Bayesian, MCMC, and Multilevel Modeling (a foray into the subjective)

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Outline

- Introduction
- 2 Prior distributions
- MCMC
- 4 MCMCglmm

Bayesian toolbox for multilevel modeling

MCMC software

- JAGS. JAGS is cross-platform, actively developed, and can be called directly from R via the rjags library. It can run any model as long as you can program it!
 - It is CLI only
- WinBUGS and/or OpenBUGS for PC. OpenBUGS is supposedly cross-platform. Similar to JAGS but more tested and with a large, active support community.
 - Can use with R via R2WinBUGS, BRugs

R software

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- glmmAK. Longitudinal ordinal regression
- MCMC diagnostics, the coda package
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Thomas Bayes



A Presbyterian minister with an itch for gambling, who now rests in Bunhill Fields.

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- In contrast, traditional frequentist statistics defines probability as the long running frequency of an event.
- Rooted in Bayes theorem
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- You can use prior knowledge.
- Inferences are based only on the data, i.e. doesn't violate likelihood principle.
- Reason for stopping the experiment doesn't affect your inferences (Carlin & Louis, 2009).
- Easier to interpret.
- More coherent as all analyses are made based on the posterior.
- Any question can be answered through Bayesian analysis.
- Bayes procedures possess numerous optimality properties.
 - Can calculate actual probability of null hypothesis being true.
 - Ability to test logical hypotheses
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- Assume we have a normal distribution, with a mean (μ) and variance (σ^2) and some data.
- The likelihood is defined as the probability of the data given the parameters, $Pr(\mathbf{y}|\mu,\sigma^2)$
- This is a conditional distribution, we conditioned on the model parameters which are taken as fixed and known.
- Isn't this odd? We've already observed the data, and we don't know what the parameter values are. How can they be fixed and known?
- Aren't we really interested in conditioning the parameters on the data because the parameters aren't observed?
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$$Pr(\mu, \sigma^2 | \mathbf{y}) = \frac{Pr(\mathbf{y} | \mu, \sigma^2) Pr(\mu, \sigma^2)}{Pr(\mathbf{y})}$$

Conceptually

$$Posterior = \frac{Likelihood*Prior}{Marginal}$$

Fortunately for us it simplifies ... a little

$$Pr(\mu, \sigma^2 | \mathbf{y}) \propto Pr(\mathbf{y} | \mu, \sigma^2) Pr(\mu, \sigma^2)$$

So ... what is the elephant in the room?

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The elephant is ...

Prior distribution

$Pr(\mu, \sigma^2)$

Why?

What is this?

How do we handle this?

How do we get rid of this?

Do we want to get rid of this?

Does it have any use?

Does it have any harm?

How can we marginalize this?

Is it useful?

- Bayes thereom, and by extension Bayesian, forces us to incorporate priors
- Priors can be very useful
 - ullet Imagine your study is only one of a 1000 studies on topic X.
 - You can formally synthesize all these results into your models
 - Gives you a stronger model because it's based on 1000+1 studies not just 1!?!
 - Is it cheating!
 - Philsophically, doesn't science build on science? Our very hypotheses on previous studies? Our models and our data are not isolated, objective icebergs!

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- If our results are truly unique and we incorporate previous data into our priors we might not see this in our results.
- Priors are subjective!
- With a small sample size, priors have a large effect on our results.
- Choice of your priors can have a profound impact on your inferences
- MLE estimates are 'more objective'
- Aren't economists Bayesian? Oh no ...

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- Confession: I would describe myself as a subjective Bayesian!
 - I believe priors should be informative and guide our models.
 - Bayesian is accepted in ecology.
 - However, I'm not foolish!
- Priors need to be based on sound evidence and must be justifiable.
- When in doubt, use non-informative, uniform priors
 - Estimates are similar to MLE in most instances
- Guess what ... you're already using Bayesian!
 - Estimation of random effects in longitudinal analyses and HLM, BIC, IRT!

