

# dclone: Data Cloning in R

by Péter Sólymos

**Abstract** The **dclone** R package contains low level functions for implementing maximum likelihood estimating procedures for complex models using data cloning and Bayesian Markov Chain Monte Carlo methods with support for JAGS, WinBUGS and OpenBUGS.

## Introduction

Hierarchical models, including generalized linear models with mixed random and fixed effects, are increasingly popular. The rapid expansion of applications is largely due to the advancement of the Markov Chain Monte Carlo (MCMC) algorithms and related software (Gelman et al., 2003; Gilks et al., 1996; Lunn et al., 2009). Data cloning is a statistical computing method introduced by Lele et al. (2007). It exploits the computational simplicity of the MCMC algorithms used in the Bayesian statistical framework, but it provides the maximum likelihood point estimates and their standard errors for complex hierarchical models. The use of the data cloning algorithm is especially valuable for complex models, where the number of unknowns increases with sample size (i.e. with latent variables), because inference and prediction procedures are often hard to implement in such situations.

The **dclone** R package (Sólymos, 2010) provides infrastructure for data cloning. Users who are familiar with Bayesian methodology can instantly use the package for maximum likelihood inference and prediction. Developers of R packages can build on the low level functionality provided by the package to implement more specific higher level estimation procedures for users who are not familiar with Bayesian methodology. This paper demonstrates the implementation of the data cloning algorithm, and presents a case study on how to write high level functions for specific modeling problems.

## Theory of data cloning

Imagine a hypothetical situation where an experiment is repeated by  $k$  different observers, and all  $k$  experiments happen to result in exactly the same set of observations,  $y^{(k)} = (y, y, \dots, y)$ . The likelihood function based on the combination of the data from these  $k$  experiments is  $L(\theta, y^{(k)}) = [L(\theta, y)]^k$ . The location of the maximum of  $L(\theta, y^{(k)})$  exactly equals the location of the maximum of the function  $L(\theta, y)$ , and the Fisher information matrix based on this likelihood is  $k$  times the Fisher information matrix based on  $L(\theta, y)$ .

One can use MCMC methods to calculate the posterior distribution of the model parameters ( $\theta$ ) conditional on the data. Under regularity conditions, if  $k$  is large, the posterior distribution corresponding to  $k$  clones of the observations is approximately normal with mean  $\hat{\theta}$  and variance  $1/k$  times the inverse of the Fisher information matrix. When  $k$  is large, the mean of this posterior distribution is the maximum likelihood estimate and  $k$  times the posterior variance is the corresponding asymptotic variance of the maximum likelihood estimate if the parameter space is continuous. When some of the parameters are on the boundaries of their feasible space (Stram and Lee, 1994), point estimates can be correct, but currently the Fisher information cannot be estimated correctly by using data cloning. This is an area for further research, but such situations challenge other computing techniques as well.

Data cloning is a computational algorithm to compute maximum likelihood estimates and the inverse of the Fisher information matrix, and is related to simulated annealing (Brooks and Morgan, 1995). By using data cloning, the statistical accuracy of the estimator remains a function of the sample size and not of the number of cloned copies. Data cloning does not improve the statistical accuracy of the estimator by artificially increasing the sample size. The data cloning procedure avoids the analytical or numerical evaluation of high dimensional integrals, numerical optimization of the likelihood function, and numerical computation of the curvature of the likelihood function. Interested readers should consult Lele et al. (2007, 2010) for more details and mathematical proofs for the data cloning algorithm.

## The data cloning algorithm

Consider the following Poisson generalized linear mixed model (GLMM) with a random intercept for i.i.d. observations of  $Y_i$  counts from  $i = 1, 2, \dots, n$  localities:

$$\begin{aligned} \alpha_i &\sim \text{normal}(0, \sigma^2) \\ \lambda_i &= \exp(\alpha_i + \mathbf{X}_i^T \boldsymbol{\beta}) \\ Y_i | \lambda_i &\sim \text{Poisson}(\lambda_i) \end{aligned}$$

The corresponding code for the simulation with  $\boldsymbol{\beta} = (1.8, -0.9)$ ,  $\sigma = 0.2$ ,  $x_i \sim U(0, 1)$  is:

```
> library(dclone)
> set.seed(1234)
> n <- 50
> beta <- c(1.8, -0.9)
> sigma <- 0.2
> x <- runif(n, min = 0, max = 1)
> X <- model.matrix(~ x)
```

```
> alpha <- rnorm(n, mean = 0, sd = sigma)
> lambda <- exp(alpha + drop(X %*% beta))
> Y <- rpois(n, lambda)
```

The first step in the data cloning algorithm is to construct the full Bayesian model of the problem with proper prior distributions for unknown parameters. We use flat normal priors for  $\beta$ s and for  $\log(\sigma)$ . First we use the **rjags** (Plummer, 2010b) and **coda** (Plummer et al., 2010) R packages and the JAGS (Plummer, 2010a) software for model fitting. But the **dclone** package also supports WinBUGS (Spiegelhalter et al., 2003) and OpenBUGS (Spiegelhalter et al., 2007) via the R packages **R2WinBUGS** (Sturtz et al., 2005) and **BRugs** (Thomas et al., 2006), respectively. The corresponding model in the BUGS language is:

```
> glmm.model <- function() {
+   for (i in 1:n) {
+     Y[i] ~ dpois(lambda[i])
+     lambda[i] <- exp(alpha[i] +
+       inprod(X[i,], beta[1,]))
+     alpha[i] ~ dnorm(0, tau)
+   }
+   for (j in 1:np) {
+     beta[1,j] ~ dnorm(0, 0.001)
+   }
+   log.sigma ~ dnorm(0, 0.001)
+   sigma <- exp(log.sigma)
+   tau <- 1 / pow(sigma, 2)
+ }
```

Note that instead of writing the model into a file, we store it as an R function (see JAGS and WinBUGS documentation for how to correctly specify the model in the BUGS language). Although the BUGS and R syntaxes seem similar, the BUGS model function cannot be evaluated within R. Storing the BUGS model as an R function is handy, because the user does not have to manage different files when modeling. Nevertheless, the model can be supplied in a separate file by giving its name as character.

