Markov chain Monte Carlo

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IAP-Workshop 2009 Modeling Association and Dependence in Complex Data

Catholic University of Leuven, Leuven, November, 2009

Outline

Metropolis Hastings

- Recall that MCMC constructs a transition kernel $k(\theta|\theta^{k-1})$ that yields the posterior $p(\theta|\mathbf{y})$ as the stationary distribution of the Markov chain.
- MCMC iterates are generated directly from the kernel:

$$\begin{aligned}
\theta^1|\theta^0 &\sim k(\cdot|\theta^0), \\
\theta^2|\theta^1 &\sim k(\cdot|\theta^1), \\
\theta^3|\theta^2 &\sim k(\cdot|\theta^2), \\
&\vdots \\
\theta^k|\theta^{k-1} &\sim k(\cdot|\theta^{k-1})
\end{aligned}$$

Metropolis Hastings transition kernel

- Let $q(\theta^*|\theta)$ be *any* conditional density. Under kernel $k(\cdot|\theta^{k-1})$,

$$\theta^k|\theta^{k-1} \left\{ \begin{array}{ll} \sim \frac{q(\theta|\theta^{k-1})\rho(\theta^{k-1},\theta)}{\int q(\theta|\theta^{k-1})\rho(\theta^{k-1},\theta)d\theta} & \text{with prob. } 1 - s(\theta^{k-1}) \\ = \theta^{k-1} & \text{with prob. } s(\theta^{k-1}) \end{array} \right\}$$

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- where

$$\rho(\theta^{k-1},\theta) = \min\left\{1, \frac{p(\theta|y)p(\theta)q(\theta^{k-1}|\theta)}{p(\theta^{k-1}|y)p(\theta^{k-1})q(\theta|\theta^{k-1})}\right\}.$$

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- $s(\theta^{k-1})$ is the probability of $\theta^k = \theta^{k-1}$, or of θ^k staying at where it is currently:

$$s(\theta^{k-1}) = 1 - \int_{\theta\in\Theta} q(\theta|\theta^{k-1})\rho(\theta^{k-1},\theta)d\theta.$$

- Simulating the chain is easier than it might first appear. Iterate k is generated from θ^{k-1} according to
  1. Draw $\theta^* \sim q(\cdot|\theta^{k-1})$ independent of $u \sim U(0,1)$.
  2. If $u \leq \rho(\theta^{k-1}, \theta^*) = \min\left\{1, \frac{p(\theta^*|y)p(\theta^*)q(\theta^{k-1}|\theta^*)}{p(\theta^{k-1}|y)p(\theta^{k-1})q(\theta^*|\theta^{k-1})}\right\}$ then $\theta^k = \theta^*$ otherwise $\theta^k = \theta^{k-1}$.

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- In theory, under mild conditions, $\theta^k \xrightarrow{\mathcal{D}} p(\theta|y)$.
- In reality, k is nowhere near ∞ and $q(\cdot|\theta^{k-1})$ needs to be picked in an intelligent way.

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- Also called a random walk chain.
- Used *a lot*. Often $\boldsymbol{\theta}^* \sim N_p(\boldsymbol{\theta}, \mathbf{S})$ for some $\mathbf{S}$. "Tuning" required to get good $\mathbf{S}$.

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- When is $\rho = 1$? This is the case for Gibbs sampling...
- Often $q(\cdot) = N_p(\cdot|\hat{\theta}, \hat{\mathbf{\Sigma}})$.

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\theta_1^k &\sim p(\theta_1 | \theta_2 = \theta_2^{k-1}, \theta_3 = \theta_3^{k-1}, y) \\
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- Generalizes to any $\boldsymbol{\theta} = (\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_p)'$.
- Need to be able to sample from all full conditional distributions!

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- For example $\rho(\boldsymbol{\theta}_1^{k-1}, \boldsymbol{\theta}_1^*|\boldsymbol{\theta}_2^{k-1}, \boldsymbol{\theta}_3^{k-1}, y) = 1$. Show this!

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- Gibbs sampler is sequence of special M-H steps where candidate is always accepted.
- Reviewed and reintroduced by Gelfand and Smith (1990).

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- Prior $\mu \sim N(m, t^{-1})$ independent of $\tau \sim \Gamma(a, b)$.
- Full conditionals:

$$\begin{aligned} \mu|\tau, y &\sim N\left(\frac{n\tau\bar{y} + mt}{n\tau + t}, \frac{1}{n\tau + t}\right) \\ \tau|\mu, y &\sim \Gamma\left(a + 0.5n, b + 0.5\sum_{i=1}^{n}(y_i - \mu)^2\right) \end{aligned}$$

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- MCMC iterates $\{(\mu^k, \tau^k)\}_{k=1}^{M}$ generated by first picking μ^0 and τ^0. Maybe $\mu^0 = m$ and $\tau = a/b$ (why?). Then...

