The family Argument for glmnet

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Introduction

The glmnet package fits a generalized linear model (GLM) via penalized maximum likelihood. Concretely, it solves the problem

\[
\min_{\beta_0, \beta} \frac{1}{N} \sum_{i=1}^{N} w_i l_i(y_i, \beta_0 + \beta^T x_i) + \lambda \left[ \frac{1 - \alpha}{2} \| \beta \|_2^2 + \alpha \| \beta \|_1 \right]
\]

over a grid of values of \( \lambda \) covering the entire range. In the equation above, \( l_i(y_i, \eta_i) \) is the negative log-likelihood contribution for observation \( i \). \( \alpha \in [0, 1] \) is a tuning parameter which bridges the gap between the lasso (\( \alpha = 1 \), the default) and ridge regression (\( \alpha = 0 \)), while \( \lambda \) controls the overall strength of the penalty.

glmnet solves the minimization problem above very efficiently for a limited number of built-in (hardwired) families. To fit these model families, one should specify the family argument to glmnet as a character string. The families that can be fit efficiently this way are the penalized Gaussian ("gaussian"), binomial ("binomial"), and Poisson ("poisson") GLMs, along with a few other special cases: the Cox model ("cox"), multinomial regression ("multinomial"), and multi-response Gaussian ("mgaussian"). Details for how to fit these models can be found in the vignette “An Introduction to glmnet”.

Apart from these built-in families, glmnet also allows the user to fit a penalized regression model for any GLM by allowing the family argument to be any legitimate GLM family object, as used by the stats:glm function.

Using class “family” objects for the family argument

The family argument to glmnet can be the result of a call to a family function. (To learn more about family functions in R, run ?family in the R console.) All the functionality of glmnet applies to these new families, and hence their addition expands the scope of glmnet considerably. In particular,

- All the methods, such as plot and predict, work as before;
- Large and sparse \( x \) matrices can be taken as input;
• The user can put upper and lower bound constraints on parameters;
• `cv.glmnet` can be used for selecting the tuning parameters;
• `relax = TRUE` can be specified for fitting unpenalized models to the active sets;
• `offsets` can be provided;
• Penalty strengths, standardization, and other options to `glmnet` work as before.

When the `family` argument is a class "family" object, `glmnet` fits the model for each value of `lambda` with a proximal Newton algorithm, also known as iteratively reweighted least squares (IRLS). The outer loop of the IRLS algorithm is coded in R, while the inner loop solves the weighted least squares problem with the elastic net penalty, and is implemented in Fortran. The R code exploits warm starts as it iterates down the path, and so is reasonably efficient.

More on GLM families

A GLM is linear model for a response variable whose conditional distribution belongs to a one-dimensional exponential family. Apart from Gaussian, Poisson and binomial families, there are other interesting members of this family, e.g. Gamma, inverse Gaussian, negative binomial, to name a few. A GLM consists of 3 parts:

1. A linear predictor: \( \eta_i = \sum_{j=1}^{p} \beta_j x_{ij} \),
2. A link function: \( \eta_i = g(\mu_i) \), and
3. A random component: \( y_i \sim f(\cdot | \mu_i) \).

The user gets to specify the link function \( g \) and the family of response distributions \( f(\cdot | \mu) \), and fitting a GLM amounts to estimating the parameter \( \beta \) by maximum likelihood.

In R, these 3 parts of the GLM are encapsulated in an object of class `family` (run `?family` in the R console for more details). A `family` object is a list of GLM components which allows functions such as `stats:glm` to fit GLMs in R. As an example, the code below shows the constituent parts for the binomial GLM, which is what is used to fit linear logistic regression:

```r
fam <- binomial()
class(fam)
#> [1] "family"
names(fam)
#> [1] "family" "link" "linkfun" "linkinv" "variance"
#> [6] "dev.resids" "aic" "mu.eta" "initialize" "validmu"
#> [11] "valideta" "simulate"
```

This is a list of functions and expressions that get used in the iteratively reweighted least squares (IRLS) algorithm for fitting the GLM.

`glmnet` can fit penalized GLMs for any family as long as the family can be expressed as a `family` object. In fact, users can make their own families, or customize existing families, just as they can for regular GLMs.

Generally this option should be used only if the desired family is not included in the built-in list. The reason is that the entire path algorithm for the built-in families is implemented in Fortran, and so will be faster.

Fitting Gaussian, binomial and Poisson GLMs

First, we demonstrate how we can use this new version of `glmnet` to fit ordinary least squares with the elastic net penalty. We set up some fake data:

```r
set.seed(1)
x <- matrix(rnorm(500), ncol = 5)
y <- rowSums(x[, 1:2]) + rnorm(100)
```
The function calls below demonstrate how we would fit the model with the old and new family parameter options. To fit a linear regression by least squares, we want to use the Gaussian family. There is a hard-wired option for this, specified via family="gaussian" (which is also the default for glmnet). Now we can also use family = gaussian() to fit the same model.

```r
library(glmnet)
oldfit <- glmnet(x, y, family = "gaussian")
newfit <- glmnet(x, y, family = gaussian())
```

glmnet distinguishes these two cases because the first is a character string, while the second is a GLM family object. Of course if we really wanted to fit this model, we would use the hard-wired version, because it is faster. Here we want to show that they are equivalent, up to machine precision.