We also have to define the data as elements of a named list along with the names of nodes that we want to monitor (we can also set up initial values, number of burn-in iterations, number of iterations for the posterior sample, thinning values, etc.; see **dclone** package documentation for details). Now we can do the Bayesian inference by calling the `jags.fit` function:

```
> dat <- list(Y = Y, X = X, n = n,
+   np = ncol(X))
> mod <- jags.fit(dat,
+   c("beta", "sigma"), glmm.model, n.iter = 1000)
```

The output `mod` is an "mcmc.list" object, which can be explored by methods such as `summary` or `plot` provided by the **coda** package.

The **dclone** package provides the `bugs.fit` wrapper function for WinBUGS/OpenBUGS. The BUGS model needs to be changed to run smoothly in WinBUGS/OpenBUGS:

```
> glmm.model.bugs <- function() {
+   for (i in 1:n) {
+     Y[i] ~ dpois(lambda[i])
+     lambda[i] <- exp(alpha[i] +
+       inprod(X[i,], beta[1,]))
+     alpha[i] ~ dnorm(0, tau) %_ I(-5, 5)
+   }
+   for (j in 1:np) {
+     beta[1,j] ~ dnorm(0, 0.01) %_ I(-5, 5)
+   }
+   log.sigma ~ dnorm(0, 0.01) %_ I(-5, 5)
+   sigma <- exp(log.sigma)
+   tau <- 1 / pow(sigma, 2)
+ }
```

In the `bugs.fit` function, the settings besides the `data`, `params`, `model`, and `inits` arguments follow the settings in the `bugs/openbugs` functions in the **R2WinBUGS** package. This leads to some differences between the arguments of the `jags.fit` and the `bugs.fit` functions. For example `bugs.fit` uses `n.thin` instead of `thin`, and `n.burnin` is equivalent to `n.adapt + n.update` as compared to `jags.fit`. The `bugs.fit` can return the results either in "mcmc.list" or "bugs" format. The reason for leaving different arguments for `jags.fit` and `bugs.fit` is that the aim of the **dclone** package is not to make the MCMC platforms interchangeable, but to provide data cloning facility for each. It is easy to adapt an existing BUGS code for data cloning, but it sometimes can be tricky to adapt a JAGS code to WinBUGS and vice versa, because of differences between the two dialects (i.e. truncation, censoring, autoregressive priors, etc., see Plummer (2010b)).

Here are the results from the three MCMC platforms:

```
> mod.wb <- bugs.fit(dat, c("beta", "sigma"),
+   glmm.model.bugs, DIC = FALSE, n.thin = 1)
> mod.ob <- bugs.fit(dat, c("beta", "sigma"),
+   glmm.model.bugs, program = "openbugs",
+   DIC = FALSE, n.thin = 1)
> sapply(list(JAGS = mod, WinBUGS = mod.wb,
+   OpenBUGS = mod.ob), coef)
           JAGS WinBUGS OpenBUGS
beta[1]  1.893   1.910  1.9037
beta[2] -1.050  -1.074  -1.0375
sigma    0.161   0.130   0.0732
```

The idea in the next step of the data cloning algorithm is that instead of using the likelihood for the observed data, we use the likelihood corresponding to  $k$  copies (clones) of the data. Actually cloning (repeating) the data  $k$  times is important if the model includes unobserved (latent) variables: in this way latent variables are cloned as well, thus contributing to the likelihood. We can use the `rep` function to repeat the data vectors, but it is less convenient for e.g. matrices or data frames. Thus, there is the **dclone** generic function with methods for various R object classes:

```
> dclone(1:5, 1)
```

```
[1] 1 2 3 4 5
> dclone(1:5, 2)

[1] 1 2 3 4 5 1 2 3 4 5
attr(,"n.clones")
[1] 2
attr(,"n.clones") attr(,"method")
[1] "rep"

> dclone(matrix(1:4, 2, 2), 2)

      [,1] [,2]
[1,]    1    3
[2,]    2    4
[3,]    1    3
[4,]    2    4
attr(,"n.clones")
[1] 2
attr(,"n.clones") attr(,"method")
[1] "rep"

> dclone(data.frame(a=1:2, b=3:4), 2)

      a b
1_1 1 3
2_1 2 4
1_2 1 3
2_2 2 4
```

The number of clones can be extracted by the `nclones` function; it returns `NULL` for  $k = 1$  and  $k$  otherwise.