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- Confession: I would describe myself as a subjective Bayesian!
 - I believe priors should be informative and guide our models.
 - Bayesian is accepted in ecology.
 - However, I'm not foolish!
- Priors need to be based on sound evidence and must be justifiable.
- When in doubt, use non-informative, uniform priors
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The legendary R. A. Fischer on probability

"The probability of any event is the ratio between the value at which an expectation depending on the happening of the event ought to be computed, and the value of the thing expected upon its happening." (In Aldrich, 2008)

• But then again, Fischer didn't believe smoking caused cancer.

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How can prior distributions affect our results?

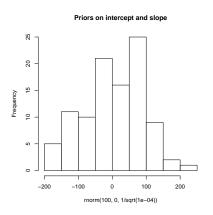
Let's take a look at rjags

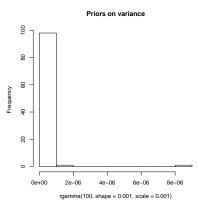
```
> require(rjags)
> dat0 <- na.omit(dat0)
> N <- nrow(dat0)
> Y <- datO$ACT ENGL
> x <- datO$ACT MATH
> dump(list=c("N","Y","x"),file="lr.data")
> datalr <- read.data(file="lr.data".format="iags")
> datalr
$x
[1] 14 19 26 15 19 18 17 13 15 16 22 21 19 18 19 16 19 20 22 25 21 19 21 12 18
[26] 21 20 20 26 21 21 24 20 20 22 23 17 18 20 19 16 19 15 29 26 17 18 20 17 16
[51] 20 17 16 15 17 16 28 20 25 22 26 18 25 18 22 19 26
$Y
[1] 16 25 24 21 17 13 18 19 16 19 17 19 15 23 21 20 16 22 18 18 14 19 22 10 13
[26] 21 18 18 16 18 24 28 25 16 16 17 14 15 18 22 15 18 10 23 19 22 20 21 16 19
[51] 18 15 12 16 19 19 27 16 23 16 23 19 25 19 25 19 20
$N
[1] 67
```

Exploring priors

```
> print(m1 <- jags.model(file="lr8920prior1.bug",data=datalr))
Compiling model graph
   Resolving undeclared variables
   Allocating nodes
  Graph Size: 197
JAGS model:
model {
   for (i in 1:N) {
          Y[i] ~ dnorm(mu[i], tau)
          mu[i] \leftarrow alpha + beta * (x[i] - x.bar)
 x.bar <- mean(x)
 alpha ~ dnorm(0.0, 1.0E-4)
 beta ~ dnorm(0.0, 1.0E-4)
  sigma <- 1.0/sqrt(tau)
 tau ~ dgamma(1.0E-3, 1.0E-3)
Fully observed variables:
NYx
```

What do these priors look like?





Prior distributions MCMC MCMCglmm

Posterior distribution from prior 1

```
> prior1 <- coda.samples(m1,variable.names=c("alpha","beta","sigma","tau"),n.iter=5000,thin=10)
> summary(prior1)
Iterations = 10:5000
Thinning interval = 10
Number of chains = 1
Sample size per chain = 500
1. Empirical mean and standard deviation for each variable,
```

plus standard error of the mean:

```
SD Naive SE Time-series SE
alpha 18.73395 0.42902 0.0191865 0.0221243
beta 0.51495 0.12166 0.0054406 0.0051588
sigma 3.42628 0.63731 0.0285015 0.0247560
                             0.0006959
      0.08829 0.01595 0.0007132
tan
```

2. Quantiles for each variable:

```
2.5%
                  25%
                         50%
                                  75%
                                       97.5%
alpha 17.82418 18.47420 18.7603 18.98205 19.5555
     0.27909 0.44618 0.5155 0.58573 0.7579
sigma 2.88946 3.19051 3.3846 3.59386 4.0401
      0.06127 0.07742 0.0873 0.09824 0.1198
tau
```

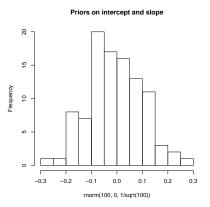
Maximum likelihood estimates

The posterior distribution estimate of the slope is nearly identical to the maximum likelihood estimate. But the intercept is a little different. What happens if we decrease the variance?

