mombf package vignette

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This manual shows how to use the mombf library to compute Moment (MOM) and inverse Moment (iMOM) Bayes factors and to perform Bayesian model selection using non-local priors. See Johnson and Rossell (2010) for an introduction to non-local priors.

The intuitive appeal of MOM and iMOM priors is that they represent prior beliefs under the alternative hypothesis which are fundamentally different from those under the null hypothesis. Mathematically, when the null hypothesis is true they present better convergence rates than BF resulting from most standard procedures. When the alternative hypothesis is true, they present the same convergence rates as most standard procedures. Additionally, in some high dimensional setups the posterior probability assigned to the correct model when using local priors is guaranteed to converge to 0, whereas for non-local priors it converges to 1.

The routines implement a Gibbs sampling scheme to perform Bayesian model selection in linear model setups. Also, we provide routines to compute both exact and approximate BF and marginal densities for linear regression models, and approximate BF for generalized linear models. Approximate BF can also be obtained in other situations where the regression coefficients are asymptotically normally distributed and sufficient. Finally, the library also contains routines to evaluate the prior density and to elicit the prior parameters by specifying the mode *a priori* of the standardized regression coefficients.

In Section 1 we briefly review the definition of the MOM and iMOM priors, and we present routines to evaluate them. In Section 2 we analyze Hald's data with linear models and compute Bayes factors to assess whether some predictors can be dropped from the model. Section 3 shows the analysis of some simulated logistic regression data.

1 Mom and iMom priors

We implement both product and quadratic non-local priors. Quadratic non-local priors are historically the first form of non-local priors that were introduced, and are primarily targeted to the comparison of only two hypotheses. Instead, product priors focus on the more general variable selection problem, where one wants de determine which coefficients are zero within a vector of p coefficients.

Let $\boldsymbol{\theta}' = (\boldsymbol{\theta}_1', \boldsymbol{\theta}_2')$ be the vector of regression coefficients, ϕ be a dispersion parameter (*i.e.* the residual variance in a linear regression setup)

1.1 Product non-local priors

The product non-local prior for $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)$ is simply defined as the product of the univariate non-local priors, i.e. $\pi(\boldsymbol{\theta}) = \prod_{i=1}^p \pi(\theta_i)$, where $\pi(\cdot)$ is a non-local prior density.

The product normal MOM prior of order r is defined as $\pi(\boldsymbol{\theta}|\phi) =$

$$\left(\prod_{i=1}^{p} \frac{\theta_{1i}^{2r}}{(\tau\phi)^{r}(2r-1)!!}\right) N(\boldsymbol{\theta}; \mathbf{0}, \tau\phi I), \tag{1}$$

where I is the $p \times p$ identity matrix and τ is a prior dispersion parameter.

The product normal MOM prior of order r is defined as $\pi(\boldsymbol{\theta}|\phi) =$

$$\left(\prod_{i=1}^{p} \frac{\theta_{1i}^{2r}}{(\tau\phi)^{r}(2r-1)!!}\right) N(\boldsymbol{\theta}; \mathbf{0}, \tau\phi I), \tag{2}$$

where I is the $p \times p$ identity matrix and τ is a prior dispersion parameter and !! denotes the double factorial.

1.2 Quadratic non-local priors

Suppose that the goal is to test $H_0: \boldsymbol{\theta}_1 = \boldsymbol{\theta}_0$ versus $H_1 = \boldsymbol{\theta}_1 \neq \boldsymbol{\theta}_0$. Consider the quadratic distance $Q(\boldsymbol{\theta}_1) = (\boldsymbol{\theta}_1 - \boldsymbol{\theta}_0)^T V_1^{-1}(\boldsymbol{\theta}_1 - \boldsymbol{\theta}_0)/(n\tau\phi)$, where $\boldsymbol{\theta}_1$ is a $p_1 \times 1$ dimensional real vector, V_1 is a $p_1 \times p_1$ positive definite matrix and $\tau > 0$ is a scalar. We set V_1 to be proportional to the asymptotic covariance matrix of the maximum likelihood estimate $\hat{\boldsymbol{\theta}}_1$. For instance, in a linear regression setup with design matrix X we set $V_1 = (X'X)^{-1}$.

