

Bayesian Networks in Educational Assessment

Estimating Parameters with MCMC

Roy Levy
Arizona State University
Roy.Levy@asu.edu

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MCMC 1

Bayesian Inference: Expanding Our Context

MCMC 2

Posterior Distribution

Posterior distribution for **unknowns** given **knowns** is

$$p(\text{unknowns} | \text{knowns}) \propto p(\text{knowns} | \text{unknowns}) p(\text{unknowns})$$

Inference about examinee latent variables (θ) given observables (\mathbf{x})

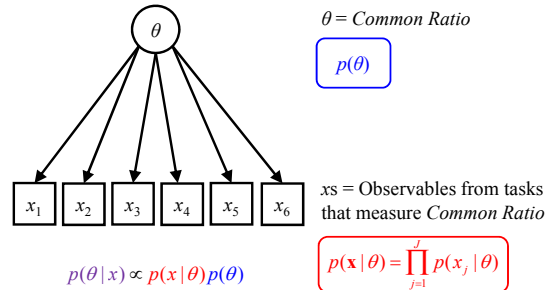
$$p(\theta | \mathbf{x}) \propto p(\mathbf{x} | \theta) p(\theta)$$

Example: ACED Bayes Net Fragment for *Common Ratio*

- θ = Common Ratio
- \mathbf{x} = Observables from tasks that measure *Common Ratio*

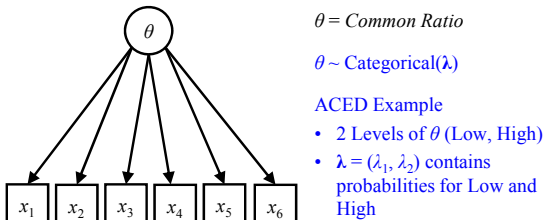
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Bayes Net Fragment



MCMC 4

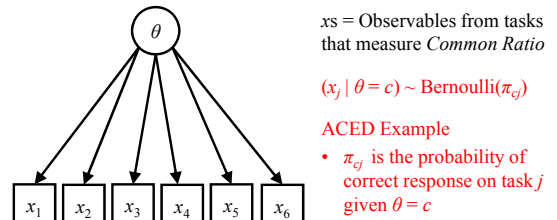
Probability Distribution for the Latent Variable



	θ (Common Ratio)	
	1	2
Prob.	λ_1	λ_2

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Probability Distribution for the Observables



	$p(x_j \theta)$	
θ	0	1
1	$1 - \pi_{1j}$	π_{1j}
2	$1 - \pi_{2j}$	π_{2j}

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Bayesian Inference

$$p(\theta | \mathbf{x}) \propto p(\mathbf{x} | \theta) p(\theta)$$

If the λ s and π s are unknown, they become subject to posterior inference too

θ (Common Ratio)		
	1	2
Prob.	λ_1	λ_2

$p(x_j \theta)$		
θ	0	1
1	$1 - \pi_{1j}$	π_{1j}
2	$1 - \pi_{2j}$	π_{2j}

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Bayesian Inference

$$p(\theta | \mathbf{x}) \propto p(\mathbf{x} | \theta) p(\theta)$$

$p(x_j \theta)$		
θ	0	1
1	$1 - \pi_{1j}$	π_{1j}
2	$1 - \pi_{2j}$	π_{2j}

A convenient choice for prior distribution is the beta distribution

$$\pi_{cj} \sim \text{Beta}(\alpha_{\pi_c}, \beta_{\pi_c})$$

ACED Example: $\pi_{1j} \sim \text{Beta}(1, 1)$ $\pi_{2j} \sim \text{Beta}(1, 1)$

For first task, constrain ($\pi_{21} > \pi_{11}$) to resolve indeterminacy in the latent variable and avoid label switching

