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 with 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</pre>
```

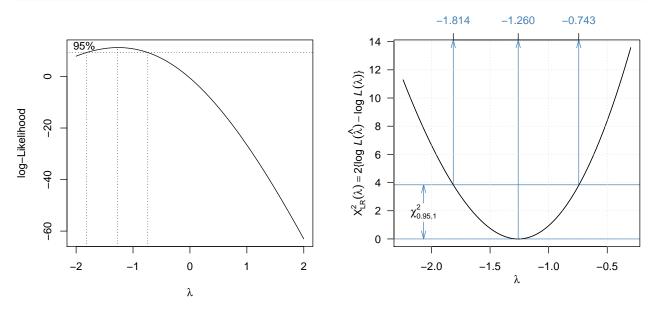


Figure 1: Box-cox, old and new displays

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</pre>
```

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

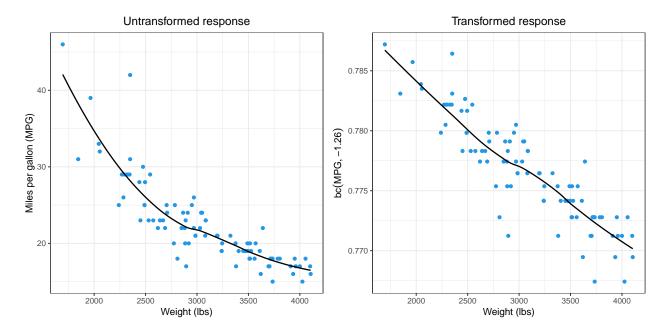


Figure 2: The Box-Cox transformation effect

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

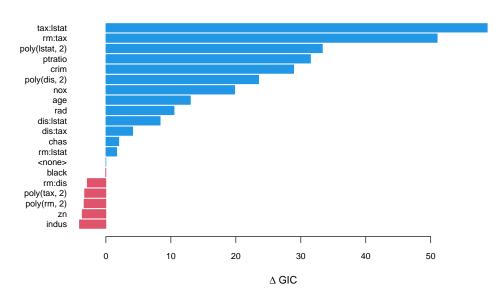
commonly are.

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.

Model:

$$\label{eq:medv} \begin{split} \text{medv} &\sim \text{crim} + \text{zn} + \text{indus} + \text{chas} + \text{nox} + \text{rm} + \text{age} + \text{dis} + \text{rad} + \\ \text{tax} &+ \text{ptratio} + \text{black} + \text{lstat} + (\text{rm} + \text{tax} + \text{lstat} + \text{dis})^2 + \\ \text{poly(dis, 2)} &+ \text{poly(rm, 2)} + \text{poly(tax, 2)} + \text{poly(lstat, 2)} \end{split}$$



	\mathbf{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*.

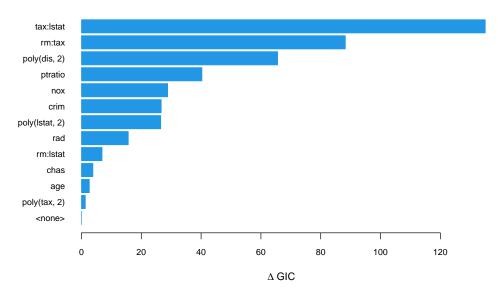
With all stepwise methods it is critically important to notice that the whole picture can change once any change is made to the current model. This terms which appear "promising" at this stage may not seem so once any variable is removed from the model or some other variable brought into it. This is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

Model: medv ~ crim + chas + nox + rm + age + rad + tax + ptratio + lstat + poly(lstat, 2) + poly(dis, 2) + poly(tax, 2) + rm:lstat + tax:lstat + rm:tax