Gibbs sampler...

$$
\begin{aligned}
\mu^1 &\sim N\left(\frac{n\tau^0\bar{y}+mt}{n\tau^0+t}, \frac{1}{n\tau^0+t}\right) \\
\tau^1 &\sim \Gamma\left(a+0.5n, b+0.5\sum_{i=1}^{n}(y_i-\mu^1)^2\right) \\
\mu^2 &\sim N\left(\frac{n\tau^1\bar{y}+mt}{n\tau^1+t}, \frac{1}{n\tau^1+t}\right) \\
\tau^2 &\sim \Gamma\left(a+0.5n, b+0.5\sum_{i=1}^{n}(y_i-\mu^2)^2\right) \\
\mu^3 &\sim N\left(\frac{n\tau^2\bar{y}+mt}{n\tau^2+t}, \frac{1}{n\tau^2+t}\right) \\
\tau^3 &\sim \Gamma\left(a+0.5n, b+0.5\sum_{i=1}^{n}(y_i-\mu^3)^2\right), \text{etc...}
\end{aligned}
$$

In R...

Let's look at fitting a simple normal model to $n = 30$ young rats whose weights were measured weekly for five weeks. Only the first week is considered here.

```
#################################################################################
# Weight of n=30 rats in grams; ll is log posterior distribution for model given in notes
#################################################################################
ll=function(mean,precision,data,a,b,m,t){
 ll=0
 for(i in 1:length(data)){ll=ll+dnorm(data[i],mean,1/sqrt(precision),log=TRUE)}
 ll=ll+dnorm(mean,m,1/sqrt(t),log=TRUE)
 ll=ll+dgamma(precision,a,b,log=TRUE)
}

weight=c(151,145,147,155,135,159,141,159,177,134,160,143,154,171,163,160,142,156,157,
         152,154,139,146,157,132,160,169,157,137,153)
MCtotal=1000
mean=1:MCtotal; precision=1:MCtotal # store MCtotal MCMC iterates here
```

Random walk proposal M-H: R code

```
#############################################################################
# Metropolis-Hastings, random walk proposal for (mean,precision)
#############################################################################
mean[1]=mean(weight); precision[1]=1/var(weight) # starting values
a=0.01; b=0.01; m=150; t=0.1                     # prior values
for(i in 2:MCtotal){
 mean.star=rnorm(1,mean[i-1],1); prec.star=rnorm(1,precision[i-1],0.001)
 rho=exp(ll(mean.star,prec.star,weight,a,b,m,t)-ll(mean[i-1],precision[i-1],weight,a,b,m,t))
 u=runif(1)
 if(u<=rho){ mean[i]=mean.star; precision[i]=prec.star }
 if(u>rho) { mean[i]=mean[i-1]; precision[i]=precision[i-1] }
}

sum(mean[2:MCtotal]-mean[1:(MCtotal-1)]!=0)/(MCtotal-1) # accept rate for (mu,tau)
plot(mean,precision) # Monte Carlo estimate of posterior
quantile(mean,c(0.025,0.5,0.975)) # 95% CI and posterior median mu
quantile(precision,c(0.025,0.5,0.975)) # 95% CI and posterior median tau
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Independence proposal M-H: R code

```
#############################################################################
# Metropolis-Hastings, independence proposal for (mean,precision)
#############################################################################
mean[1]=mean(weight); precision[1]=1/var(weight) # starting values
a=0.01; b=0.01; m=150; t=0.1                     # prior values
for(i in 2:MCtotal){
 mean.star=rnorm(1,152,2); prec.star=rnorm(1,0.008,0.002)
 rho=exp(ll(mean.star,prec.star,weight,a,b,m,t)-ll(mean[i-1],precision[i-1],weight,a,b,m,t)
     -dnorm(mean.star,152,2,log=TRUE)+dnorm(mean[i-1],152,2,log=TRUE)
     -dnorm(prec.star,0.008,0.002,log=TRUE)+dnorm(precision[i-1],0.008,0.002,log=TRUE))
 u=runif(1)
 if(u<=rho){ mean[i]=mean.star; precision[i]=prec.star }
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Gibbs sampling: R code

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# Gibbs sampler for (mean,precision)
#############################################################################
mean[1]=mean(weight); precision[1]=1/var(weight) # starting values
a=0.01; b=0.01; m=150; t=0.1; n=length(data)     # prior values
for(i in 2:MCtotal){
 mu.var=1/(n*precision[i-1]+t)
 mu.mean=mu.var*(n*precision[i-1]*mean(weight)+m*t)
 mean[i]=rnorm(1,mu.mean,sqrt(mu.var))
 precision[i]=rgamma(1,a+0.5*n,b+0.5*sum((weight-mean[i])**2))
}

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- WinBUGS suffers in terms of analyzing the output though. Complex analyses require imputting WinBUGS output into R or SAS anyway.
- After today, all examples will be almost exclusively in DPpackage, but it's good to know about BUGS, BayesX, etc.

How does WinBUGS sample the posterior?

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- Bad point: there are precious few practical ways to improve mixing in a Gibbs sampler.

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- Metropolis step. (Tierney, 1994). Unrestricted range.