The BUGS data specification might contain some elements that we do not want to clone (e.g. "np", the number of columns of the design matrix in this case). Thus the `dclone` method has different behaviour for lists, than for non list classes (including data frames). We can define which elements should not be cloned, or which should be multiplied by  $k$  instead of being cloned  $k$  times.

```
> dat2 <- dclone(dat, n.clones = 2,
+ multiply = "n", unchanged = "np")
> nclones(dat2)

[1] 2
attr(,"method")
      Y      X      n      np
"rep" "rep" "multi" NA
```

The "method" attribute of the cloned object stores this information. There are three different ways of cloning (besides NA standing for unchanged): "rep" is for (longitudinal) repetitions, "multi" is for multiplication, and "dim" is repeating the data along an extra dimension (see later).

Now we do the model fitting with  $k = 2$ . The "mcmc.list" object inherits the information about the cloning:

```
> mod2 <- jags.fit(dat2,
+ c("beta", "sigma"), glmm.model, n.iter = 1000)
```

Similarly, the `bugs.fit` function takes care of the cloning information passed through the data argument:

```
> mod.wb2 <- bugs.fit(dat2, c("beta", "sigma"),
+ glmm.model.bugs, DIC = FALSE, n.thin = 1)
> mod.ob2 <- bugs.fit(dat2, c("beta", "sigma"),
+ glmm.model.bugs, program = "openbugs",
+ DIC = FALSE, n.thin = 1)
```

And here are the results based on  $k = 2$  for the three MCMC platforms:

```
> sapply(list(JAGS = mod2, WinBUGS = mod.wb2,
+ OpenBUGS = mod.ob2), coef)

      JAGS WinBUGS OpenBUGS
beta[1] 1.918   1.905   1.896
beta[2] -1.114  -1.080  -1.078
sigma   0.207   0.187   0.243
```

For some models, indexing can be more complex, and simple repetitions of the data ("rep" method) are not appropriate. In case of non independent data (time series or spatial autoregressive models), cloning should be done over an extra dimension to ensure that clones are independent. For this purpose, one can use the `dcdim` function:

```
> (obj <- dclone(dcdim(data.matrix(1:5)), 2))

      clone.1 clone.2
[1,]        1        1
[2,]        2        2
[3,]        3        3
[4,]        4        4
[5,]        5        5
attr(,"n.clones")
[1] 2
attr(,"n.clones") attr(,"method")
[1] "dim"
attr(,"n.clones") attr(,"method") attr(,"drop")
[1] TRUE
```

If data cloning consists of repetitions of the data, our BUGS model usually does not need modifications. If we add an extra dimension to the data, the BUGS model and the data specification must reflect the extra dimension, too.

To demonstrate this, we consider a model and data set from Ponciano et al. (2009). They used the single-species population growth data from laboratory experiments of Gause (1934) with *Paramecium aurelia*. Gause initiated liquid cultures on day 0 at a concentration of two individuals per 0.5 cm<sup>3</sup> of culture media. Then, on days 2–19, he took daily 0.5 cm<sup>3</sup> samples of the microbe cultures and counted the number of cells in each sample. Ponciano et al. (2009) fitted discrete time stochastic models of population dynamics to describe Gause's data taking into account both process noise and observation error. The Beverton-Holt model incorporates a latent variable component ( $N_t$ ,  $t = 0, 1, \dots, q$ ) to describe an unobserved time series of actual population abundance. The latent variable component contains density dependence ( $\beta$ ) and stochastic process noise ( $\sigma^2$ ). The

model incorporates a Poisson observation component to account for variability caused by sampling:

$$\begin{aligned}\mu_t &= \log(\lambda) + \log(N_{t-1}) - \log(1 + \beta N_{t-1}) \\ \log(N_t) &\sim \text{normal}(\mu_t, \sigma^2) \\ Y_t | N_t &\sim \text{Poisson}(N_t)\end{aligned}$$

$\lambda$  is the finite rate of increase in population abundance. The corresponding BUGS model is:

```
> beverton.holt <- function() {
+   for (j in 1:k) {
+     for(i in 2:(n+1)){
+       Y[(i-1),j] ~ dpois(exp(log.N[i,j]))
+       log.N[i,j] ~ dnorm(mu[i,j], 1 / sigma^2)
+       mu[i,j] <- log(lambda) + log.N[(i-1),j]
+         - log(1 + beta * exp(log.N[(i-1),j]))
+     }
+     log.N[1,j] ~ dnorm(mu0, 1 / sigma^2)
+   }
+   beta ~ dlnorm(-1, 1)
+   sigma ~ dlnorm(0, 1)
+   tmp ~ dlnorm(0, 1)
+   lambda <- tmp + 1
+   mu0 <- log(lambda) + log(2) - log(1 + beta * 2)
+ }
```

Note that besides the indexing for the time series, the model contains another dimension for the clones. We define the data set by using the `dcdim` method for cloning the observations. We include an element `k = 1` that will be multiplied to indicate how many clones (columns) are in the data, while `n` (number of observations) remains unchanged:

```
> paurelia <- c(17, 29, 39, 63, 185, 258, 267,
+ 392, 510, 570, 650, 560, 575, 650, 550,
+ 480, 520, 500)
> bhdat <- list(Y=dcdim(data.matrix(paurelia)),
+ n=length(paurelia), k=1)
> dcbhdat <- dclone(bhdat, n.clones = 5,
+ multiply = "k", unchanged = "n")
> bhmod <- jags.fit(dcbhdat,
+ c("lambda","beta","sigma"), beverton.holt,
+ n.iter=1000)
> coef(bhmod)
```

```
beta lambda sigma
0.00218 2.18755 0.12777
```

Results compare well with estimates in Ponciano et al. (2009) ( $\hat{\beta} = 0.00235$ ,  $\hat{\lambda} = 2.274$ ,  $\hat{\sigma} = 0.1274$ ).