	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)
1	233.292	6087.899	15.658	19.486	0.000
1	128.612	5983.219	6.882	10.742	0.001
1	92.617	5947.224	3.829	7.736	0.006
1	78.635	5933.242	2.638	6.568	0.011
1	62.892	5917.499	1.293	5.253	0.022
		5854.607	0.000		
	1 1	1 233.292 1 128.612 1 92.617 1 78.635	1 233.292 6087.899 1 128.612 5983.219 1 92.617 5947.224 1 78.635 5933.242 1 62.892 5917.499	1 233.292 6087.899 15.658 1 128.612 5983.219 6.882 1 92.617 5947.224 3.829 1 78.635 5933.242 2.638 1 62.892 5917.499 1.293	1 233.292 6087.899 15.658 19.486 1 128.612 5983.219 6.882 10.742 1 92.617 5947.224 3.829 7.736 1 78.635 5933.242 2.638 6.568 1 62.892 5917.499 1.293 5.253

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
```

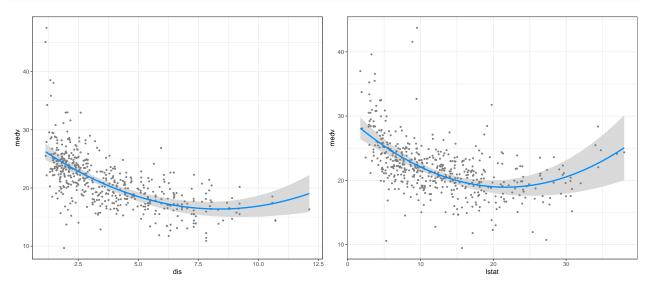


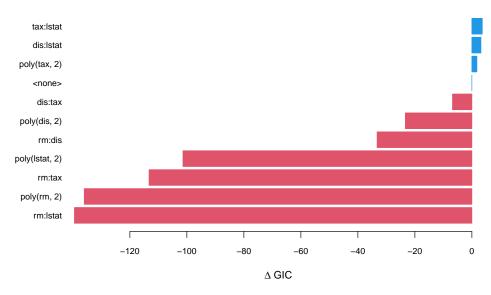
Figure 3: Two component visualisations for the Boston house price model

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)
```

Model: medv ~ crim + zn + indus + chas + nox + rm + age + dis + rad + tax + ptratio + black + lstat



	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.

	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	$8.1439 \\ 0.0000$	18.6193	3e-04

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.

	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 Cylinders	1 5	1.490 0.901 0.732	79.688 2.097 0.000	89.042 3.956	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,