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Bayesian Inference

$$p(\theta | \mathbf{x}) \propto p(\mathbf{x} | \theta) p(\theta)$$

A convenient choice for the prior distribution is the Dirichlet distribution

$$\lambda \sim \text{Dirichlet}(\alpha_\lambda) \quad \alpha_\lambda = (\alpha_{\lambda_1}, \alpha_{\lambda_2})$$

which generalizes the Beta distribution to the case of multiple categories

ACED Example: $\lambda = (\lambda_1, \lambda_2) \sim \text{Dirichlet}(1, 1)$

θ (Common Ratio)		
	1 (Low)	2 (High)
Prob.	λ_1	λ_2

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Model Summary

$\theta_i \sim \text{Categorical}(\lambda)$

$\lambda \sim \text{Dirichlet}(1, 1)$

$(x_{ij} | \theta_i = c) \sim \text{Bernoulli}(\pi_{cj})$

$\pi_{11} \sim \text{Beta}(1, 1)$

$\pi_{21} \sim \text{Beta}(1, 1) \quad I(\pi_{21} > \pi_{11})$

$\pi_{cj} \sim \text{Beta}(1, 1)$ for others obs.

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JAGS Code

JAGS Code

MCMC 11

JAGS Code

```

for (i in 1:n){
  for(j in 1:J){
    x[i,j] ~ dbern(pi[theta[i],j])
  }
}

```

Referencing the table for π s in terms of $\theta = 1$ or 2

$p(x_j \theta)$		
θ	0	1
1	$1 - \pi_{1j}$	π_{1j}
2	$1 - \pi_{2j}$	π_{2j}

MCMC 12

JAGS Code

```
pi[1,1] ~ dbeta(1,1)          pi_11 ~ Beta(1, 1)
pi[2,1] ~ dbeta(1,1) T(pi[1,1],) pi_21 ~ Beta(1, 1) I(pi_21 > pi_11)

for(c in 1:C){                pi_cj ~ Beta(1, 1) for remaining observables
  for(j in 2:J){
    pi[c,j] ~ dbeta(1,1)
  }
}
```

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JAGS Code

```
for (i in 1:n){                theta_i ~ Categorical(lambda)
  theta[i] ~ dcat(lambda[])
}

lambda[1:C] ~ ddirch(alpha_lambda[])   lambda ~ Dirichlet(1, 1)
for(c in 1:C){
  alpha_lambda[c] <- 1
}
```

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Markov Chain Monte Carlo

MCMC 15

Estimation in Bayesian Modeling

- Our “answer” is a posterior distribution
 - All parameters treated as random, not fixed
- Contrasts with frequentist approaches to inference, estimation
 - Parameters are fixed, so estimation comes to finding the single best value
 - “Best” here in terms of a criterion (ML, LS, etc.)
- Peak of a mountain vs. mapping the entire terrain of peaks, valleys, and plateaus (of a landscape)

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What's In a Name?

Markov chain *Monte Carlo*

- Construct a sampling algorithm to *simulate* or *draw from* the posterior.
- Collect many such draws, which serve to empirically approximate the posterior distribution, and can be used to empirical approximate summary statistics.

Monte Carlo Principle:

Anything we want to know about a random variable θ can be learned by sampling many times from $f(\theta)$, the density of θ .

-- Jackman (2009)

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What's In a Name?

Markov *chain* Monte Carlo

- Values really generated as a sequence or chain
- t denotes the step in the chain
- $\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \dots, \theta^{(t)}, \dots, \theta^{(T)}$
- Also thought of as a time indicator

Markov chain Monte Carlo

- Follows the Markov property...