We define an improper prior density on θ_2 proportional to 1, and in the situation where ϕ is unknown we specify an independent improper prior on ϕ proportional to $1/\sqrt{\phi}$.

1.2.1 Mom prior

Let $\pi_Z(\boldsymbol{\theta}_1)$ be a prior density for $\boldsymbol{\theta}_1$ for which $E_{\pi_Z}[Q(\boldsymbol{\theta}_1)^k]$ is finite. We define the quadratic MOM prior as

$$\pi_M(\boldsymbol{\theta}_1) = \frac{Q(\boldsymbol{\theta}_1)^k}{E_{\pi_Z}[Q(\boldsymbol{\theta}_1)^k]} \pi_Z(\boldsymbol{\theta}_1). \tag{3}$$

The package currently implements normal MOM priors (where π_Z is the gprior of Zellner and Siow (1980), i.e. $\pi_Z(\boldsymbol{\theta}_1) = N(\boldsymbol{\theta}_0, n\tau\phi V_1)$) and T MOM priors (where π_Z is a multivariate T with $\nu \geq 3$ degrees of freedom). Both for normal and T MOM priors only the case k=1 is currently implemented. For the normal MOM prior the normalization constant is $E_{\pi_Z}(Q(\boldsymbol{\theta})^k) = \prod_{i=0}^{k-1}(p_1+2i)$, i.e. the k^{th} raw moment of a chi-square distribution with p_1 degrees of freedom. For k=1 this simplifies to $E_{\pi_Z}(Q(\boldsymbol{\theta})^k) = 1$. For the T MOM prior and k=1 the normalization constant is $E_{\pi_Z}(Q(\boldsymbol{\theta})^k) = d\frac{\nu}{\nu-2}$.

1.2.2 iMom prior

The quadratic iMom prior on θ_1 is

$$\pi_I(\boldsymbol{\theta}_1) = c_I \ Q(\boldsymbol{\theta}_1)^{-\frac{\nu + p_1}{2}} \exp\left[Q(\boldsymbol{\theta}_1)^{-k}\right],\tag{4}$$

where

$$c_I = \left| \frac{V_1^{-1}}{n\tau\phi} \right|^{1/2} \frac{k}{\Gamma(\nu/2k)} \frac{\Gamma(p_1/2)}{\pi^{p_1/2}}.$$
 (5)

As $Q(\boldsymbol{\theta}_1)$ increases, the influence of the exponential term in (4) disappears and the tails of π_I are of the same order as those of a multivariate T with ν degrees of freedom. Several authors have found appealing to set $\nu=1$ (Bayarri and Garcia-Donato, 2007), which is the default value in our routines. Currently the library only implements the case k=1.

1.3 Evaluating the Mom and iMom priors

The functions dmom and dimom evaluate the Mom and iMom priors, respectively. Set the argument penalty=='product' for the product priors and penalty=='quadratic' for the quadratic priors. Setting the argument baseDensity='normal' in dmom (the default) returns the normal MOM density, baseDensity='t' returns the t MOM density. The functions pmom and pimom evaluate the distribution functions, and qmom and qimom return quantiles. Currently pmom and qmom are only implemented for the normal MOM. Let's set the prior parameter tau = 1 and plot the Mom and iMom priors in

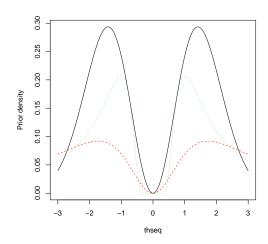


Figure 1: Moment and inverse Moment priors for tau = 1

a univariate setting for $\theta_1 \in (-3,3)$. Notice that in the univariate case the product and quadratic priors are equivalent.

```
> library(mombf)
> tau <- 1
> thseq <- seq(-3,3,length=1000)
> plot(thseq,dmom(thseq,tau=tau),type='l',ylab='Prior density')
> lines(thseq,dmom(thseq,tau=tau,baseDensity='t',penalty='quadratic',nu=3),lty=2,col=2)
> lines(thseq,dimom(thseq,tau=tau),lty=3,col=3)
```