Alternate priors with small variances

```
> print(m2 <- jags.model(file="lr8920prior2.bug",data=datalr))
Compiling model graph
   Resolving undeclared variables
   Allocating nodes
  Graph Size: 197
JAGS model:
model {
   for (i in 1:N) {
          Y[i] ~ dnorm(mu[i], tau)
          mu[i] \leftarrow alpha + beta * (x[i] - x.bar)
 x.bar <- mean(x)
 alpha ~ dnorm(0.0, 100)
 beta ~ dnorm(0.0, 100)
  sigma <- 1.0/sqrt(tau)
 tau ~ dgamma(1.0E-3, 1.0E-3)
Fully observed variables:
NYx
```

What do these alternate priors look like?



I bet this will have an enormous impact!

Posterior distribution from prior 2

```
> prior2 <- coda.samples(m2,variable.names=c("alpha","beta","sigma","tau"),n.iter=5000,thin=10)
  1**************** 100%
> summary(prior2)
Iterations = 10.5000
Thinning interval = 10
Number of chains = 1
Sample size per chain = 500
1. Empirical mean and standard deviation for each variable,
  plus standard error of the mean:
          Mean
                     SD Naive SE Time-series SE
alpha 0.045119 0.341613 1.528e-02 1.453e-02
beta 0.013496 0.105259 4.707e-03 4.841e-03
sigma 19.366620 1.742587 7.793e-02 7.326e-02 tau 0.002731 0.000495 2.214e-05 2.127e-05
2. Quantiles for each variable:
          2.5%
                     25%
                              50%
                                        75%
                                                97.5%
alpha -0.165544 -0.034142 0.031131 0.093523 0.230392
beta -0.193316 -0.055528 0.009584 0.082081 0.211800
sigma 16.482919 18.133185 19.282952 20.382879 22.999065
      0.001891 0.002407 0.002689 0.003041 0.003681
```

alpha and beta got pulled towards zero and sigma balloned!

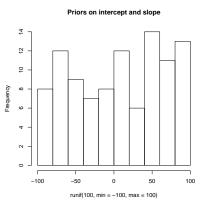
This time with uniform priors

This time lets set set the priors on alpha and beta to be uniform.

```
Compiling model graph
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  Graph Size: 197
JAGS model:
model {
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          Y[i] ~ dnorm(mu[i], tau)
          mu[i] \leftarrow alpha + beta * (x[i] - x.bar)
 x.bar <- mean(x)
 alpha ~ dunif(-100, 100)
 beta ~ dunif(-100, 100)
 sigma <- 1.0/sqrt(tau)
 tau ~ dgamma(1.0E-3, 1.0E-3)
Fully observed variables:
NYx
```

> print(m3 <- jags.model(file="lr8920prior3.bug",data=datalr))

3rd priors



What do you think the posterior distribution will look like?

Posterior distribution from prior 3

2. Quantiles for each variable:

```
2.5% 25% 50% 75% 97.5% alpha 17.96480 18.43754 18.74745 19.02622 19.4980 beta 0.30025 0.44335 0.51497 0.59273 0.7369 sigma 2.81918 3.18651 3.33087 3.56174 4.0542 tau 0.06084 0.07883 0.09013 0.09848 0.1258
```

Very similar to MLE

- I'd like you guys to break up into groups of 3.
- Using my code and data, tweak the model, and run it!
- Run jags.model() then coda.samples()
- Try it with a few different priors and repeat the process for the same priors.
- What were your priors? How did they affect your estimates?
 Do you get the same estimates when you ran the same priors again? What if you used set.seed()?

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- Priors can greatly affect your estimates, especially the choice of the variance!
- When *n* increases, the influence of priors goes down
 - How big does *n* need to be? Bigger than 67 apparently
 - For "fixed effects" estimates, n doesn't need to be as big as it does for variance and "random effects"
- Should examine posterior modes, posterior means, and Bayesian confidence intervals. If these are similar to MLE then you are good to go! If not worry?
- Can also do sensitivity analysis of posterior distribution under different prior specifications.
- For GLMM and LMM, when in doubt use non-informative uniform priors on fixed effects and non-informative inverse Wishart on residuals & random effects (discussed later).
 Results will be similar to MLE.

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How do we estimate posterior distributions?