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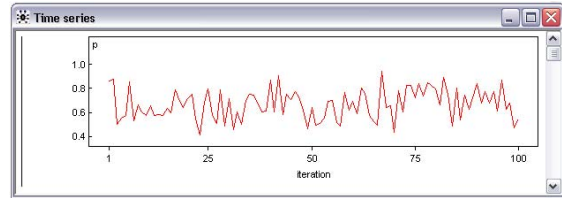
The Markov Property

- Current state depends on previous position
 - Examples: weather, checkers, baseball counts & scoring
- Next state conditionally independent of past, given the present
 - Akin to a full mediation model
- $p(\theta^{t+1} | \theta^0, \theta^{t-1}, \theta^{t-2}, \dots) = p(\theta^{t+1} | \theta^t)$



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Visualizing the Chain: Trace Plot



MCMC 20

Markov Chain Monte Carlo

- Markov chains are *sequences of numbers* that have the Markov property
 - Draws in cycle $t+1$ depend on values from cycle t , but given those not on previous cycles (Markov property)
- Under certain assumptions Markov chains reach *stationarity*
- The collection of values converges to a distribution, referred to as a stationary distribution
 - Memoryless: It will “forget” where it starts
 - Start anywhere, will reach stationarity if regularity conditions hold
 - For Bayes, set it up so that this is the posterior distribution
- Upon convergence, samples from the chain approximate the stationary (posterior) distribution

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Assessing Convergence

MCMC 22

Diagnosing Convergence

- With MCMC, convergence to a *distribution*, not a point
- ML:
 - Convergence is when we’ve reached the highest point in the likelihood,
 - The highest peak of the mountain
- MCMC:
 - Convergence when we’re sampling values from the correct distribution,
 - We are mapping the entire terrain accurately

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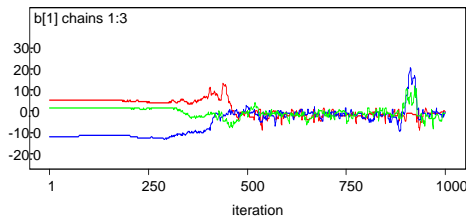
Diagnosing Convergence

- A properly constructed Markov chain is guaranteed to converge to the stationary (posterior) distribution...eventually
- Upon convergence, it will sample over the full support of the stationary (posterior) distribution...over an ∞ number of draws
- In a finite chain, no guarantee that the chain has converged or is sampling through the full support of the stationary (posterior) distribution
- Many ways to diagnose convergence
- Whole software packages dedicated to just assessing convergence of chains (e.g., R packages ‘coda’ and ‘boa’)

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Gelman & Rubin's (1992) Potential Scale Reduction Factor (PSRF)

- Run **multiple** chains from dispersed starting points
- Suggest convergence when the chains come together
- If they all go to the same place, it's probably the stationary distribution



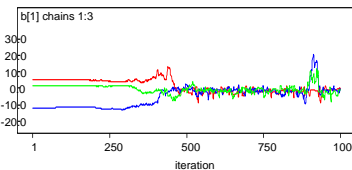
mCMC 25

Gelman & Rubin's (1992) Potential Scale Reduction Factor (PSRF)

- An analysis of variance type argument
- $PSRF$ or $R =$

$$\frac{\text{Total Variance}}{\text{Within Chain Variance}} = \frac{\text{Between Chain Variance} + \text{Within Chain Variance}}{\text{Within Chain Variance}}$$

- If there is substantial between-chain variance, will be $\gg 1$



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Gelman & Rubin's (1992) Potential Scale Reduction Factor (PSRF)

- Run **multiple** chains from dispersed starting points
- Suggest convergence when the chains come together
- Operationalized in terms of partitioning variability
- Run multiple chains for $2T$ iterations, discard first half
- Examine between and within chain variability
- Various versions, modifications suggested over time

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Potential Scale Reduction Factor (PSRF)

- For any θ , for any chain c the within-chain variance is

$$W_c = \frac{1}{T-1} \sum_{t=1}^T (\theta_{(c)}^{(t)} - \bar{\theta}_{(c)})^2$$

- For all chains, the pooled within-chain variance is

$$W = \frac{1}{C} \sum_{c=1}^C W_c = \frac{1}{C(T-1)} \sum_{c=1}^C \sum_{t=1}^T (\theta_{(c)}^{(t)} - \bar{\theta}_{(c)})^2$$

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Potential Scale Reduction Factor (PSRF)

