Using the package `glmBfp`:
a binary regression example.

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3rd August 2017
This short vignette shall introduce into the usage of the package glmBfp. For more information on the methodology, see Sabanés Bové and Held (2011). There you can also find the references for the other tools mentioned here.

If you have any questions or critique concerning the package, write an email to me: daniel.sabanesbove@ifspm.uzh.ch. Many thanks in advance!

0.1 Pima Indians diabetes data

We will have a look at the Pima Indians diabetes data, which is available in the package MASS:

```r
> library(MASS)
> pima <- rbind(Pima.tr, Pima.te)
> pima$hasDiabetes <- as.numeric(pima$type == "Yes")
> pima.nObs <- nrow(pima)
```

**Setup** For \( n = 532 \) women of Pima Indian heritage, seven possible predictors for the presence of diabetes are recorded. We would like to investigate with a binary regression, which of them are relevant, and what form the statistical association has – is it a linear effect, or rather a nonlinear effect? Here we will model possible nonlinear effects with the fractional polynomials.

First, we need to decide on the prior distributions to use. We are going to use the generalised hyper-\( g \) priors for GLMs (Sabanés Bové and Held, 2011). They are automatic and are supposed to yield reasonable results. We only need to specify which hyper-prior to put on the factor \( g \). One possible choice is the Zellner-Siow hyper-prior which says \( g \sim IG(1/2, n/2) \):

```r
> library(glmBfp)
> ## define the prior distributions for g which we are going to use:
> prior <- InvGammaGPrior(a=1/2,
+   b=pima.nObs/2)
> ## (the warning can be ignored)
```

This corresponds to the F1 prior in Sabanés Bové and Held (2011). Another possible choice is the hyper-\( g/n \) prior. For this there is no special constructor function, instead you can directly specify the log prior density, as follows:

```r
> ## You may also use the hyper-g/n prior:
> prior.f2 <- CustomGPrior(logDens=function(g)
+   - log(pima.nObs) - 2 * log(1 + g / pima.nObs))
```

**Stochastic model search** Next, we will do a stochastic search on the (very large) model space to find “good” models. Here we have to decide on the model prior, and in this example we use the sparse type which was also used in the paper. We use a chainlength
of 100, which is very small but enough for illustration purposes (usually one should use at least 10,000 as a rule of thumb), and save all models (in general nModels is the number of models which are saved from all visited models). Finally, we decide that we do not want to use OpenMP acceleration (this would parallelise loops over all observations on all cores of your processor) and that we want to do higher order correction for the Laplace approximations. In order to be able to reproduce the analysis, it is advisable to set a seed for the random number generator before starting the stochastic search.

```r
> set.seed(102)
> time.pima <-
+   system.time(models.pima <-
+     glmBayesMfp(type ~
+                     bfp(npreg) +
+                     bfp(glu) +
+                     bfp(bp) +
+                     bfp(skin) +
+                     bfp(bmi) +
+                     bfp(ped) +
+                     bfp(age),
+                     data=pima,
+                     family=binomial("logit"),
+                     priorSpecs=
+                     list(gPrior=prior,
+                         modelPrior="sparse"),
+                     nModels=1e3L,
+                     chainlength=1e1L,
+                     method="sampling",
+                     useOpenMP=FALSE,
+                     higherOrderCorrection=TRUE))

Starting sampler...
0%______________________________________________________________100%
----------
Number of non-identifiable model proposals: 0
Number of total cached models: 9
Number of returned models: 9

> time.pima

        user  system elapsed
       0.372   0.004   0.427

> attr(models.pima, "numVisited")

[1] 9
```
We see that the search took 0 seconds, and 9 models were found. Now, if we want to have a table of the found models, with their posterior probability, the log marginal likelihood, the log prior probability, and the powers for every covariate and the number of times that the sampler encountered that model:

```r
> table.pima <- as.data.frame(models.pima)
> table.pima

         posterior logMargLik logPrior age bmi bp glu npreg ped skin
  1 5.752526e-01 -265.8779 -11.849169  1   -0.5
  2 4.036782e-01 -266.2321 -11.849169  2   -0.5
  3 7.971175e-03 -270.1569 -11.849169  2   3
  4 6.638447e-03 -268.2604 -13.928611  0   2   -0.5
  5 6.134410e-03 -272.4983 -9.769728   2
  6 3.250886e-04 -273.3564 -11.849169  3   2
  7 2.089908e-20 -310.6396 -11.849169  2
  8 2.131992e-23 -317.5274 -11.849169  2   3
  9 2.726801e-31 -339.8609 -7.690286
```

