Practical Considerations for WinBUGS Users

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Issues in MCMC use for Bayesian model fitting

- Deciding how many chains to run
- Choosing initial values
- Assessing whether sampler has "converged"
- Choosing model parameterizations and MCMC algorithms that will lead to convergence in a reasonable amount of time
- Using correlated samples for estimation and inference
  - adjusting estimates of standard errors

Using MCMC for Bayesian inference (idealized sequence!)

- specify a Bayesian model
- construct a Markov chain whose target distribution is the joint posterior distribution of interest
- run the chain until output converges in distribution to draws from the target distribution
- base inference regarding unknown quantities in model on output of subsequent iterations of the chain

Convergence assessment

- How many initial iterations need to be discarded in order that remaining samples are drawn from a distribution close enough to the true stationary distribution to be usable for estimation and inference?
  - "burn-in"
- Has the sampler traversed the entire support of the posterior distribution?
  - "support"
- How many (dependent) samples are needed in order to provide the desired precision in estimation and inference?
  - "variance"

Using MCMC for Bayesian inference (more realistic sequence)

1. specify a Bayesian model
2. construct a Markov chain whose target distribution is the joint posterior distribution of interest
3. run one or more chain(s) as long as you can stand it
4. assess convergence
   - retune model parameterization, Markov chain algorithm, priors, etc.
   - or increase number of iterations
   - return to step 3 or continue to step 5 as appropriate
5. base inference regarding unknown quantities in model on portion of output identified during convergence assessment

Suggested steps in WinBUGS

- run a minimum of 3 parallel chains from overdispersed initial values
- monitor all unknown model quantities beginning from the first iteration
  - if not feasible to monitor all, then monitor at least representative samples of each *kind* of parameter
  - let WinBUGS help you determine how many early iterations to throw out for burn-in
- inspect the following WinBUGS output to evaluate sampler performance
  - history plots
  - autocorrelation plots
  - Brooks, Gelman, and Rubin diagnostic
  - Monte Carlo errors
- decide whether to
  - discard some initial burn-in iterations and use remaining sampler output for inference
  - or take some corrective action
    * run more iterations
    * change parameterization of model

Initial values

- Initial values are not like priors!
  - Priors are part of the model specification.
  - Priors must *not* be derived from the current dataset.
  - Initial values are part of the computing process.
  - Initial values can be derived from the current dataset.
- Choosing initial values
  - Run more than one chain with initial values selected to give you information about sampler performance.
  - Initial values may be generated from priors.
  - Initial values may be based on frequentist estimates.
    * e.g. mle, mle - 4 standard errors, mle + 4 standarde rrors

- Initial values may be chosen systematically to represent extreme regions of the parameter space.
- Initial values must be specified for variance components
  - WinBUGS usually can automatically generate initial values for other parameters
  - But it's often advantageous to specify even those WinBUGS can generate

History plots: Early graphical methods of convergence assessment

- trajectories of sampler output for each model unknown
- can quickly reveal failure to reach stationarity
- can give qualitative information about sampler behavior
- cannot confirm that any of the three aspects of convergence have occurred

Convergence diagnostics

- Statistical methods applied to the *output* of MCMC samplers in an effort to assess convergence.
- Gelman and Rubin (1992): Early diagnostic comparing variance between/within multiple chains
  - requires running multiple parallel chains from overdispersed initial values
  - applied to each univariate quantity of interest
  - always applied to last half of sampler output (i.e., assumes that first half of sampler output is burn-in)
  - computes "potential scale reduction factor": the factor by which the scale parameter of the estimated marginal distribution might shrink if sampling were continued indefinitely

- Brooks and Gelman (1998)
  - corrected computation of Gelman and Rubin (1992) potential scale reduction factor
  - propose a multivariate potential scale reduction factor to simultaneous assessment of convergence of all model unknowns
  - extended method to other measures besides estimate of posterior variance, particularly widths of credible sets

Gelman-Rubin convergence diagnostic in WinBUGS

- obtain in graphical form using "GRdiag" button on Inference menu
- plots the following versus iteration
  - width of central 80% interval constructed from pooled runs (plotted in green)
  - average width of 80% intervals constructed from each run (plotted in blue)
  - ratio $R = \frac{pooled}{within}$ in red
- both widths are scaled so maximum values are 1
- convert plot to numeric output by
  - double-clicking on plot
  - then control-left-mouse-click on the window)
- want to see:
  - BGR R (value of numeric diagnostic) close to 1
  - convergence of both pooled- and within-interval widths to stability

Monte Carlo error

- on "Stats" output
- similar to standard error of the mean, but adjusted for autocorrelated sample
- it will get smaller as more iterations are run
- use it to guide your decision as to how many iterations you need to run after burn-in is done

Software for MCMC convergence assessment

- Rudimentary facilities built into WinBUGS
- BOA (Bayesian Output Analysis)
  - developed in 1999 by Brian Smith of University of Iowa
  - includes all the convergence diagnostics/output analysis features in WinBUGS and much more
  - available for free download from

    `http://www.public-health.uiowa.edu/BOA/`
  - use "Coda" button on WinBUGS Inference menu to export WinBUGS output to a file that BOA can process
- downside: by definition canned software cannot perform problem-specific convergence assessment procedures

Recommendations

- Learn as much as possible about model before ever running an MCMC sampler.
  - maximum likelihood
  - noniterative Bayesian approximations
  - numerical mode-finding
  - simplified models
- Pre-assess burn-in time if possible; then run a single chain.
  - how to do this is beyond scope of this course
- If this is not possible, run a small number $(3-5?)$ of parallel chains from overdispersed starting values.
- Monitor
  - all types of model parameters, not only parameters of substantive interest
  - sample paths graphically
  - autocorrelations
  - cross-correlations between parameters
- Apply more than one diagnostic, including one or more that uses information about the specific model.

Conclusions

- MCMC methods have enabled the fitting of complex, realistic models.
- Use of MCMC methods requires careful attention to
  - model parameterization
  - MCMC sampler algorithms
  - choice of initial values
  - convergence assessment
  - output analysis
- Ongoing research in theoretical verification of convergence, MCMC acceleration, and exact sampling holds great promise.