The iMOM prior assigns the lowest density for θ_1 in a neighborhood of 0, whereas the normal MOM prior assigns the largest density. We can also plot the corresponding distribution functions.

```
> library(mombf)
> plot(thseq,pmom(thseq,tau=tau),type='l',ylab='Prior cdf')
> lines(thseq,pimom(thseq,tau=tau),lty=3,col=3)
```

2 Bayes factors for linear regression models

This section focuses on computing Bayes factors to compare two models. The examples use quadratic non-local priors. For examples using product non-local priors see Section 4.

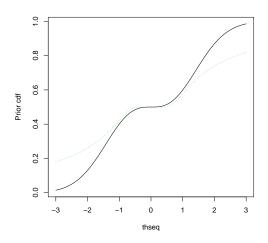


Figure 2: Moment and inverse Moment cdf for tau = 1

2.1 Linear model fit and prior elicitation

The Hald data contains 13 observations, a continuous response variable and 4 predictors. We start by loading the data and fitting a linear regression model.

```
> data(hald)
> dim(hald)
[1] 13 5
> lm1 <- lm(hald[,1] ~ hald[,2] + hald[,3] + hald[,4] + hald[,5])
> summary(lm1)
Call:
lm(formula = hald[, 1] ~ hald[, 2] + hald[, 3] + hald[, 4] +
    hald[, 5])
Residuals:
    Min
             1Q Median
                              3Q
                                     Max
-3.1750 -1.6709
                0.2508 1.3783
                                  3.9254
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)
             62.4054
                         70.0710
                                   0.891
                                           0.3991
                                   2.083
                                           0.0708 .
hald[, 2]
              1.5511
                         0.7448
hald[, 3]
                                           0.5009
              0.5102
                         0.7238
                                   0.705
hald[, 4]
              0.1019
                         0.7547
                                   0.135
                                           0.8959
hald[, 5]
             -0.1441
                         0.7091
                                  -0.203
                                           0.8441
```

```
Signif. codes: 0 âĂŸ***âĂŹ 0.001 âĂŸ**âĂŹ 0.01 âĂŸ*âĂŹ 0.05 âĂŸ.âĂŹ 0.1 âĂŸ âĂŹ 1
```

Residual standard error: 2.446 on 8 degrees of freedom Multiple R-squared: 0.9824, Adjusted R-squared: 0.9736 F-statistic: 111.5 on 4 and 8 DF, p-value: 4.756e-07

The goal is to obtain Bayes factors to assess whether any one predictor can be dropped from the model. First, we specify the prior parameter τ based on considerations about the standardized regression coefficient (θ_1^2/ϕ) . Notice that $\theta_1/\sqrt{\phi}$ is the signal-to-noise ratio or standardized effect size. To find the g value that gives a prior mode at $\pm .2$, we use the function mode2g. For instance, for the regression coefficient associated to hald[,2] we would do as follows.

```
> prior.mode <- .2^2
> V <- summary(lm1)$cov.unscaled
> diag(V)
 (Intercept)
                hald[, 2]
                              hald[, 3]
                                             hald[, 4]
                                                           hald[, 5]
820.65457471
               0.09271040
                              0.08756026
                                            0.09520141
                                                          0.08403119
> taumom <- mode2g(prior.mode,prior='normalMom')</pre>
> tautmom <- mode2g(prior.mode,prior='tMom',nu=3)</pre>
> tauimom <- mode2g(prior.mode,prior='iMom')</pre>
> taumom
[1] 0.02
> tautmom
[1] 0.01333333
> tauimom
[1] 0.04
```