- The between-chain variance is

$$B = \frac{T}{C-1} \sum_{c=1}^C (\bar{\theta}_{(c)} - \bar{\theta})^2$$

- The estimated variance is

$$\hat{V}ar(\theta) = (T-1/T)W + (1/T)B$$

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Potential Scale Reduction Factor (PSRF)

- The potential scale reduction factor is

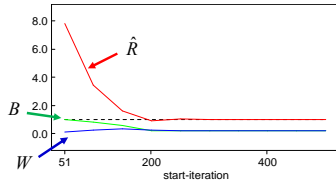
$$\hat{R} = \sqrt{\frac{\hat{V}ar(\theta)}{W}}$$

- If close to 1 (e.g., < 1.1) for all parameters, can conclude convergence

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Potential Scale Reduction Factor (PSRF)

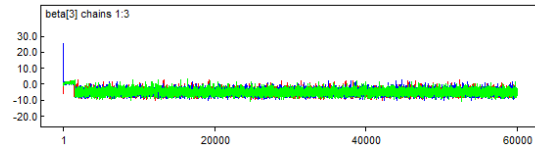
- Examine it over “time”, look for $\hat{R} \rightarrow 1$, stability of B and W
- If close to 1 (e.g., < 1.2 , or < 1.1) can conclude convergence



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Assessing Convergence: No Guarantees

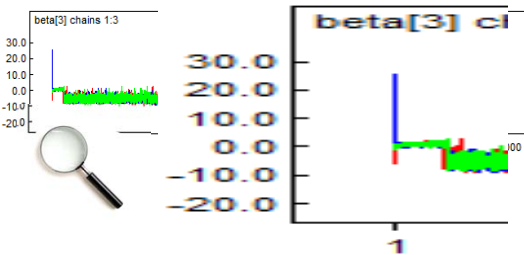
Multiple chains coming together does not guarantee they have converged



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Assessing Convergence: No Guarantees

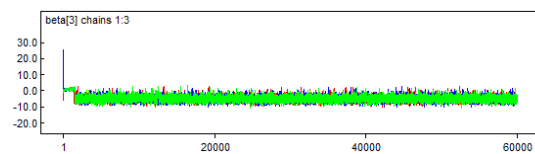
multiple chains come together does not guarantee they have converged



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Assessing Convergence: No Guarantees

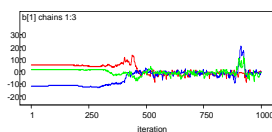
Multiple chains coming together does not guarantee they have converged



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Assessing Convergence

- Recommend running multiple chains far apart and determine when they reach the same “place”
 - PSRF criterion an approximation to this
 - Akin to starting ML from different start values and seeing if they reach the same maximum
 - Here, convergence to a distribution, not a point
- A chain hasn't converged until **all** parameters converged
 - Brooks & Gelman multivariate PSRF



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Serial Dependence

MCMC 36

Serial Dependence

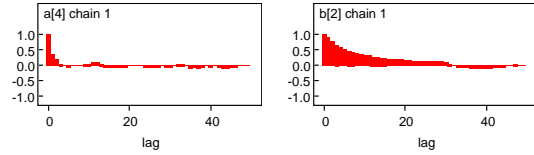
- Serial dependence between draws due to the dependent nature of the draws (i.e., the Markov structure)
- $p(\theta^{(t+1)} | \theta^{(t)}, \theta^{(t-1)}, \theta^{(t-2)}, \dots) = p(\theta^{(t+1)} | \theta^{(t)})$



- However there is a *marginal* dependence across multiple lags
- Can examine the autocorrelation across different lags

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Autocorrelation



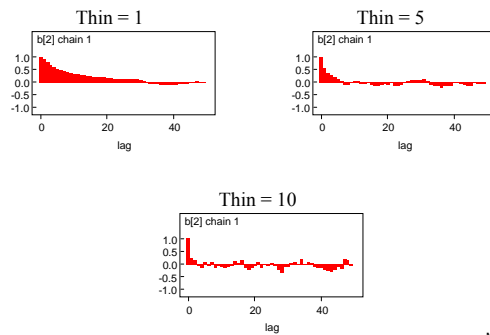
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Thinning

- Can “thin” the chain by dropping certain iterations
- Thin = 1 → keep every iteration
- Thin = 2 → keep every other iteration (1, 3, 5,...)
- Thin = 5 → keep every 5th iteration (1, 6, 11,...)
- Thin = 10 → keep every 10th iteration (1, 11, 21,...)
- Thin = 100 → keep every 100th iteration (1, 101, 201,...)