## Iterative model fitting

We can use the `dc.fit` function to iteratively fit the same model with various `k` values as described in Lele et al. (2010). The function takes similar arguments to `dclone` and `jags.fit` (or `bugs.fit`, if flavour = "bugs" is used). Because the information in the data overrides the priors by increasing the

number of clones, we can improve MCMC convergence by making the priors more informative during the iterative fitting process. We achieve this by modifying the BUGS model for the Poisson GLMM example:

```
> glmm.model.up <- function() {
+   for (i in 1:n) {
+     Y[i] ~ dpois(lambda[i])
+     lambda[i] <- exp(alpha[i] +
+       inprod(X[i,], beta[1,]))
+     alpha[i] ~ dnorm(0, 1/sigma^2)
+   }
+   for (j in 1:np) {
+     beta[1,j] ~ dnorm(pr[j,1], pr[j,2])
+   }
+   log.sigma ~ dnorm(pr[(np+1),1], pr[(np+1),2])
+   sigma <- exp(log.sigma)
+   tau <- 1 / pow(sigma, 2)
+ }
```

We also define a function to update the priors. The function returns values for flat prior specification in the first iteration, and uses the updated posterior means (via the `coef` method) and data cloning standard errors (via the `dcsd` method) in the rest, because priors that have large probability mass near the maximum likelihood estimate require fewer clones to achieve the desired accuracy.

```
> upfun <- function(x) {
+   if (missing(x)) {
+     np <- ncol(X)
+     return(cbind(rep(0, np+1),
+       rep(0.001, np+1)))
+   } else {
+     ncl <- nclones(x)
+     if (is.null(ncl))
+       ncl <- 1
+     par <- coef(x)
+     se <- dcsd(x)
+     log.sigma <- mcmcapply(x[, "sigma"], log)
+     par[length(par)] <- mean(log.sigma)
+     se[length(se)] <- sd(log.sigma) * sqrt(ncl)
+     return(cbind(par, se))
+   }
+ }
```

Finally, we define prior specifications as part of the data ("pr"), and provide the updating function in the `dc.fit` call:

```
> updat <- list(Y = Y, X = X, n = n,
+ np = ncol(X), pr = upfun())
> k <- c(1, 5, 10, 20)
> dcmmod <- dc.fit(updat, c("beta", "sigma"),
+ glmm.model.up, n.clones = k, n.iter = 1000,
+ multiply = "n", unchanged = "np",
+ update = "pr", updatefun = upfun)
```

```
> summary(dcmmod)

Iterations = 1001:2000
Thinning interval = 1
Number of chains = 3
Sample size per chain = 1000
Number of clones = 20
```

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

```

      Mean      SD DC SD Naive SE
beta[1]  1.894 0.0368 0.164 0.000671
beta[2] -1.082 0.0734 0.328 0.001341
sigma    0.278 0.0256 0.114 0.000467
Time-series SE R hat
beta[1]      0.00259 1.01
beta[2]      0.00546 1.01
sigma        0.00194 1.04

```

- Quantiles for each variable:

```

      2.5%  25%  50%  75%  97.5%
beta[1]  1.823 1.869 1.89 1.920 1.964
beta[2] -1.230 -1.133 -1.08 -1.029 -0.943
sigma    0.226 0.260 0.28 0.296 0.323

```

The summary contains data cloning standard errors (DC SD) and  $\hat{R}$  values for MCMC chain convergence (Gelman and Rubin, 1992).

## Diagnostics

We can see how the increase in the number of clones affects our inferences on single nodes by using the `dctable` function. This function retrieves the information stored during the iterative fitting process (or can be used to compare more than one fitted model). Only the last MCMC object is returned by `dc.fit`, but descriptive statistics of the posterior distribution are stored in each step (Figure 1). The asymptotic convergence can be visually evaluated by plotting the posterior variances scaled by the variance for the model at  $k = 1$  (or the smallest  $k$ ). If scaled variances are decreasing at a  $1/k$  rate and have reached a lower bound (say  $< 0.05$ ), the data cloning algorithm has converged. If scaled variances are not decreasing at the proper rate, that might indicate identifiability issues (Lele et al., 2010). On the log scale, this graph should show an approximately linear decrease of  $\log(\text{scaled variance})$  vs.  $\log(k)$  for each parameter (Figure 2).

```

> dct <- dctable(dcmmod)
> plot(dct)

> plot(dct, type="log.var")

```

Lele et al. (2010) introduced diagnostic measures for checking the convergence of the data cloning algorithm which are based on the joint posterior distribution and not only on single parameters. These include calculating the largest eigenvalue of the posterior variance covariance matrix (`lambda.max.diag`), or calculating the mean squared error and another correlation-like fit statistic ( $r^2$ ) based on a  $\chi^2$  approximation (`chisq.diag` with a `plot` method). The maximum eigenvalue reflects the degeneracy of the pos-

terior distribution, while the two fit measures reflect the adequacy of the normal approximation. All three statistics should converge to zero as  $k$  increases. If this happens, different prior specifications are no longer influencing the results (Lele et al., 2007, 2010).