We can check the obtained τ values by plotting the prior density.

```
> thseq <- seq(-1,1,length=1000)
> plot(thseq,dmom(thseq,V1=nrow(hald)*V[2,2],tau=taumom),type='l',xlab='theta/sigma',ylab='Pri
> lines(thseq,dmom(thseq,V1=nrow(hald)*V[2,2],tau=tautmom,baseDensity='t',nu=3,penalty='quadra
> lines(thseq,dimom(thseq,V1=nrow(hald)*V[2,2],tau=tauimom),lty=3,col=3)
> abline(v=.2,lty=2,col='gray')
```

Another way to specify g is by finding the value that assigns a desired prior probability to a certain interval. This can be achieved with the function priorp2g. For instance, to find the g value that gives 5% probability to the interval (-0.2,0.2) we use the following code.

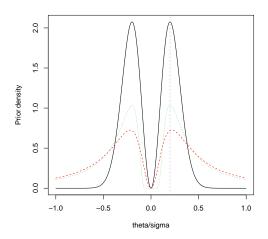


Figure 3: Hald data. Mom and iMom priors for a regression coefficient. The prior mode for θ_1/σ is set at ± 0.2

```
> a <- .2; priorp <- .05
> taumom2 <- priorp2g(priorp=priorp,q=a,prior='normalMom')
> tauimom2 <- priorp2g(priorp=priorp,q=-a,prior='iMom')
> taumom2
[1] 0.113686
> tauimom2
[1] 0.07682918
```

2.2 Bayes factor computation

Bayes factors can be easily computed using the functions mombf and imombf. The normal Mom BF can be computed in explicit form, the T MOM BF require computing a one dimensional integral and the iMom BF a two dimensional integral (regardless of the dimensionality of θ_1). The numerical integration can be achieved either via adaptive quadratures (as implemented in the routines integrate) by setting method='adapt', or via Monte Carlo simulation by setting method='MC'. When ϕ is unknown, method=='adapt' combines integrate with the quantile method of Johnson (1992). The parameter nquant determines the number of quantiles of the posterior distribution of ϕ at which to evaluate the integral. The default nquant=100 usually gives a fairly good approximation. For Monte Carlo integration, the argument B specifies the number of Monte Carlo samples.

In our example, for computational speed we use B=100000, even though in real examples a higher value can be used to ensure proper accuracy. For comparison, we also compute the Bayes factors that would be obtained under Zellner's g-prior with the default value g=1. which can be achieved with the function zellnerbf. Notice that g corresponds to τ in our notation. For reproducibility, we set the random number generator seed to the date this code was written.

We assess the Monte Carlo error by re-computing the iMom BF with a different set of Monte Carlo samples. We find the error to be acceptable.

```
> imombf(lm1,coef=2,g=tauimom,method='MC',B=10^5)
[,1]
[1,] 1.711051
```

We now assess the sensitivity to the prior mode specification. For illustration purposes, we exclude the T MOM and iMom BF as these take longer to compute. The estimated standardized regression coefficient is

```
> sr <- sqrt(sum(lm1$residuals^2)/(nrow(hald)-5))
> thest <- coef(lm1)[2]/sr
> thest
hald[, 2]
0.6341364
```

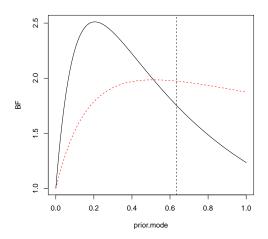


Figure 4: Hald data. BF obtained for Mom and Zellner's g-prior for several prior mode specifications.