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Thinning



MCMC 40

Thinning

- Can “thin” the chain by dropping certain iterations
- Thin = 1 → keep every iteration
- Thin = 2 → keep every other iteration (1, 3, 5,...)
- Thin = 5 → keep every 5th iteration (1, 6, 11,...)
- Thin = 10 → keep every 10th iteration (1, 11, 21,...)
- Thin = 100 → keep every 100th iteration (1, 101, 201,...)
- Thinning *does not* provide a better portrait of the posterior
 - A loss of information
- May want to keep, and account for time-series dependence
- Useful when data storage, other computations an issue
 - *I want 1000 iterations, rather have 1000 approximately independent iterations*
- Dependence *within* chains, but none *between* chains

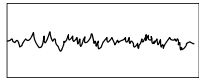
MCMC 41

Mixing

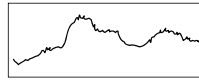
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Mixing

- We don't want the sampler to get "stuck" in some region of the posterior, or ignore a certain area of the posterior
- Mixing refers to the chain "moving" throughout the support of the distribution in a reasonable way



relatively good mixing



relatively poor mixing

MCMC 43

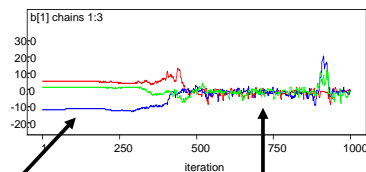
Mixing

- Mixing \neq convergence, but better mixing usually leads to faster convergence
- Mixing \neq autocorrelation, but better mixing usually goes with lower autocorrelation (and cross-correlations between parameters)
- With better mixing, then for a given number of MCMC iterations, get more information about the posterior
 - Ideal scenario is independent draws from the posterior
- With worse mixing, need more iterations to (a) achieve convergence and (b) achieve a desired level of precision for the summary statistics of the posterior

MCMC 44

Mixing

- Chains may mix differently at different times
- Often indicative of an adaptive MCMC algorithm



relatively poor mixing

relatively good mixing

MCMC 45

Mixing

- Slow mixing can also be caused by high dependence between parameters
 - Example: multicollinearity
- Reparameterizing the model can improve mixing
 - Example: centering predictors in regression

MCMC 46

Stopping the Chain(s)

MCMC 47

When to Stop The Chain(s)

- Discard the iterations prior to convergence as *burn-in*
- How many more iterations to run?
 - As many as you want ☺
 - As many as time provides
- Autocorrelation complicates things
- Software may provide the "MC error"
 - Estimate of the sampling variability of the sample mean
 - Sample here is the sample of iterations
 - Accounts for the dependence between iterations
 - Guideline is to go at least until MC error is less than 5% of the posterior standard deviation
- Effective sample size
 - Approximation of how many independent samples we have

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Steps in MCMC in Practice

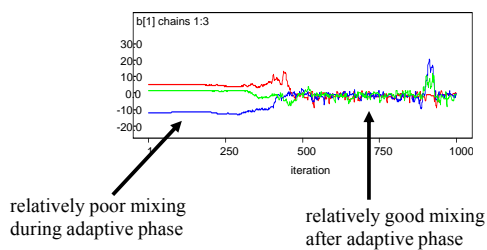
MCMC 49

Steps in MCMC (1)

- Setup MCMC using any of a number of algorithms
 - Program yourself (have fun ☺)
 - Use existing software (BUGS, JAGS)
- Diagnose convergence
 - Monitor trace plots, PSRF criteria
- Discard iterations prior to convergence as *burn-in*
 - Software may indicate a minimum number of iterations needed
 - A lower bound