These measures and multivariate  $\hat{R}$  values for MCMC chain convergence (Brooks and Gelman, 1997) are calculated during the iterations by `dc.fit` as well, and can be retrieved by the function `dcdiag`:

```

> dcdiag(dcmmod)

      n.clones lambda.max ms.error r.squared r.hat
1           1   0.11538   0.1282   0.02103  1.66
2           5   0.02225   0.0229   0.00277  1.02
3          10   0.01145   0.0383   0.00612  1.01
4          20   0.00643   0.0241   0.00173  1.03

```

The data cloning algorithm requires that MCMC chains are properly mixed and the posterior distribution is nearly degenerate multivariate normal. These requirements have been satisfied in the case of the Poisson GLMM model.  $\hat{R}$  values show better mixing properties of the MCMC chains with higher  $k$  values, and in this example it is expected, because we have used informative priors near the maximum likelihood estimates for the cases  $k > 1$ .

The functions `dctable` and `dcdiag` can be used to determine the number of clones required for a particular model and data set. Also, these diagnostic functions can alert the modeller when the model contains non-identifiable parameters. Lele et al. (2010) gives several examples; here we consider the normal-normal mixture:

$$\mu_i \sim \text{normal}(\gamma, \tau^2)$$

$$Y_i | \mu_i \sim \text{normal}(\mu_i, \sigma^2)$$

where the parameters  $(\gamma, \sigma^2 + \tau^2)$  are known to be identifiable, but  $(\gamma, \sigma^2, \tau^2)$  are not.

We simulate random observations under this model ( $\gamma = 2.5, \sigma = 0.2, \tau = 0.5$ ) and fit the corresponding BUGS model:

```

> gamma <- 2.5
> sigma <- 0.2
> tau <- 0.5
> set.seed(2345)
> mu <- rnorm(n, gamma, tau)
> Y <- rnorm(n, mu, sigma)
> nn.model <- function() {
+   for (i in 1:n) {
+     Y[i] ~ dnorm(mu[i], prec1)
+     mu[i] ~ dnorm(gamma, prec2)
+   }
+   gamma ~ dnorm(0, 0.001)
+   log.sigma ~ dnorm(0, 0.001)
+   sigma <- exp(log.sigma)
+   prec1 <- 1 / pow(sigma, 2)
+   log.tau ~ dnorm(0, 0.001)
+   tau <- exp(log.tau)
+   prec2 <- 1 / pow(tau, 2)
+ }
> nndat <- list(Y = Y, n = n)

```

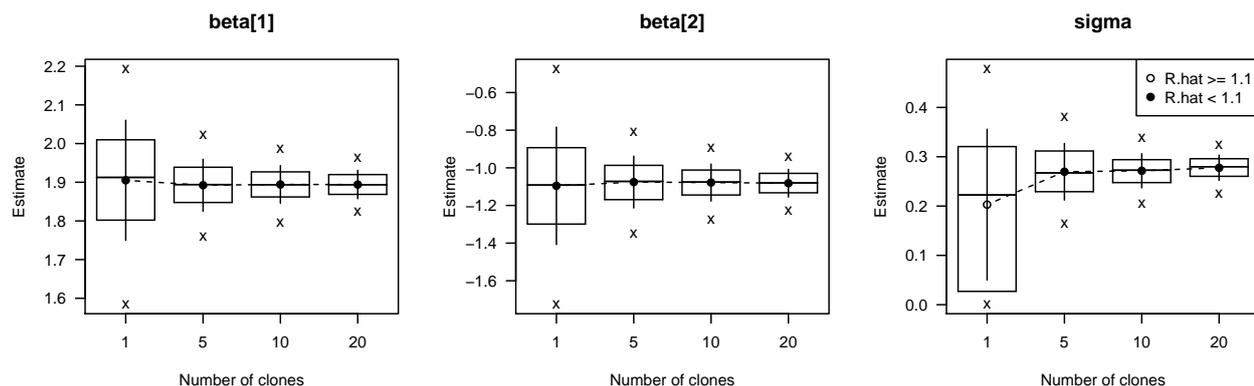


Figure 1: Summary statistics for the Poisson mixed model example. Means are converging towards the maximum likelihood estimates (points), standard errors (vertical lines) are getting shorter with increasing number of clones (95 and 50% quantile ranges and median also depicted).