Recall for a simple linear regressioen of a normally distributed variable...

$$Pr(\mu, \sigma^2 | \mathbf{y}) \propto Pr(\mathbf{y} | \mu, \sigma^2) Pr(\mu, \sigma^2)$$

- In order to calculate the posterior distribution often requires integrating out many variables, taking integrals of integrals.
 - Imagine the case of a GLMM, where you have to estimate your fixed effects, variances, and random effects.
 - This can not be derived analytically and requires approximation.
- MCMC provides a way to estimate the posterior distribution.
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- The first thing that you need for MCMC are starting values
- This will help to speed up convergence and reduce wasted wandering
- All estimated parameters require starting values
- These may be generated by the program
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- After we've initialized our chain we need to decide where to go next and start sampling from our posterior distribution!
- To do this we generate a candidate destination and decide whether we should move there or stay put.
- One way to do this is using a Metropolis-Hastings (MH) algorithm.
- During the first iteration, a random set of coordinates are picked from a multivariate normal distribution and compared to the intial coordinates.
- If the posterior probability is greater for the new coordinates, than we move to the new coordinates.

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Metropolis-Hastings continued

- If the posterior probability is lower, than we may stay or we may go.
- Once this iteration is complete, we repeat this again with our coordinates at the end of the last iteration becoming our base line coordinates.
- We repeat this over and over again depending upon how many iterations we've specified.
- Iterations are saved and we examine them when we look at the posterior distribution.
- Pros: Easy to write your own algorithms, less mathematical
- Cons: Very slow to converge!

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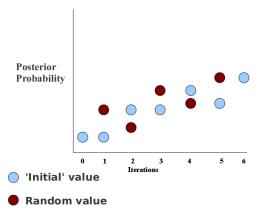
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MH conceptually



Gibbs sampling

A special case of MH

- In MH, we could move in multiple directions simulatenously, i.e. we moved for both μ and σ^2 .
- However, we could have moved in just one direction at a time, for example move in the direction of μ conditioned on some value of σ^2 say 1.
- Mathematically then, $Pr(\mu|\sigma^2=1,\mathbf{y})$

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- \bullet First, let's move in the direction of μ conditioned on some value of σ^2
- We could generate a new candidate randomly and ask if it's posterior probability is higher but ...
- We often know the equation for this conditional distribution, this is Gibbs Sampling
- We know we're at $\sigma^2=1$, so why don't we just calculate μ directly.
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 - They should be free from pattern
 - Each plot should have roughly a horizontal line with no ascending/descending pattern
- Next you should look at autocorrelation between iterations.
 - Iterations have a tendency to be autocorrelated and are not independent.
 - Should examine this empirically and thin out your chain
- There are lots of helpful diagnostic tools in the coda package
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- Can estimate very complex models.
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- Developer extremely helpful and active on r-sig-mixed models mailing list.
- Can calculate actual p-values, 95% Bayesian confidence intervals, Deviance information criterion.

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Specifying a MCMCglmm() model

Default arguments to MCMCglmm()

```
MCMCglmm(fixed, random=NULL, rcov= units, family="gaussian", mev=NULL, data,start=NULL, prior=NULL, tune=NULL, pedigree=NULL, nodes="ALL", scale=TRUE, nitt=13000, thin=10, burnin=3000, pr=FALSE, pl=FALSE, verbose=TRUE, DIC=TRUE, singular.ok=FALSE, saveX=FALSE, saveZ=FALSE, slice=FALSE)
```

fixed and **random** fixed and random effects formulae: **rcov** residual Cov structure; **family** probability family; **mev** specify measurement error (meta-analysis); data data; start starting values; **prior** the priors; **tune** Cov matrix for proposed latent variable; **pedigree**, **nodes**, and **scale** useful for genetics; **nitt** # of iterations; thin thinning interval; burnin # of burn-ins; pr and pl save posterior of random effects and latent variables; verbose get output; **DIC** Deviance information criterion; **singular.ok** when false linear dependencies in fixed effects are removed; saveX and **saveZ** save fixed effects and random effects matrix: **slice** use slice sampling (type of MCMC).

Labdosage data set

We'll use the labdosage.txt file. I believe you all are familiar with it?