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Adapting MCMC → Automatic Discard



MCMC 51

Steps in MCMC (2)

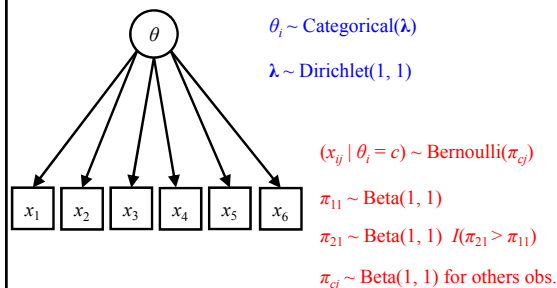
- Run the chain for a desired number of iterations
 - Understanding serial dependence/autocorrelation
 - Understanding mixing
- Summarize results
 - Monte Carlo principle
 - Densities
 - Summary statistics

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ACED Example

MCMC 53

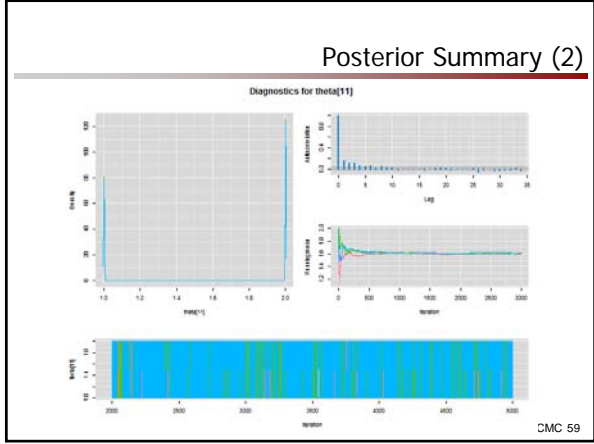
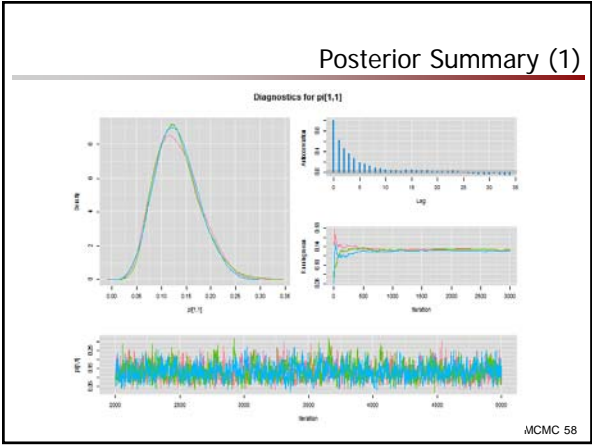
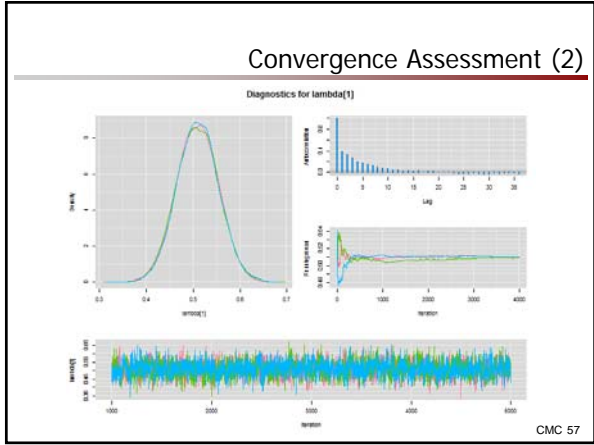
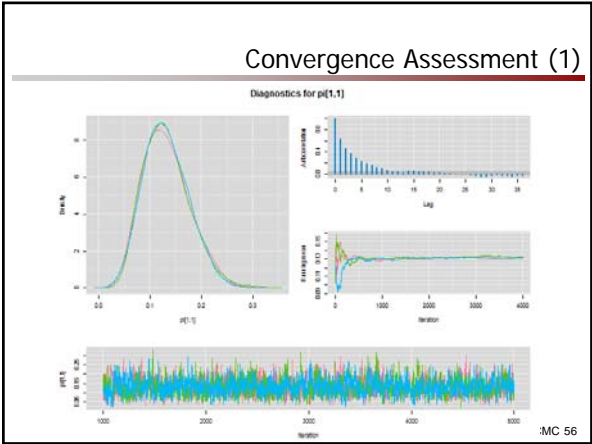
Model Summary