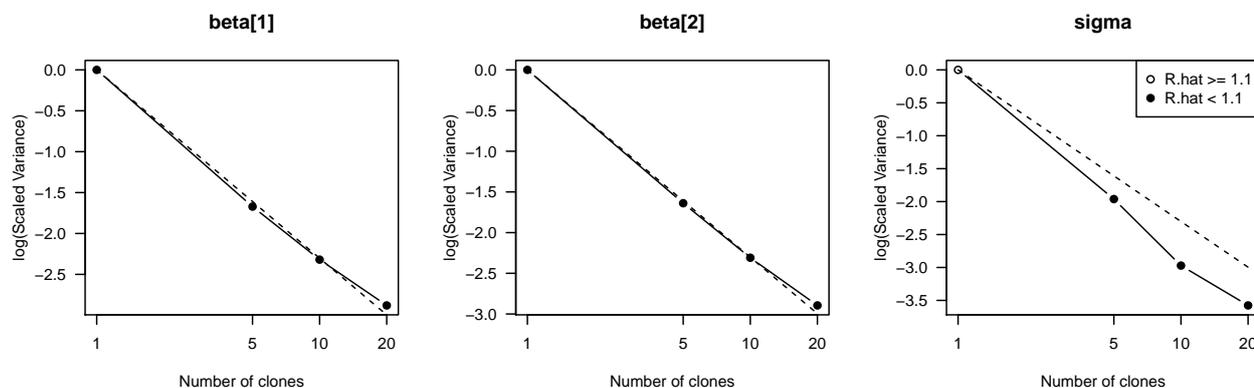


Figure 2: Convergence diagnostics for data cloning based on the Poisson mixed model example. Log of Scaled Variances should decrease linearly with  $\log(k)$ , the scaled variance value close to zero ( $< 0.05$ ) indicates convergence of the data cloning algorithm.

```
> nnmod <- dc.fit(nndat, c("gamma","sigma","tau"),
+ nn.model, n.clones=c(1,10,20,30,40,50),
+ n.iter=1000, multiply="n")
> dcdiag(nnmod)
  n.clones lambda.max ms.error r.squared r.hat
1         1    0.0312  0.508  0.02985  1.18
2        10    0.0364  0.275  0.00355  2.06
3        20    1.2617  1.111  0.13714 50.15
4        30    0.1530  0.753  0.10267 12.91
5        40    1.7972  0.232  0.03770 92.87
6        50    1.8634  0.241  0.04003 15.72
> vars <- mcmcapply(nnmod[,c("sigma","tau")],
+ array)^2
> sigma^2 + tau^2
[1] 0.29
> summary(rowSums(vars))
  Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 0.21  0.23   2.87   3.00   6.04   6.84
```

The high  $r.hat$  and the variable  $\lambda.max$  and fit statistic values that are not converging to zero indicate possible problems with identifiability.

## Inference and prediction

We can explore the results with methods defined for "mcmc.list" objects (many such methods are available in the `coda` package, e.g. `summary`, `plot`, etc.). The `dclone` package adds a few more methods: `coef` returns the mean of the posterior, `dcsd` the data cloning standard errors. Any function returning a scalar statistic can be passed via the `mcmcapply` function:

```
> coef(dcmmod)
beta[1] beta[2]  sigma
 1.894  -1.082  0.278
```

```
> dcsd(dcmmod)

beta[1] beta[2]  sigma
  0.164  0.328  0.114

> mcmcapply(dcmmod, sd) * sqrt(ncolones(dcmmod))
```

```
beta[1] beta[2]  sigma
  0.164  0.328  0.114
```

The asymptotic multivariate normality can be used to get Wald-type confidence intervals for the estimates based on the inverse of the Fisher information matrix. The `vcov` method returns the inverse Fisher information matrix, the `confint` method calculates confidence intervals assuming multivariate normality for MCMC objects with  $k > 1$ :

```
> confint(dcmmod)

          2.5 % 97.5 %
beta[1]  1.5718  2.217
beta[2] -1.7253 -0.438
sigma    0.0534  0.502
```

```
> vcov(dcmmod)

          beta[1] beta[2]  sigma
beta[1]  0.02705 -0.04604 -0.00291
beta[2] -0.04604  0.10783 -0.00156
sigma   -0.00291 -0.00156  0.01308
```

Confidence intervals can also be obtained via parametric bootstrap or based on profile likelihood (Ponciano et al., 2009), but these are not currently available in the `dclone` package and often require substantial user intervention.

These methods are handy when we make predictions. We can use the maximum likelihood estimates and the variance-covariance matrix defined as a multivariate normal node in the BUGS model. For the Poisson mixed model example, the BUGS model for prediction will look like:

```
> glmm.pred <- function() {
+   for (i in 1:n) {
+     Y[i] ~ dpois(lambda[i])
+     lambda[i] <- exp(mu[i])
+     mu[i] <- alpha[i] +
+       inprod(X[i,], beta[1,])
+     alpha[i] ~ dnorm(0, tau)
+   }
+   tmp[1:(np+1)] ~ dmnorm(param[,], prec[,])
+   beta[1,1:np] <- tmp[1:np]
+   sigma <- tmp[(np+1)]
+   tau <- 1 / pow(sigma, 2)
+ }
```

Now we add the estimates and the precision matrix `prec` to the data (the `make.symmetric` function prevents some problems related to matrix symmetry and numerical precision), and define `X` for the predictions (now we simply use the observed values of the covariates). Then do the modeling as usual by sampling the node "lambda":

```
> prec <- make.symmetric(solve(vcov(dcmmod)))
> prdat <- list(X = X, n = nrow(X), np = ncol(X),
+   param = coef(dcmmod), prec = prec)
> prmod <- jags.fit(prdat, "lambda", glmm.pred,
+   n.iter = 1000)
```

## Writing high level functions

Suppose we want to provide a user friendly function to fit the Poisson mixed model with random intercept. We are now modeling the observed abundances (count based on point counts) of the Ovenbird (*Seiurus aurocapilla*) as a function of ecological site characteristics (upland/lowland, `uplow`) and percentage of total human disturbance around the sites (`thd` in the ovenbird data set). Data were collected from 182 sites in the Northern Boreal region of Alberta, Canada, between 2003 and 2008. Data were collected by the Alberta Biodiversity Monitoring Institute and are available at <http://www.abmi.ca>.

Our goal is to determine the effect of human disturbance on Ovenbird abundance, by controlling for site characteristics. But we know that other factors not taken into account, e.g. the amount of deciduous forest, might influence the abundance as well (Hobson and Bayne, 2002). So the random intercept will account for this unexplained environmental variability. The Poisson error component will account for random deviations from expected abundances ( $\lambda_i$ ) and observed counts ( $Y_i$ ) represent a realization of this quantity.

