consider a refinement of this model by stepwise means, but rather than use the large model as the starting point, we begin with a more modest one which has no quadratic terms.

```
base_model <- lm(medv ~ ., Boston)
gic_model <- step_GIC(base_model, scope = list(lower = ~1, upper = formula(big_model)))
drop_term(gic_model) %>% plot() %>% kable(booktabs = TRUE, digits = 3)
```



	Df	Sum of Sq	RSS	delta_GIC	F Value	Pr(F)
tax:lstat	1	1853.126	7707.733	135.034	154.780	0.000
rm:tax	1	1172.351	7026.958	88.244	97.919	0.000
poly(dis, 2)	2	919.601	6774.208	65.596	38.404	0.000
ptratio	1	537.017	6391.624	40.293	44.854	0.000
nox	1	393.819	6248.426	28.828	32.893	0.000
crim	1	367.257	6221.864	26.672	30.675	0.000
poly(lstat, 2)	1	365.333	6219.940	26.516	30.514	0.000

	Df	Sum of Sq	RSS	delta_GIC	F Value	Pr(F)
rad	1	233.292	6087.899	15.658	19.486	0.000
rm:lstat	1	128.612	5983.219	6.882	10.742	0.001
chas	1	92.617	5947.224	3.829	7.736	0.006
age	1	78.635	5933.242	2.638	6.568	0.011
poly(tax, 2)	1	62.892	5917.499	1.293	5.253	0.022
			5854.607	0.000		

The model is likely to be over-fitted. To follow up on this we could look at profiles of the fitted terms as an informal way of model 'criticism'.

```
capture.output(suppressWarnings({
   g1 <- visreg(gic_model, "dis", plot = FALSE)
   g2 <- visreg(gic_model, "lstat", plot = FALSE)
   plot(g1, gg = TRUE) + plot(g2, gg = TRUE)
})) -> void
```

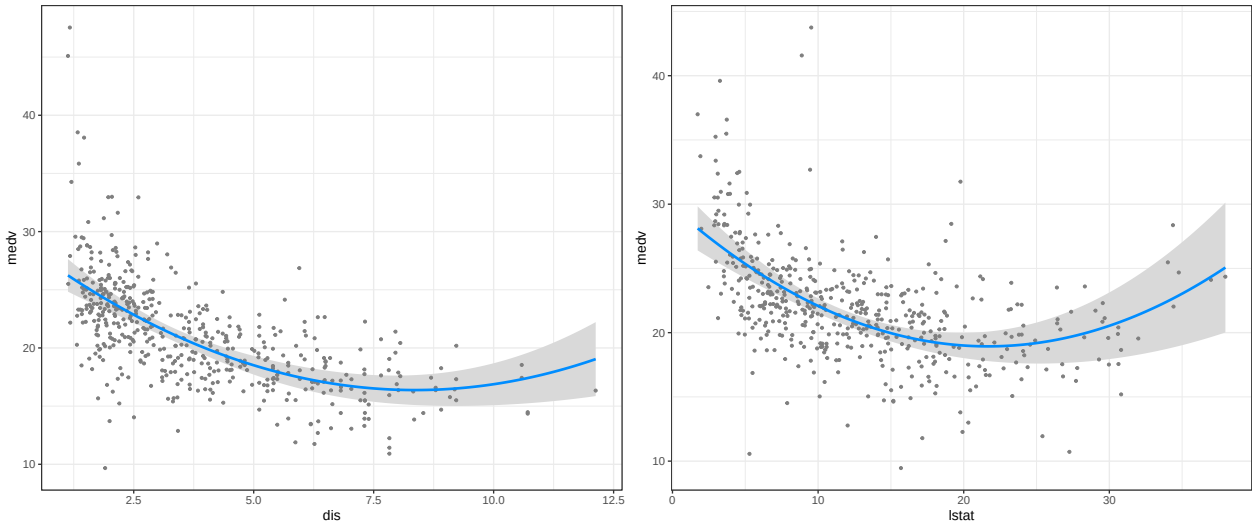
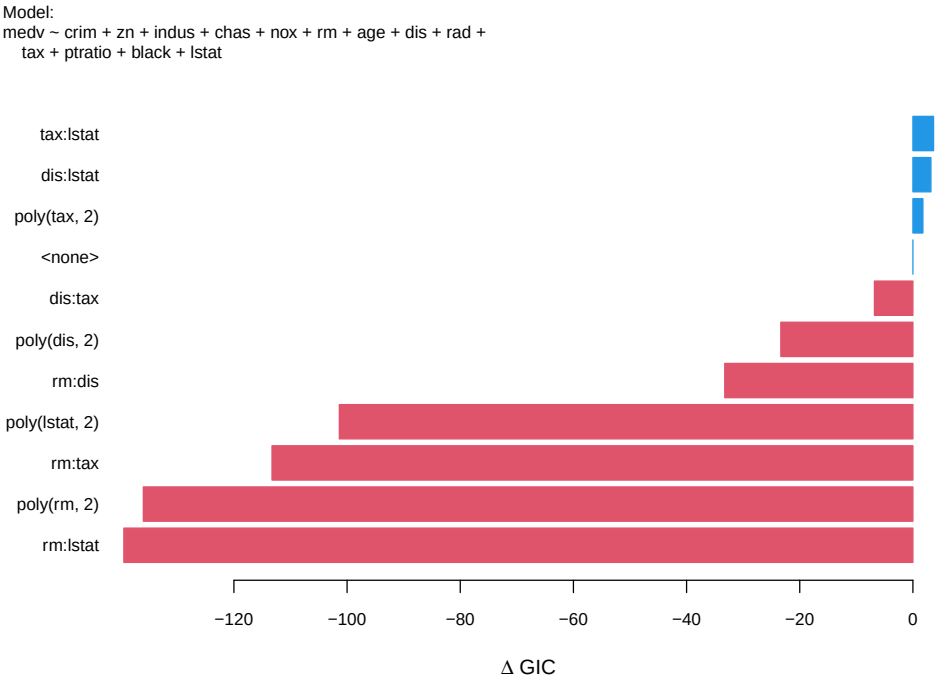