Note that while `frequency` refers to the frequency of the models in the sampling chain, thus providing a Monte Carlo estimate of the posterior model probabilities, `posterior` refers to the renormalised posterior model probabilities. The latter has the advantage that ratios of posterior probabilities between any two models are exact, while the former is unbiased (but obviously has larger variance).

**Inclusion probabilities** The estimated marginal inclusion probabilities for all covariates are also saved:

```r
> round(attr(models.pima, "inclusionProbs"),2)

       age bmi bp glu npreg ped skin
0.00 0.00 0.01 1.00 0.00 0.00 0.99
```

**Sampling model parameters** If we now want to look at the estimated covariate effects in the estimated MAP model which has the configuration given in the last seven columns of `table.pima`, then we first need to generate parameter samples from that model:

```r
> ## MCMC settings
> mcmcOptions <- McmcOptions(iterations=1e4L,
+                            burnin=1e3L,
+                            step=2L)
> ## get samples from the MAP model
> set.seed(634)
> mapSamples <- sampleGlm(models.pima[1L],
+                          mcmc=mcmcOptions,
+                          useOpenMP=FALSE)
```
Taking the linear approximation method

Finished MCMC simulation with acceptance ratio 0.868

With the function `McmcOptions`, we have defined an S4 object of MCMC settings, comprising the number of iterations, the length of the burn-in, the thinning step (here save every second iteration), and here the acceptance rate was 0.87). Note that you can also get predictive samples for new data points via the `newdata` option of `sampleGlm`. The result `mapSamples` has the following structure:

```r
> str(mapSamples)
```

List of 5

$ tbf : logi FALSE

$ acceptanceRatio: num 0.868

$ logMargLik :List of 5

..$ estimate : Named num -266

..- attr(*, "names")= chr "numeratorTerms"

..$ standardError : num [1, 1] 0.00237

..$ numeratorTerms : num [1:4500] 0.542 0.657 0.664 0.619 0.559 ...

..$ denominatorTerms : num [1:4500] 1 1 0.989 1 1 ...

..$ highDensityPointLogUnPosterior: num -266

$ coefficients : num [1:3, 1:4500] -0.932 4.211 -5.46 -0.827 3.745 ...

..- attr(*, "dimnames")=List of 2

.. ..$ : chr [1:3] "(Intercept)" "glu" "skin"

.. ..$ : NULL

$ samples :Formal class 'GlmBayesMfpSamples' [package "glmBfp"] with 8 slots

.. ...@ fitted : num [1:532, 1:4500] -2.29 2.55 -2.11 1.66 -1.6 ...

.. ...- attr(*, "dimnames")=List of 2

.. ... ...$ : chr [1:532] "1" "2" "3" "4" ...

.. ... ...$ : NULL

.. ...@ predictions : logi[0,0]

.. ...@ fixCoefs :List of 1

.. ... ...$ (Intercept): num [1, 1:4500] -0.932 -0.827 -0.932 -0.936 -1.073 ...

.. ... ...- attr(*, "dimnames")=List of 2

.. ... ... ...$ : chr "(Intercept)"

.. ... ... ...$ : NULL

.. ...@ z : num [1:4500] 5.32 5.44 7.19 5.08 5.57 ...

.. ...@ bfpCurves :List of 2

.. ... ...$ glu : num [1:327, 1:4500] -3.05 -3.02 -3.01 -2.99 -2.96 ...