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ACED Example
 See 'ACED Analysis.R' for Running the analysis in R
 See Following Slides for Select Results

MCMC 55



Posterior Summary (3)

	Mean	SD	Naive SE	Time-series SE	0.025	0.25	0.5	0.75	0.975	Median	95% HPD Lower	95% HPD Upper
lambda[1]	0.51	0.04	0	0	0.42	0.48	0.51	0.54	0.6	0.51	0.43	0.6
lambda[2]	0.49	0.04	0	0	0.4	0.46	0.49	0.52	0.58	0.49	0.4	0.57
p[1,1]	0.13	0.04	0	0	0.06	0.1	0.13	0.16	0.23	0.13	0.05	0.22
p[2,1]	0.84	0.04	0	0	0.75	0.81	0.84	0.87	0.91	0.84	0.75	0.92
p[1,2]	0.22	0.05	0	0	0.12	0.18	0.22	0.26	0.33	0.22	0.12	0.33
p[2,2]	0.98	0.02	0	0	0.93	0.97	0.99	0.99	1	0.99	0.94	1
p[1,3]	0.02	0.01	0	0	0	0.01	0.02	0.03	0.06	0.02	0	0.05
p[2,3]	0.19	0.04	0	0	0.12	0.17	0.19	0.22	0.28	0.19	0.12	0.27
p[1,4]	0.03	0.02	0	0	0.01	0.02	0.03	0.04	0.07	0.03	0	0.06
p[2,4]	0.23	0.05	0	0	0.15	0.2	0.23	0.26	0.33	0.23	0.15	0.33
p[1,5]	0.15	0.04	0	0	0.08	0.12	0.15	0.17	0.22	0.15	0.08	0.22
p[2,5]	0.64	0.05	0	0	0.53	0.6	0.64	0.67	0.74	0.64	0.53	0.74
p[1,6]	0.17	0.04	0	0	0.1	0.14	0.17	0.2	0.25	0.17	0.1	0.25
p[2,6]	0.82	0.05	0	0	0.72	0.79	0.82	0.86	0.92	0.82	0.73	0.92
theta[1]	2	0.06	0	0	2	2	2	2	2	2	2	2
theta[2]	1	0.02	0	0	1	1	1	1	1	1	1	1
theta[3]	1	0.01	0	0	1	1	1	1	1	1	1	1
theta[4]	1.97	0.17	0	0	1	2	2	2	2	2	2	2
theta[5]	1.17	0.38	0	0.01	1	1	1	1	2	1	1	2
theta[6]	1	0.01	0	0	1	1	1	1	1	1	1	1
theta[7]	1.01	0.07	0	0	1	1	1	1	1	1	1	1

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Summary and Conclusion

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Summary

- Dependence on initial values is “forgotten” after a sufficiently long run of the chain (memoryless)
- Convergence to a *distribution*
 - Recommend monitoring multiple chains
 - PSRF as approximation
- Let the chain “burn-in”
 - Discard draws prior to convergence
 - Retain the remaining draws as draws from the posterior
- Dependence across draws induce autocorrelations
 - Can thin if desired
- Dependence across draws within and between parameters can slow mixing
 - Reparameterizing may help

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Wise Words of Caution

Beware: MCMC sampling can be dangerous!

-- Spiegelhalter, Thomas, Best, & Lunn (2007)
(WinBUGS User Manual)

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