Figure 3: Two component visualisations for the Boston house price model

The case for curvature appears to be fairly weak, in each case with departure from a straight line dependence depending on a relatively few observations with high values for the predictor. (Notice how hard you have to work to prevent `visreg` from generating unwanted output.)

As an example of `add_term`, consider going from what we have called the `base_model` to the `big_model`, or at least what might be the initial step:

```
add_term(base_model, scope = formula(big_model), k = "gic") %>%
   plot() %>% kable(booktabs = TRUE, digits = 3)
```



	Df	Sum of Sq	RSS	delta_GIC	F Value	Pr(F)
tax:lstat	1	10.105	11068.680	3.652	0.448	0.503
dis:lstat	1	20.414	11058.371	3.180	0.906	0.342
poly(tax, 2)	1	51.266	11027.518	1.766	2.283	0.131
			11078.785	0.000		
dis:tax	1	236.466	10842.318	-6.804	10.708	0.001
poly(dis, 2)	1	585.089	10493.696	-23.341	27.376	0.000
rm:dis	1	788.628	10290.157	-33.252	37.630	0.000
poly(lstat, 2)	1	2084.780	8994.005	-101.374	113.812	0.000
rm:tax	1	2293.787	8784.998	-113.272	128.201	0.000
poly(rm, 2)	1	2679.861	8398.923	-136.013	156.664	0.000
rm:lstat	1	2736.760	8342.024	-139.452	161.082	0.000

So in this case, your best first step would be to *add* the term which most decreases the criterion, that is, the one nearest the bottom of the table (or display).

Non-gaussian models

For a non-gaussian model consider the Quine data (`?quine`) example discussed in the *MASS* book. We begin by fitting a full negative binomial model and refine it using a stepwise algorithm.

```
quine_full <- glm.nb(Days ~ Age*Eth*Sex*Lrn, data = quine)
drop_term(quine_full) %>% kable(booktabs = TRUE, digits = 4)
```

	Df	delta_AIC	LRT	Pr(Chi)
		0.0000		
Age:Eth:Sex:Lrn	2	-2.5962	1.4038	0.4956

```
quine_gic <- step_GIC(quine_full)
drop_term(quine_gic) %>% kable(booktabs = TRUE, digits = 4)
```

	Df	delta_GIC	LRT	Pr(Chi)
Eth:Sex:Lrn	1	8.9298	12.4216	4e-04
Age:Sex	3	8.1439	18.6193	3e-04
		0.0000		

So GIC refinement has led to the same model as in the *MASS* book, which in more understandable form would be written `Days ~ Sex/(Age + Eth*Lrn)`. Note also that the default test is in this case the likelihood ratio test.