.. ... ...- attr(*, "scaledGrid")= num [1:327, 1] 0.56 0.567 0.57 0.574 0.581 ...

.. ... ... ...$ : NULL

```
It is a list with the acceptanceRatio of the Metropolis-Hastings proposals, an MCMC estimate for the log marginal likelihood including an associated standard error (logMargLik), the coefficients samples of the model, and an S4 object samples. This S4 object includes the fitted samples on the linear predictor scale (in our case on the log Odds Ratio scale), possibly predictions samples, samples of the intercept (fixed), samples of \( z = \log(g) \), samples of the fractional polynomial curves (bfpCurves), coefficients of uncertain but fixed form covariates (ucCoefs), the shifts and scales applied to the original covariates (shiftScaleMax) and the number of samples (nSamples). You can read more details on the results on the help page by typing ?"GlmBayesMfpSamples-class" in R.

If we wanted to get posterior fitted values on the probability scale, we can use the following code:

```r
> mapFit <- rowMeans(plogis(mapSamples$samples@fitted))
> head(mapFit)

   1       2       3       4       5       6
0.1017081 0.8967206 0.1096366 0.7864968 0.1794264 0.1412198
```

We can also analyse the MCMC output in greater detail by applying the functions in the coda package:

```r
> library(coda)
> coefMcmc <- mcmc(data=t(mapSamples$coefficients),
+ start=mcmcOptions@burnin + 1,
+ thin=mcmcOptions@step)
> str(coefMcmc)

mcmc [1:4500, 1:3] -0.932 -0.827 -0.932 -0.936 -1.073 ...
- attr(*, "dimnames")=List of 2
```
$ : NULL
$. : chr [1:3] "(Intercept)" "glu^1" "skin^-0.5"
attr(*, "mcpar") = num [1:3] 1001 9999 2

> ## standard summary table for the coefficients:
> summary(coefMcmc)

Iterations = 1001:9999
Thinning interval = 2
Number of chains = 1
Sample size per chain = 4500

1. Empirical mean and standard deviation for each variable, plus standard error of the mean:

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>SD</th>
<th>Naive SE</th>
<th>Time-series SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Intercept)</td>
<td>-0.9298</td>
<td>0.1144</td>
<td>0.001705</td>
<td>0.001812</td>
</tr>
<tr>
<td>glu^1</td>
<td>3.8503</td>
<td>0.3963</td>
<td>0.005907</td>
<td>0.006548</td>
</tr>
<tr>
<td>skin^-0.5</td>
<td>-4.0626</td>
<td>1.0093</td>
<td>0.015046</td>
<td>0.017079</td>
</tr>
</tbody>
</table>

2. Quantiles for each variable:

<table>
<thead>
<tr>
<th></th>
<th>2.5%</th>
<th>25%</th>
<th>50%</th>
<th>75%</th>
<th>97.5%</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Intercept)</td>
<td>-1.158</td>
<td>-1.008</td>
<td>-0.929</td>
<td>-0.8514</td>
<td>-0.7113</td>
</tr>
<tr>
<td>skin^-0.5</td>
<td>-6.053</td>
<td>-4.736</td>
<td>-4.057</td>
<td>-3.3781</td>
<td>-2.1071</td>
</tr>
</tbody>
</table>

> autocorr(coefMcmc)

, , (Intercept)

<table>
<thead>
<tr>
<th></th>
<th>(Intercept)</th>
<th>glu^1</th>
<th>skin^-0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lag 0</td>
<td>1.0000000000</td>
<td>-0.198545301</td>
<td>0.22364820</td>
</tr>
<tr>
<td>Lag 2</td>
<td>0.0605853522</td>
<td>-0.021893505</td>
<td>0.02726208</td>
</tr>
<tr>
<td>Lag 10</td>
<td>-0.009556659</td>
<td>0.011005546</td>
<td>0.02048678</td>
</tr>
<tr>
<td>Lag 20</td>
<td>-0.008033578</td>
<td>0.001619819</td>
<td>-0.02348717</td>
</tr>
<tr>
<td>Lag 100</td>
<td>0.0090202422</td>
<td>-0.025143099</td>
<td>-0.01664317</td>
</tr>
</tbody>
</table>

, , glu^1

<table>
<thead>
<tr>
<th></th>
<th>(Intercept)</th>
<th>glu^1</th>
<th>skin^-0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lag 0</td>
<td>-0.198545301</td>
<td>1.000000000</td>
<td>0.033350565</td>
</tr>
<tr>
<td>Lag 2</td>
<td>-0.015649028</td>
<td>0.102578846</td>
<td>-0.011644669</td>
</tr>
<tr>
<td>Lag 10</td>
<td>-0.006802564</td>
<td>-0.007056528</td>
<td>-0.009870305</td>
</tr>
<tr>
<td>Lag 20</td>
<td>0.0254576882</td>
<td>-0.016328556</td>
<td>-0.004131433</td>
</tr>
</tbody>
</table>
Lag 100  0.010054085  0.004816710  0.006559927

, , skin^-0.5

(Intercept)   glu^1   skin^-0.5
Lag 0  0.22364820  0.0333505647  1.0000000000
Lag 2  0.05308624  0.0007788737  0.086390518
Lag 10  0.01053958 -0.0013760574  0.0004120857
Lag 20 -0.02397061  0.0008594713 -0.0206584865
Lag 100 -0.02560623 -0.0044481064 -0.0312199771

> ## etc.
> plot(coefMcmc)
> ## samples of z:
> zMcmc <- mcmc(data=mapSamples$samples@z,
+            start=mcmcOptions@burnin + 1,
+            thin=mcmcOptions@step)
> plot(zMcmc)
> ## etc.
Curve estimates  Now we can use the samples to plot the estimated effects of the MAP model covariates, with the `plotCurveEstimate` function. For example:

```r
> plotCurveEstimate(termName="skin",
+                    samples=mapSamples$samples)
```
Model averaging  Model averaging works in principle similar to sampling from a single model, but multiple model configurations are supplied and their respective log posterior probabilities. For example, if we wanted to average the top three models found, we would do the following:

```r
> set.seed(312)
> bmaSamples <-
+    sampleBma(models.pima[1:3],
+                mcmc=mcmcOptions,
+                useOpenMP=FALSE,
+                nMargLikSamples=1000)
```
Starting sampling ...
Now at model 1 ...
Taking the linear approximation method
0%______________________________________________________________________________________________100%
----------------------------------------------------------------------------------------------------
Finished MCMC simulation with acceptance ratio 0.875

Now at model 2 ...
Taking the linear approximation method
0%______________________________________________________________________________________________100%
-----------------------------------------------------------------------------------------------------
Finished MCMC simulation with acceptance ratio 0.864

Now at model 3 ...
Taking the linear approximation method
0%______________________________________________________________________________________________100%
----------------------------------------------------------------------------------------------------
Finished MCMC simulation with acceptance ratio 0.886

> ## look at the list element names:
> names(bmaSamples)

[1] "modelData" "samples"

> ## now we can see how close the MCMC estimates ("margLikEstimate")
> ## are to the ILA estimates ("logMargLik") of the log marginal likelihood:
> bmaSamples$modelData[, c("logMargLik", "margLikEstimate")]

   logMargLik margLikEstimate
1  -265.8779    -265.8792
2  -266.2321    -266.2333
3  -270.1569    -270.1514

> ## the "samples" list is again of class "GlmBayesMfpSamples":
> class(bmaSamples$samples)

[1] "GlmBayesMfpSamples"
attr("package")
[1] "glmBfp"

Then internally, first the models are sampled, and for each sampled model so many
samples are drawn as determined by the model frequency in the model average sample.
The result is a list with two elements: modelData is similar to the table.pima, and
contains in addition to that the BMA probability and frequency in the sample, the
MCMC acceptance ratios (which should be high). On the second element samples,
which is again of class GlmBayesMfpSamples, the above presented functions can again
be applied (e.g. plotCurveEstimate).
Bibliography