There are slight differences in the algorithms used to compute the solutions, so some of the equality tests run using testthat::expect_equal might fail. However, these same tests can be made to pass by decreasing the thresh option in both function calls:

```r
thresh <- 1e-18
oldfit <- glmnet(x, y, family="gaussian", thresh = thresh)
newfit <- glmnet(x, y, family = gaussian(), thresh = thresh)
```

```r
# tests for equality
library(testthat)
for (key in c("a0", "beta", "df", "dim", "lambda", "dev.ratio", "nulldev", "offset", "nobs")) {
  expect_equal(oldfit[[key]], newfit[[key]])
}
```

Next, we demonstrate the function calls for the binomial and Poisson GLM families.

```r
biny <- ifelse(y > 0, 1, 0)  # binary data
cnty <- ceiling(exp(y))      # count data

# fitting binomial GLMs the old and new way
oldfit <- glmnet(x, biny, family = "binomial")
newfit <- glmnet(x, biny, family = binomial())

# fitting Poisson GLMs the old and new way
oldfit <- glmnet(x, cnty, family = "poisson")
newfit <- glmnet(x, cnty, family = poisson())
```

Timing comparisons

In the examples above, the new version is simply replicating existing functionality in glmnet. For these GLMs, we recommend specifying the GLM family as a character string for computational efficiency. The figures below illustrate that existing code for these GLM families is more efficient than the new code, especially for the Gaussian case.

(In the figures, n and p denote the number of observations and features respectively. Each point is the mean of 5 simulation runs. Note that both the x and y axes are on a log scale.)

Fitting other GLMs

The real power of using class "family" objects for the family argument is in fitting GLMs other than the three in the previous section. For example, performing probit regression with the elastic net penalty is as
Figure 1: Timing comparisons for Gaussian family

Figure 2: Timing comparisons for binomial family
simple as the code below:

```r
newfit <- glmnet(x, biny, family = binomial(link = "probit"))
```

For the *complementary log-log* link we would specify `family = binomial(link = "cloglog")`.

We can fit nonlinear least-squares models by using a different link with the Gaussian family; for example `family = gaussian(link = "log")`.

For count data, we can fit a quasi-Poisson model that allows for overdispersion:

```r
newfit <- glmnet(x, cnty, family = quasipoisson())
```

The negative binomial is often used to model over-dispersed count data (instead of Poisson regression), and is also easy:

```r
library(MASS)
newfit <- glmnet(x, cnty, family = negative.binomial(theta = 5))
```

There are many other families, including `quasi` where users can customize their own families. There are additional specialized families such as `statmod:tweedie` for overdispersed count data.

### Class "glmnetfit" objects

If `glmnet` is called with a class "family" object as its argument, it returns an object with class

```r
class(newfit)

#> [1] "glmnetfit" "glmnet"
```

This is similar to the hard-wired classes; for example a `family = "gaussian"` fit has class

```r
fit <- glmnet(x, y, family = "gaussian")
class(fit)

#> [1] "elnet" "glmnet"
```

Importantly, both these inherit from class "glmnet", and so all the S3 methods such as `plot`, `predict`, `coef`, and `print` will work out the box.

### Step size halving within iteratively reweighted least squares (IRLS)

For the built-in families, `glmnet` solves the optimization problem for non-Gaussian families via iteratively reweighted least squares (IRLS). In each iteration a unit Newton step is taken, and the algorithm terminates when the unit Newton step fails to decrease the deviance sufficiently. Because the algorithm is forced to take a unit step, this can result in non-convergence of the algorithm in some cases.

Here is an example of the non-convergence for Poisson data. The `stats:glm` function converges and gives us coefficients that are reasonably close to the truth:

```r
set.seed(2020)
n <- 100
p <- 4
x <- matrix(runif(n * p, 5, 10), n)
y <- rpois(n, exp(rowMeans(x)))

# glm fit
glmfit <- glm(y ~ x - 1, family = poisson)
coef(glmfit)
```
Fitting `glmnet` with `lambda = 0` is equivalent to fitting an unregularized GLM. If we use `glmnet` with `family = "poisson"`, we encounter an issue with non-convergence:

```r
oldfit <- glmnet(x, y, family = "poisson", standardize = FALSE,
                  intercept = FALSE, lambda = 0)
```

This divergence happens because the unit Newton step was too large. However, if a `family` object is passed to the `family` argument of `glmnet`, the IRLS algorithm will perform step size halving. After computing the Newton step, the algorithm checks if the new solution has infinite (or astronomically large) objective function value or if it results in invalid $\eta$ or $\mu$. If so, the algorithm halves the step size repeatedly until these invalid conditions no longer hold.

The code below shows that this step size halving avoids the divergence we were experiencing in our running example:

```r
glmnet.control(mxitnr = 50)  # increase maximum no. of IRLS iterations allowed
newfit <- glmnet(x, y, family = poisson(), standardize = FALSE,
                  intercept = FALSE, lambda = 0)
```

In the process, `glmnet` warns the user that an infinite objective function value was encountered and that step size halving was done to address the issue. The coefficients are close to those obtained by `stats:glm`, and can be made to be numerically indistinguishable by tightening the convergence criteria in both function calls.

```r
thresh <- 1e-15
glmfit <- glm(y ~ x-1, family = poisson,
              control = list(epsilon = thresh, maxit = 100))
newfit <- glmnet(x, y, family = poisson(), standardize = FALSE, intercept = FALSE,
                 lambda = 0, thresh = thresh)
```

In the process, `glmnet` warns the user that an infinite objective function value was encountered and that step size halving was done to address the issue. The coefficients are close to those obtained by `stats:glm`, and can be made to be numerically indistinguishable by tightening the convergence criteria in both function calls.
# coef(glmfit) doesn't have intercept but coef(newfit does)

```r
expect_equal(as.numeric(coef(glmfit)),
              as.numeric(coef(newfit))[2:5])
```