For a different example, consider an alternative way to model the MPG data, rather than transforming to an inverse scale, using a generalized linear model with an inverse link and a gamma response.

```
mpg0 <- glm(MPG.city ~ Weight + Cylinders + EngineSize + Origin,
            family = Gamma(link = "inverse"), data = Cars93)
drop_term(mpg0) %>% kable(booktabs = TRUE, digits = 3)
```

	Df	Deviance	delta_AIC	F value	Pr(F)
Weight	1	1.032	34.400	38.499	0.000
Cylinders	5	0.867	7.919	3.790	0.004
		0.708	0.000		
Origin	1	0.721	-0.566	1.516	0.222
EngineSize	1	0.712	-1.560	0.465	0.497

```
mpg_gic <- step_down(mpg0, k = "gic")       ## simple backward elimination, mainly used for GLMMs
drop_term(mpg_gic) %>% kable(booktabs = TRUE, digits = 3)
```

	Df	Deviance	delta_GIC	F value	Pr(F)
Weight	1	1.490	79.688	89.042	0.000
Cylinders	5	0.901	2.097	3.956	0.003
		0.732	0.000		

We can see something of how well the final model is performing by looking at a slightly larger model fitted on the fly in `ggplot`:

```
ggplot(Cars93) + aes(x = Weight, y = MPG.city, colour = Cylinders) + geom_point() +
   geom_smooth(method = "glm", method.args = list(family = Gamma), formula = y ~ x) +
   ylab("Miles per gallon (city driving)") + scale_colour_brewer(palette = "Dark2")
```

The function `step_down` is a simple implementation of backward elimination with the sole virtue that it works for (Generalised) Linear Mixed Models, or at least for the fixed effect component of them, whereas other stepwise methods do not (yet). As fitting GLMMs can be very slow, going through a full stepwise process could be very time consuming in any case.

Scaling functions

When a function such as `base::scale`, `stats:poly` or `splines:ns` (also exported from `MASSExtra`) is used in modelling it is important that the fitted model object has enough information so that when it is used in prediction for new data, the same transformation can be put in place with the new predictor variable values. Setting up functions in such a way to enable this is a slightly tricky exercise. It involves writing a method function for the S3 generic function `stats::makepredictcall`. To illustrate this we have supplied four simple functions that employ the technique.

- `zs` ("z-score") is essentially the same as `base::scale` with the default argument settings,