> head(dos)

```
    id
    group time count

    1.1
    1
    2mg
    1
    5

    1.2
    1
    2mg
    2
    2

    1.3
    1
    2mg
    3
    2

    1.4
    1
    2mg
    4
    5

    1.5
    1
    2mg
    5
    2

    1.6
    1
    2mg
    6
    4
```

Specifying priors on a random intercepts model with Poisson data

- *B-structure* priors on 'fixed effects'; *G-structure* priors on 'random effects'; *R-structure* priors on residual variance.
- Default B is $\mu = 0$, V=I*1e+10, G and R are nu=0, V=1, alpha.mu=1, and alpha.V=0.
- B is multivariate normal; G and R are inverse Wishart with Cauchy parameter expansion (Gelman, 2006)
- Default B is weak and essentially uniformative, G and R are both weakly informative.

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Specifying a random intercepts model continued

> prior<-list(R=list(V=1, nu=0.002), G=list(G1=list(V=1, nu=0.002)))

Summary statistics - Fixed effects

```
> # Summary of 'Fixed Effects'
> summary(m1$Sol)
Tterations = 3001:12991
Thinning interval = 10
Number of chains = 1
Sample size per chain = 1000
1. Empirical mean and standard deviation for each variable,
   plus standard error of the mean:
                          SD Naive SE Time-series SE
(Intercept) 1.93977 0.080995 0.0025613 0.0030749
           -0.05646 0.006811 0.0002154 0.0002181
time
2. Quantiles for each variable:
               2.5%
                         25%
                                  50%
                                          75%
                                                 97.5%
(Intercept) 1.78134 1.88190 1.93970 1.99740 2.09185
           -0.06871 -0.06132 -0.05666 -0.05219 -0.04249
time
> HPDinterval(m1$Sol)
                 lower
                             upper
(Intercept) 1.78774756 2.09483939
          -0.06889096 -0.04286956
attr(, "Probability")
Γ17 0.95
```

Summary statistics - Random effects

- > # Summary of 'Random Effects
 > summary(m1\$VCV)
- Empirical mean and standard deviation for each variable, plus standard error of the mean:

```
        Mean
        SD
        Naive SE Time-series SE

        id
        0.2815
        0.06264
        0.0019809
        0.001970

        units
        0.2424
        0.02490
        0.0007873
        0.001281
```

2. Quantiles for each variable:

```
2.5% 25% 50% 75% 97.5% id 0.1865 0.2372 0.2727 0.3174 0.4166 units 0.1997 0.2248 0.2410 0.2577 0.2959
```

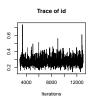
> HPDinterval(m1\$VCV)

```
lower upper
id 0.1728576 0.3990647
units 0.1967859 0.2921864
attr(,"Probability")
[1] 0.95
```

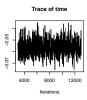
Trace plots of 'fixed' and 'random' effects

















Autocorrelations of iterations

```
> autocorr(m1$Sol)
, , (Intercept)
       (Intercept) time
Lag 0 1.00000000 -0.49419125
Lag 10 0.08802531 -0.07252791
Lag 50 0.06445487 -0.04806522
Lag 100 -0.02629911 0.06327561
Lag 500 0.03672346 -0.04482030
, , time
       (Intercept)
                         time
Lag 0 -0.49419125 1.00000000
Lag 10 0.02048099 0.04815938
Lag 50 -0.04384447 0.03041308
Lag 100 -0.01538620 -0.03313733
Lag 500 -0.00999942 0.02657281
```

How does this compare with glmer()

```
> m1.glmer <- glmer(count ~ 1 + time + (1 | id), family="poisson",data=dos)</pre>
```

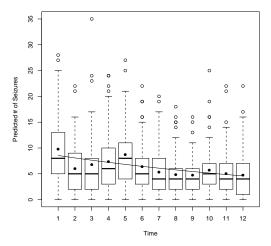
Effect	MCMCglmm	lme4
Intercept	1.9398	2.0389
Time	-0.0565	-0.0546
id	0.2815	0.2652

Very similar! This is great! Additionally, the standard errors were similar too with MCMCglmm being slightly smaller.