Here is the high level function for fitting the Poisson mixed model built on data cloning with a simple `print`, `summary` and `predict` method:

```
> glmmPois <- function(formula,
+ data = parent.frame(), n.clones, ...) {
+   lhs <- formula[[2]]
+   Y <- eval(lhs, data)
+   formula[[2]] <- NULL
+   rhs <- model.frame(formula, data)
+   X <- model.matrix(attr(rhs, "terms"), rhs)
+   dat <- list(n = length(Y), Y = Y,
+     X = X, np = ncol(X))
+   dcdat <- dclone(dat, n.clones,
+     multiply = "n", unchanged = "np")
+   mod <- jags.fit(dcdat, c("beta", "sigma"),
+     glmm.model, ...)
+   coefs <- coef(mod)
+   names(coefs) <- c(colnames(X),
+     "sigma")
+   rval <- list(coefficients = coefs,
+     call = match.call(),
+     mcmc = mod, y = Y, x = rhs,
+     model = X, formula = formula)
+   class(rval) <- "glmmPois"
+   rval
+ }
> print.glmmPois <- function(x, ...) {
+   cat("glmmPois model\n\n")
+   print(format(coef(x), digits = 4),
```

```

+     print.gap = 2, quote = FALSE)
+   cat("\n")
+   invisible(x)
+ }
> summary.glmmPois <- function(object, ...) {
+   x <- cbind("Estimate" = coef(object),
+     "Std. Error" = dcsd(object$mcmc),
+     confint(object$mcmc))
+   cat("Call:", deparse(object$call,
+     width.cutoff = getOption("width")),
+     "\n", sep="\n")
+   cat("glmmPois model\n\n")
+   printCoefmat(x, ...)
+   cat("\n")
+   invisible(x)
+ }
> predict.glmmPois <- function(object,
+ newdata = NULL, type = c("mu", "lambda", "Y"),
+ level = 0.95, ...){
+   prec <- solve(vcov(object$mcmc))
+   prec <- make.symmetric(prec)
+   param <- coef(object)
+   if (is.null(newdata)) {
+     X <- object$model
+   } else {
+     rhs <- model.frame(object$formula, newdata)
+     X <- model.matrix(attr(rhs, "terms"), rhs)
+   }
+   type <- match.arg(type)
+   prdat <- list(n = nrow(X), X = X,
+     np = ncol(X), param = param, prec = prec)
+   prval <- jags.fit(prdat, type, glmm.pred, ...)
+   a <- (1 - level)/2
+   a <- c(a, 1 - a)
+   rval <- list(fit = coef(prval),
+     ci.fit = quantile(prval, probs = a))
+   rval
+ }

```

Note that the functions `glmm.model` and `glmm.pred` containing the BUGS code are used within these R functions. This implementation works fine, but is not adequate when building a contributed R package, because functions such as `dnorm` and `inprod` are not valid R objects, etc. For R packages, the best way is to represent the BUGS model as a character vector with lines as elements, and put that inside the R function. The `custommodel` function of the `dclone` package can be used to create such character vectors and pass them to other `dclone` functions via the `model` argument.

Now we fit the model for the `ovenbird` data set to estimate the effect of human disturbance on Ovenbird abundance. We fit the model using the function `glmmPois`:

```

> data(ovenbird)
> obmod <- glmmPois(count ~ uplow + thd,
+   ovenbird, n.clones = 5, n.update = 1000,
+   n.iter = 1000)

```

Then print the object and inspect the summary,

```

> obmod

```

```

glmmPois model

(Intercept)  uplowlowland      thd
          2.00312         -1.34242      -0.01647
          sigma
          1.19318

> summary(obmod)

Call:
glmmPois(formula = count ~ uplow + thd, data = ovenbird,
  n.clones = 5, n.update = 1000, n.iter = 1000)

glmmPois model

              Estimate Std. Error   2.5 % 97.5 %
(Intercept)   2.00312    0.13767  1.73328  2.27
uplowlowland -1.34242    0.21503 -1.76387 -0.92
thd           -0.01647    0.00569 -0.02763 -0.01
sigma         1.19318    0.09523  1.00653  1.38

```

Finally predict abundances as a function of disturbance (0–100%) by controlling for site characteristics (Figure 3):

```

> thd <- seq(0, 100, len = 101)
> ndata <- data.frame(uplow = rep("lowland",
+   length(thd)), thd = thd)
> levels(ndata$uplow) <- levels(ovenbird$uplow)
> obpred <- predict(obmod, ndata, "lambda")

```

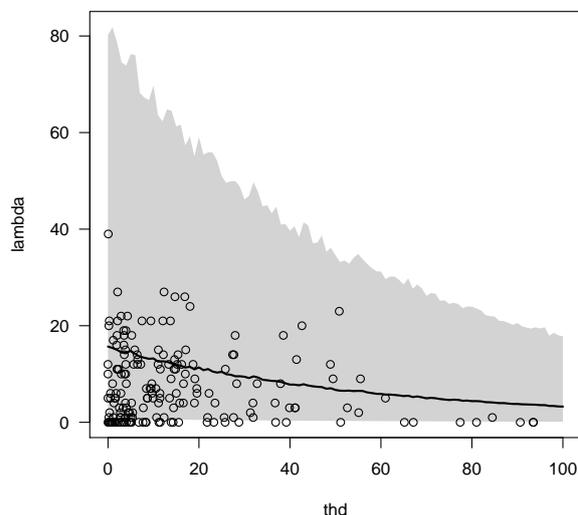


Figure 3: Expected Ovenbird abundance ( $\lambda$ ) as the function of percentage human disturbance ( $thd$ ) based on the Poisson mixed model. Line represents the mean, gray shading indicates 95% prediction intervals. Points are observations.