We define a sequence of prior modes, find the corresponding g values and compute Bayes factors. Note that mombf, imombf and zellnerbf accept g to be a vector instead of a single value. For large g vectors setting the option method='MC' in imombf can save considerable computing time, as the Monte Carlo samples need only be generated once for all g values.

```
> prior.mode <- seq(.01,1,length=100)^2
> taumom <- mode2g(prior.mode,prior='normalMom')
> bf1 <- mombf(lm1,coef=2,g=taumom)
> bf2 <- zellnerbf(lm1,coef=2,g=taumom)
> plot(prior.mode,bf1,type='l',ylab='BF')
> lines(prior.mode,bf2,lty=2,col=2)
> abline(v=thest,lty=2)
```

The highest possible BF are observed when the prior mode is slightly smaller than the estimated 0.634. As the mode converges to zero both priors converge to a point mass at zero, and hence the BF converges to 1. As the mode goes to infinity the BF goes to 0, as predicted by Lindley's paradox (Lindley, 1957). Although the Mom and Zellner BF show some sensitivity to the prior specification, any prior mode between 0 and 1 results in evidence in favor of including the variable in the model.

3 Bayes factors for generalized linear regression models

This section focuses on obtaining Bayes factors to compare two models. In the examples we use quadratic non-local priors. For examples using product non-local priors see Section 4.

As an illustration, we simulate data with 50 observations from a probit regression model. We simulate two correlated predictors with coefficients equal to log(2) and 0 (i.e. the second variable is not actually in the model). The predictors are stored in the matrix \mathbf{x} , the success probabilities in the vector \mathbf{p} and the observed responses in the vector \mathbf{y} . As in Section 2.2, for reproducibility purposes we set the random number generator seed to the date this code was written.

```
> set.seed(4*2*2008)
> n <- 50; theta <- c(log(2),0)
> x <- matrix(NA,nrow=n,ncol=2)
> x[,1] <- rnorm(n,0,1); x[,2] <- rnorm(n,.5*x[,1],1)
> p <- pnorm(x %*% matrix(theta,ncol=1))
> y <- rbinom(n,1,p)</pre>
```

Before computing Bayes factors, we fit a probit regression model with the function glm. The maximum likelihood estimates are stored in thetahat and the asymptotic covariance matrix in V.

```
> glm1 <- glm(y~x[,1]+x[,2],family=binomial(link = "probit"))
> thetahat <- coef(glm1)
> V <- summary(glm1)$cov.scaled</pre>
```

To compute Bayes factors we use the functions momknown and imomknown. These functions take as primary arguments a vector of regression coefficients and their covariance matrix, and hence they can be used in any setting where one has a statistic that is asymptotically sufficient and normally distributed. The resulting Bayes factors are approximate. The functions also allow for the presence of a dispersion parameter sigma, *i.e.* the covariance of the regression coefficients is sigma*V, but they assume that sigma is known. The probit regression model that we simulated has no over-dispersion and hence it corresponds to sigma=1. We first compare the full model with the model resulting from excluding the second covariate, setting g=0.5 for illustration (note that thetahat[1] contains the intercept).

```
> g <- .5
> bfmom.1 <- momknown(thetahat[2],V[2,2],n=n,g=g,sigma=1)
> bfimom.1 <- imomknown(thetahat[2],V[2,2],n=n,nuisance.theta=2,g=g,sigma=1)
> bfmom.1
```

```
[,1]
[1,] 4.262401
> bfimom.1
[,1]
[1,] 3.336888
```

Both priors result in evidence for including the first covariate. We now check whether the second covariate can be dropped.

Both Mom and iMom BF provide strong evidence in favor of the simpler model, i.e. excluding x[,2]. To compare the full model with the model that has no covariates (i.e. only the constant term remains) we use the same routines, passing a vector as the first argument and a matrix as the second argument.

Based on the resulting BF being close to 1, it is not clear whether the full model is preferable to the model with no covariates.

The BF can be used to easily compute posterior probabilities for each of the four considered models: no covariates, only x[,1], only x[,2] and both x[,1] and x[,2]. We assume equal probabilities a priori.

```
> prior.prob <- rep(1/4,4)
> bf <- c(bfmom.0,bfmom.1,bfmom.2,1)
> pos.prob <- prior.prob*bf/sum(prior.prob*bf)
> pos.prob
```

The model with the highest posterior probability is the one including only x[,1], *i.e.* the correct model, and the model with the lowest posterior probability is that including only x[,2].