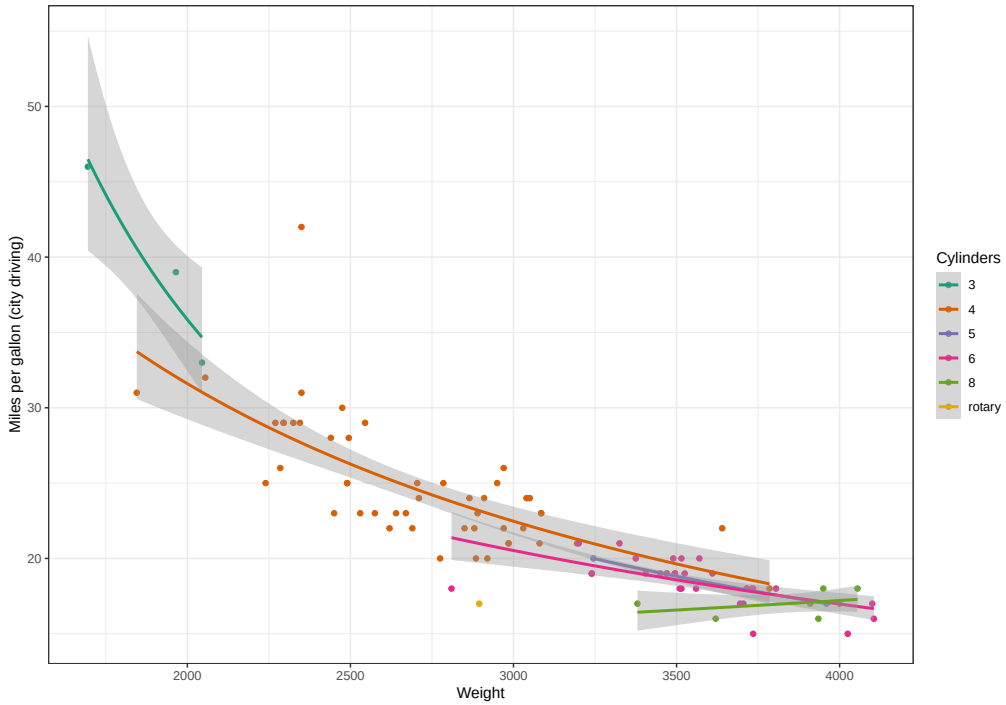


Figure 4: MPG model using a Gamma family with inverse link

- zu allows re-scaling to a fixed range of [0, 1], often used in neural network models,
- zq allows a quantile scaling where the location is the lower quartile and the scale is the inter-quartile range. In other words, the scaling is to [0,1] *within the box* of a boxplot. *(Go figure.)*
- zr allows a "robust" scaling where the location is the median and the scale uses `stats::mad`

The only real interest in these very minor convenience functions lies in how they are programmed. The following chain from the package code sets out the steps.

```
dput(MASSExtra:::makepredictcall.normalise) ## exported only as an S3 method
function (var, call)
{
    parms <- attr(var, "parms")
    call <- call[1:2]
    call[[1]] <- as.name(".normalise")
    call[names(parms)] <- parms
    call
}
dput(.normalise)                            ## an exported helper, but with a hidden name
function (x, location, scale)
{
    z <- structure(cbind(z = (x - location)/scale), parms = c(location = unname(location),
        scale = unname(scale)))
    class(z) <- c("normalise", "matrix")
    z
}
dput(zs)                                    ## the scale() equivalent
function (x)
{
    .normalise(x, mean(x), sd(x))
}
dput(zq)                                    ## the 'boxplot scaling' (based on quantiles)
```

```
function (x)
{
    .normalise(x, quantile(x, 0.25), IQR(x))
}
```

Postamble

In this final section we mainly give a list of functions provided by the package, and their origins.

We begin by giving a list of functions in the MASS package which are *not* re-exported from the MASSExtra package. If you need any of these you will need either to attach the MASS package itself, or use the qualified form MASS::<name>.

```
 [1] Shepard           area              as.fractions      bandwidth.nrd
 [5] bcv               con2tr            contr.sdif        corresp
 [9] cov.mcd           cov.mve           cov.rob           cov.trob
[13] denumerate        dose.p            enlist            eqscplot
[17] fbeta             fitdistr          frequency.polygon gamma.dispersion
[21] gamma.shape       hist.FD           hist.scott        huber
[25] hubers            is.fractions      ldahist           lm.ridge
[29] lmsreg            lmwork            loglm             loglm1
[33] lqs.formula       ltsreg            mca               mvrnorm
[37] nclass.freq       neg.bin           negexp.SSival     parcoord
[41] psi.bisquare      psi.hampel        psi.huber         rational
[45] renumerate        rms.curv          select            truehist
[49] write.matrix
```

The following objects *are* re-exported from the MASSExtra package, and hence may be used directly, if needed.

```
 [1] Null              addterm           boxcox            dropterm
 [5] fractions         ginv              glm.convert       glm.nb
 [9] glmmPQL           isoMDS            kde2d             lda
[13] lm.gls            logtrans          lqs               negative.binomial
[17] polr              qda               rlm               rnegbin
[21] sammon            stdres            stepAIC           studres
[25] theta.md          theta.ml          theta.mm          ucv
[29] width.SJ
```

The following functions are *new* to the MASSExtra package, some of which are obviously refinements of their MASS workhorse counterparts.

```
 [1] .normalise        GIC               add_term          bc
 [5] bc_inv            box_cox           default_test      drop_term
 [9] eigen2            givens_orth       gs_orth           gs_orth_modified
[13] lambda            mean_c            step_AIC          step_BIC
[17] step_GIC          step_down         var_c             vcovx
[21] which_tri         zq                zr                zs
[25] zu
```

Finally the following objects are re-exported from splines:

```
[1] bs ns
```

Only four of the MASS data sets are included in MASSExtra, namely Cars93, Boston, quine and whiteside. Other data sets from MASS itself will need to be accessed directly, e.g. MASS::immer.