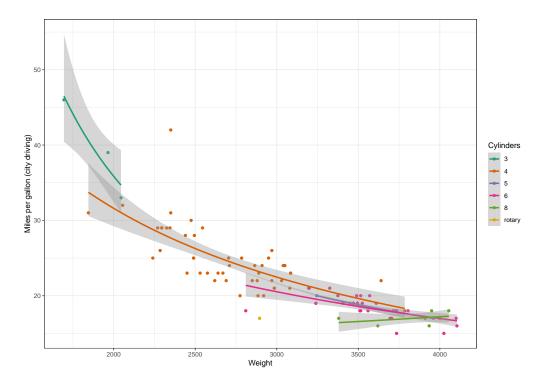


Figure 4: MPG model using a Gamma family with inverse link

- 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")</pre>
    call <- call[1:2]</pre>
    call[[1]] <- as.name(".normalise")</pre>
    call[names(parms)] <- parms</pre>
    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")</pre>
}
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))
}
```

Postabmle

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>.

character(0)

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

[1]	Null	Shepard	addterm	area
[5]	as.fractions	bandwidth.nrd	bcv	boxcox
[9]	con2tr	contr.sdif	corresp	cov.mcd
[13]	cov.mve	cov.rob	cov.trob	denumerate
[17]	dose.p	dropterm	enlist	eqscplot
[21]	fbeta	fitdistr	fractions	frequency.polygon
[25]	gamma.dispersion	gamma.shape	ginv	glm.convert
[29]	glm.nb	glmmPQL	hist.FD	hist.scott
[33]	huber	hubers	is.fractions	isoMDS
[37]	kde2d	lda	ldahist	lm.gls
[41]	<pre>lm.ridge</pre>	lmsreg	lmwork	loglm
[45]	loglm1	logtrans	lqs	lqs.formula
[49]	ltsreg	mca	mvrnorm	nclass.freq
[53]	neg.bin	negative.binomial	negexp.SSival	parcoord
[57]	polr	psi.bisquare	psi.hampel	psi.huber
[61]	qda	rational	renumerate	rlm
[65]	rms.curv	rnegbin	sammon	select
[69]	stdres	stepAIC	studres	theta.md
[73]	theta.ml	theta.mm	truehist	ucv
[77]	width.SJ	write.matrix		

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

- [1] .EmptyPrimitiveSkeletons
- [2] .MFclass
- [3] .OldClassesList
- [4] .S4methods
- [5] .ShortPrimitiveSkeletons
- [6] .TraceWithMethods
- [7] .__C__(
- [8] .__C_.NULL
- [9] .__C__.Other
- [10] .__C__.environment
- [11] .__C_.externalptr
- [12] .__C_.name
- [13] .__C__<-
- [14] .__C__ANY
- [15] $.__C_ClassUnionRepresentation$
- [16] .__C__Date

- [17] .__C__EmptyMethodsList
- [18] .__C_LinearMethodsList
- [19] .__C__MethodDefinition
- [20] .__C__MethodDefinitionWithTrace
- [21] .__C__MethodSelectionReport
- [22] .__C__MethodWithNext
- [23] .__C__MethodWithNextWithTrace
- [24] .__C_MethodsList
- [25] .__C__NULL
- [26] .__C__ObjectsWithPackage
- [27] $.__C__OptionalFunction$
- [28] .__C__POSIXct
- [29] .__C__POSIX1t
- [30] .__C__POSIXt
- [31] .__C__PossibleMethod
- [32] .__C__S3
- [33] .__C__S4
- [34] .__C__SClassExtension
- [35] .__C__SealedMethodDefinition
- [36] .__C__SuperClassMethod
- [37] .__C__VIRTUAL
- [38] .__C_activeBindingFunction
- [39] .__C_anova
- [40] .__C__anova.glm
- [41] .__C_anova.glm.null
- [42] .__C_aov
- [43] .__C_array
- [44] .__C_builtin
- [45] .__C__call
- [46] .__C__character
- [47] .__C__classGeneratorFunction
- [48] .__C_className
- [49] .__C__classPrototypeDef
- [50] .__C__classRepresentation
- [51] .__C__complex
- [52] .__C_conditionalExtension
- [53] . C data.frame
- [54] .__C__data.frameRowLabels
- [55] .__C__defaultBindingFunction
- [56] .__C__density
- [57] .__C__derivedDefaultMethod
- [58] .__C__derivedDefaultMethodWithTrace
- [59] .__C__double
- [60] .__C_dump.frames
- [61] .__C__envRefClass
- [62] $.__C__$ environment
- [63] .__C_expression
- [64] .__C__externalRefMethod
- [65] .__C__externalptr
- [66] .__C__factor
- [67] .__C__for
- [68] .__C__formula
- [69] .__C__function
- [70] $._C_{functionWithTrace}$
- [71] .__C__genericFunction
- [72] .__C__genericFunctionWithTrace

- [73] .__C__glm
- [74] .__C_glm.null
- [75] .__C__groupGenericFunction
- [76] .__C__groupGenericFunctionWithTrace
- [77] .__C_hsearch
- [78] .__C__if
- [79] .__C__integer
- [80] .__C__integrate
- [81] .__C__internalDispatchMethod
- [82] .__C_language
- [83] .__C_libraryIQR
- [84] .__C__list
- [85] .__C_listOfMethods
- [86] .__C_lm
- [87] .__C__localRefClass
- [88] .__C__logLik
- [89] .__C_logical
- [90] .__C__maov
- [91] .__C__matrix
- [92] .__C__missing
- [93] .__C__mlm
- [94] .__C__mtable
- [95] .__C__mts
- [96] .__C__name
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- [937] yinch
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- [939] zr
- [940] zs
- [941] zu

Finally the following objects are re-exported from splines:

- [1] as.polySpline asVector backSpline bs interpSpline [6] ns periodicSpline polySpline spline.des splineDesign [11] splineKnots splineOrder xyVector
- 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.