Predicted growth curve from MCMCglmm syntax

```
> beta<-colMeans(m1$Sol)
> pred<-beta[1]+beta[2]*I(1:12)
> plot(dos$count~as.factor(dos$time),xlab="Time",
    ylab="Predicted # of Seizures")
> points(tapply(dos$count, as.factor(dos$time), mean)~I(1:12),pch=16)
> lines(exp(pred+0.5*mean(rowSums(m1$VCV)))~I(1:12))
```

Predicted growth curve



Random slopes MCMCglmm model

Which model is better: Random intercepts or random slope?

```
> m1$DIC;m2$DIC
```

[1] 3871.923

[1] 3861.976

Random slopes model

- > summary(m2\$VCV)
- Empirical mean and standard deviation for each variable, plus standard error of the mean:

```
        Mean
        SD
        Naive SE
        Time-series SE

        id
        0.28073
        0.05920
        0.0018722
        0.0022649

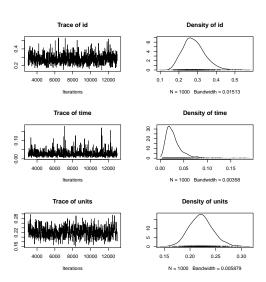
        time
        0.02867
        0.01890
        0.0005977
        0.0007020

        units
        0.22134
        0.02244
        0.0007097
        0.0009372
```

2. Quantiles for each variable:

```
2.5% 25% 50% 75% 97.5% id 0.181775 0.24027 0.27404 0.31639 0.41390 time 0.007685 0.01663 0.02452 0.03464 0.07818 units 0.180095 0.20586 0.22075 0.23545 0.26900
```

Trace plots of random slopes model



Random slopes model with a static predictor

Summary statistics: Fixed effects

- > summary(m3\$Sol)
- Empirical mean and standard deviation for each variable, plus standard error of the mean:

```
        Mean
        SD
        Naive SE
        Time-series SE

        (Intercept)
        2.05451
        0.14353
        0.0045389
        0.0050984

        time
        -0.05584
        0.01520
        0.0004808
        0.0005261

        group2mg
        -0.27097
        0.14036
        0.0044387
        0.0043285
```

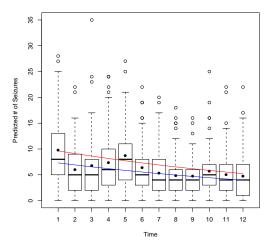
2. Quantiles for each variable:

```
2.5% 25% 50% 75% 97.5% (Intercept) 1.75796 1.9676 2.05187 2.14983 2.33057 time -0.08692 -0.0651 -0.05606 -0.04607 -0.02599 group2mg -0.53615 -0.3666 -0.27407 -0.17733 0.00905
```

Predicted growth curves syntax

> beta<-colMeans(m3\$Sol)

Growth curve



m3 with different priors

Let's set some pretty illogical priors

And the results ...

Uninformative priors	Crazy priors
2.055	2.061
-0.056	-0.056
-0.271	-0.270
0.264	0.266
0.029	0.0274
	2.055 -0.056 -0.271 0.264

With 780 data points, the likelihood already swamps the prior!

- Spend some time now in a group running different priors and different models on the data set.
- Maybe try specifying starting values?
 - start <- list(B=2.05,-0.06,-0.27)
 - random=~id + time,family="poisson",data=dos, prior=prior,start=start,verbose=FALSE)
 - I don't recommend starting values for G and R
- If you need help with syntax please ask.
- Did you find anything interesting?

- Spend some time now in a group running different priors and different models on the data set.
- Maybe try specifying starting values?

```
• start <- list(B=2.05,-0.06,-0.27)
```

- m3a <- MCMCglmm(count ~ 1 + time + group, random=~id + time,family="poisson",data=dos, prior=prior,start=start,verbose=FALSE)
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- In my opinion, it's useful to know Bayesian methods as ML approaches & least squares approaches don't always work.
- I believe that Bayesian methods will become more and more important as computers become more and more powerful.
- Bayesian frees you from the awkwardness of frequentist statistics and creates the opportunity to include prior information.
- But ... like everything there are costs to Bayesian.
- Hopefully I've give you just enough information to be dangerous

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Thanks!