Ovenbird abundance was significantly higher in upland sites, and human disturbance had a significant negative effect on expected Ovenbird abundance. Unexplained variation ( $\sigma^2 = 1.425 \pm 0.102$  SE) was

substantial, thus the choice of the Poisson mixed model makes sense for this data set.

## Summary

The data cloning algorithm is especially useful for complex models for which other likelihood based computational methods fail. The algorithm also can numerically reveal potential identifiability issues related to hierarchical models. The **dclone** package supports established MCMC software and provides low level functions to help implementing high level estimating procedures to get maximum likelihood inferences and predictions for more specialized problems based on the data cloning algorithm.

## Acknowledgements

Subhash Lele, Khurram Nadeem and Gabor Grothendieck have provided invaluable suggestions and feedback on this work. Comments of Martyn Plummer and two anonymous reviewers greatly improved the quality of the paper. Funding was provided by the Alberta Biodiversity Monitoring Institute and the Natural Sciences and Engineering Research Council.

Péter Sólymos

Alberta Biodiversity Monitoring Institute  
Department of Biological Sciences  
University of Alberta  
solymos@ualberta.ca

## Bibliography

- S. P. Brooks and A. Gelman. General methods for monitoring convergence of iterative simulations. *Journal of Computational and Graphical Statistics*, 7: 434–455, 1997.
- S. P. Brooks and B. J. T. Morgan. Optimization using simulated annealing. *Statistician*, 241–257:44, 1995.
- G. F. Gause. *The struggle for existence*. Wilkins, Baltimore, Maryland, USA, 1934.
- A. Gelman and D. B. Rubin. Inference from iterative simulation using multiple sequences. *Statistical Science*, 7:457–511, 1992.
- A. Gelman, J. Carlin, H. Stern, and D. Rubin. *Bayesian Data Analysis*. CRC Press, Boca Raton, 2 edition, 2003.
- W. Gilks, S. Richardson, and D. Spiegelhalter. *Markov Chain Monte Carlo in Practice*. Chapman & Hall, London, 1996.
- K. A. Hobson and E. M. Bayne. Breeding bird communities in boreal forest of western Canada: Consequences of “unmixing” the mixedwoods. *Condor*, 102:759–769, 2002.
- S. R. Lele, B. Dennis, and F. Lutscher. Data cloning: easy maximum likelihood estimation for complex ecological models using Bayesian Markov chain Monte Carlo methods. *Ecology Letters*, 10:551–563, 2007.
- S. R. Lele, K. Nadeem, and B. Schmuland. Estimability and likelihood inference for generalized linear mixed models using data cloning. *Journal of the American Statistical Association*, 2010. in press.
- D. Lunn, D. Spiegelhalter, A. Thomas, and N. Best. The BUGS project: Evolution, critique and future directions. *Statistics in Medicine*, 28:3049–3067, 2009. with discussion.
- M. Plummer. *JAGS Version 2.0.0 manual (April 26, 2010)*, 2010a. URL <http://mcmc-jags.sourceforge.net>.
- M. Plummer. *rjags: Bayesian graphical models using MCMC*, 2010b. URL <http://mcmc-jags.sourceforge.net>. R package version 2.0.0-2.
- M. Plummer, N. Best, K. Cowles, and K. Vines. *coda: Output analysis and diagnostics for MCMC*, 2010. URL <http://cran.r-project.org/web/packages/coda/index.html>. R package version 0.13-5.
- J. M. Ponciano, M. L. Taper, B. Dennis, and S. R. Lele. Hierarchical models in ecology: confidence intervals, hypothesis testing, and model selection using data cloning. *Ecology*, 90:356–362, 2009.
- P. Sólymos. *dclone: Data Cloning and MCMC Tools for Maximum Likelihood Methods*, 2010. URL <http://cran.r-project.org/packages=dclone>. R package version 1.2-0.
- D. Spiegelhalter, A. Thomas, N. Best, and D. Lunn. *OpenBUGS User Manual, Version 3.0.2, September 2007*, 2007. URL <http://mathstat.helsinki.fi/openbugs/>.
- D. J. Spiegelhalter, A. Thomas, N. G. Best, and D. Lunn. *WinBUGS version 1.4 users manual*. MRC Biostatistics Unit, Cambridge, 2003. URL <http://www.mrc-bsu.cam.ac.uk/bugs/>.
- D. O. Stram and J. W. Lee. Variance components testing in the longitudinal mixed effects model. *Biometrics*, 50:1171–1177, 1994.
- S. Sturtz, U. Ligges, and A. Gelman. R2WinBUGS: A package for running WinBUGS from R. *Journal of Statistical Software*, 12(3):1–16, 2005. URL <http://www.jstatsoft.org>.
- A. Thomas, B. O’Hara, U. Ligges, and S. Sturtz. Making BUGS open. *R News*, 6(1):12–17, 2006. URL <http://cran.r-project.org/doc/Rnews/>.