WinBUGS code

WinBUGS code looks a lot like R or S-plus. Here's code for fitting a simple normal model to $n = 30$ young rats whose weights were measured weekly for five weeks. Only the first week is considered here.

```
model{
 for(i in 1:n){ y[i] ~ dnorm(mu, tau) }
 mu ~ dnorm(0,0.001)
 tau ~ dgamma(0.001,0.001)
}

list(mu=150, tau=0.1)  # starting values

list(y=c(151,145,147,155,135,159,141,159,177,134,160,143,
154,171,163,160,142,156,157,152,154,139,146,157,
132,160,169,157,137,153), n=30)  # data
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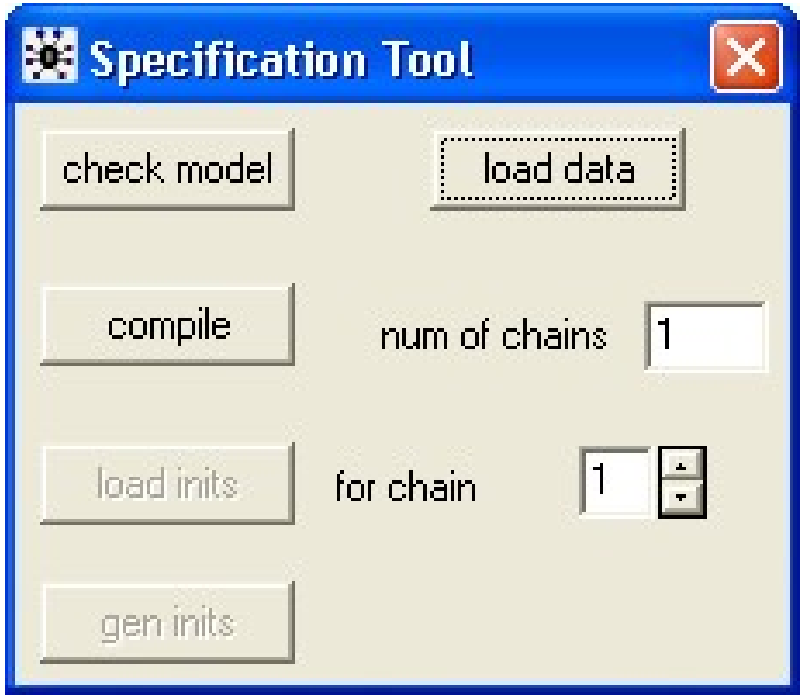
- Finally, the data is `list`ed. Data can also be listed one or more columns. Again, more on this later.

WinBUGS tools:

There are three main tools you will use frequently. The winBUGS manual explains the use of each in detail. Under **Model** in the toolbar, pick **Specification...** and the **Specification Tool** appears:



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- If the model is okay, next double click on the `list` that holds the data and click load data. WinBUGS will tell you "data loaded" if there were no problems, otherwise you'll find out something is not right with your `data` list or perhaps your `model`.

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- Click compile.

Starting values

- You can either provide intelligent starting values for the Markov chain or let WinBUGS generate them from the prior. If the prior is vague, the former is a good idea. Double click on the `list` that holds the starting values, then click load inits. You are ready to generate samples!

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- Note: you can also provide *partial* starting values, for example just the mean value in this example. This is handy in random effects models where there may be several hundred random effects. Click gen inits to simulate initial values for remaining parameters.

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- The path of the Markov chain can be monitored by clicking on trace button.

The **Update tool**

- Click the update button in the **Update Tool**. The trace plot will dynamically show the actual MCMC iterates being generated with each click of update in the **Update Tool**.

  Click update several times. Be careful, this can be quite hypnotic. Update the Markov chain until 11000 iterates are generated, i.e. until 11000 is in the **iteration** box. You can update more or less than 1000 at a time by typing a different value in the **updates** box.

- A *burn in* value can be specified in the **beg** box of the **Sample Monitor Tool**. Type “1001” in this box. We will discuss the notion of burn in carefully later, but roughly, we are throwing out the first 1000 iterates to eliminate any dependence posterior inferences might have on our starting values.

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- Go back to the **Sample Monitor Tool** and click on stats to get your posterior estimates.

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- Under **Help** you can find **Examples Vol I** and **Examples Vol II**. These examples are an excellent source of models, data, and ideas.
- The error codes in WinBUGS are mysterious. A few are explained in the manual. The most common errors have to do with defining nodes twice and when WinBUGS has trouble sampling, typically with censored data.
- WinBUGS 1.4 now gives the user some leeway in "tweaking" M-H burn-in values, allows for blocked updates, and also allows choosing update options. This can improve convergence dramatically.

et cetera...

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- `history` gives entire iteration history for all nodes being monitored. Good for assessing burn-in and convergence to posterior.
- `density` gives (marginal) posterior kernel-smoothed density estimates.
- `stats` gives posterior summary statistics.
- `coda` gives the actual Gibbs iterates for use in other programs.
- `quantiles` gives “running quantiles” useful for assessing burn-in and convergence.

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- auto cor gives the ACF for each node. Useful for determining how well the chain is mixing and/or determining thinning values.
- **Inference** then **DIC...** ultimately gives the *deviance information driterion* for a model. Basically a measure of how "complex" a model is along with an overall measure of fit. This statistic can be informally used to compare models and provides a measure of model fit penalized by complexity much in the same manner as the AIC or BIC.