4 Variable selection for linear models

We illustrate how to perform variable selection with a simple simulated dataset. We generate 100 observations for the response variable and 3 covariates. The regression coefficient for the third covariate is 0.

```
> set.seed(2011*01*18)
> x <- matrix(rnorm(100*3),nrow=100,ncol=3)
> theta <- matrix(c(1,1,0),ncol=1)
> y <- x %*% theta + rnorm(100)</pre>
```

First we need to specify the prior distribution for the regression coefficients, the model space and the residual variance. We specify a (product) iMOM prior on the coefficients with prior variance parameter tau=.131, which targets the detection of standardized effect sizes above 0.2. Regarding the model space, we use a Beta-binomial prior (binomial prior on the number of included variables with a beta hyper-prior on the Binomial success probability) as then posterior probabilities automatically adjust for multiple comparisons (Scott and Berger, 2010). Finally, for the residual variance we set a fairly non-informative inverse gamma prior.

```
> priorCoef <- new("msPriorSpec",priorType='coefficients',priorDistr='piMOM',priorPars=c(tau=.
> priorDelta <- new("msPriorSpec",priorType='modelIndicator',priorDistr='binomial',priorPars=c
> priorVar <- new("msPriorSpec",priorType='nuisancePars',priorDistr='invgamma',priorPars=c(alp.</pre>
```

The routine modelSelection implements a Gibbs sampling scheme which returns a posterior sample for the variable inclusion indicators in the slot postSample, the visited model with highest posterior probability and the marginal posterior probabilities of inclusion for each covariate. The marginal posterior probabilities are estimated via Rao-Blackwellization, i.e. averaging the posterior probability for inclusion in each Gibbs iteration, as this estimate is more precise than simply taking colMeans on the slot postSample.

```
> fit1 <- modelSelection(y=y, x=x, center=FALSE, scale=FALSE, niter=10^2,
+ priorCoef=priorCoef, priorDelta=priorDelta, priorVar=priorVar,
+ method='Laplace')
Greedy searching posterior mode... Done.
Running Gibbs sampler............ Done.</pre>
```

```
> fit1$postMode
[1] 1 1 0
> fit1$margpp
[1] 1.0000000000 1.000000000 0.0004456386
```

We see that the posterior mode chooses the correct model, and that the marginal probabilities clearly indicate that covariates 1 and 2 should be included and covariate 3 should be excluded. This illustrates an important issue: non-local priors result in a procedure which assigns high posterior probability to the true model (or the model under consideration with smallest Kullback-Leibler distance to the true model). This remains true even in high dimensions, whereas local priors typically assign negligible mass to any single model. We can see this by checking the proportion of posterior samples in which the correct model has been visited: 90 out of 90.

```
> correct <- t(fit1$postSample)==c(TRUE,TRUE,FALSE)
> table(colSums(correct)==3)

TRUE
90
```

References

- M.J. Bayarri and G. Garcia-Donato. Extending conventional priors for testing general hypotheses in linear models. *Biometrika*, 94:135–152, 2007.
- V.E. Johnson. A technique for estimating marginal posterior densities in hierarchical models using mixtures of conditional densities. *Journal of American Statistical Association*, 87:852–860, 1992.
- V.E. Johnson and D. Rossell. Prior densities for default bayesian hypothesis tests. *Journal of the Royal Statistical Society B*, 72:143–170, 2010.
- D.V. Lindley. A statistical paradox. Biometrika, 44:187–192, 1957.
- J.G. Scott and J.O Berger. Bayes and empirical Bayes multiplicity adjustment in the variable selection problem. *The Annals of Statistics*, 38(5): 2587–2619, 2010.
- A. Zellner and A. Siow. Posterior odds ratios for selected regression hypotheses, volume 1. Valencia: University Press, 1980.