Week 12: Bayesian Computations (continued)

MATH-517 Statistical Computation and Visualization

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Bayes' Rule

Let X be a random variable and θ a parameter, considered also a random variable:

$$f_{X,\theta}(x,\theta) = \underbrace{f_{X|\theta}(x \mid \theta)}_{\text{likelihood}} \underbrace{f_\theta(\theta)}_{\text{prior}} = \underbrace{f_{\theta|X}(\theta \mid x)}_{\text{posterior}} f_X(x).$$

- likelihood $=$ frequentist model
- likelihood & prior $=$ Bayesian model

Rewritten:

$$f_{\theta|X=x_0}(\theta \mid x_0) \propto f_{X|\theta}(x_0 \mid \theta) f_\theta(\theta),$$

in words: posterior $\propto$ likelihod $\times$ prior

- posterior has all the answers, but is often intractable $\Rightarrow$ MCMC

Metropolis–Hastings

Metropolis–Hastings (M–H) algorithm:

- **Input**: a proposal density $q(y \mid x)$, the target f (up to a constant)
- **for** $t = 1, 2, \ldots$, update $X^{(t-1)}$ to $X^{(t)}$ by
  - generate $U^{(t)} \sim q(\cdot \mid X^{(t-1)})$
  - define

$$\alpha(X^{(t-1)}, U^{(t)}) = \min\left\{1, \frac{f(U^{(t)})q(X^{(t-1)} \mid U^{(t)})}{f(X^{(t-1)})q(U^{(t)} \mid X^{(t-1)})}\right\}$$

  - set $X^{(t)} := U^{(t)}$ with probability $\alpha(X^{(t-1)}, U^{(t)})$
  - otherwise set $X^{(t)} := X^{(t-1)}$

Metropolis–Hastings

- Under some conditions (see last week's lecture), the chain is ergodic (geometrically or uniformly)
- Metropolis–Hastings: extremely versatile approach to MCMC, but a good proposal (yielding good mixing rate/exploration of space) can be hard to find
- For the common random walk M–H, this is a scaling issue
  - too small and the chain will move too slowly; too large and the proposals will usually be rejected

Adaptive M–H: few words

- trial and error
  - if the acceptance rate seems too high, then we increase the proposal scaling
  - if the acceptance rate seems too low, then we decrease the scaling
- or let the computer decide on the fly
  - suppose we have a family $\{P_\gamma\}_{\gamma \in \mathcal{Y}}$ of possible Markov chains, each with stationary distribution $f(\cdot)$. Let the computer choose among them! At iteration n, use Markov chain P_{Γ_n}, where $\Gamma_n \in \mathcal{Y}$ chosen according to some adaptive rules (depending on chain's history, etc.)
  - example: optimal proposal depends on the covariance matrix of the target, then take the empirical covariance at each step n
  - $\Rightarrow$ Markov property and stationarity are destroyed. Will it still converge? Use "finite adaptation", i.e., stop adapting after a while

Gibbs Sampler

Idea: take advantage of the hierarchical structure, i.e., decompose the multidimensional distribution into *full conditionals* and draw from those in a cyclic manner

- not as universal as M–H, since calculation of the conditional distributions not always possible

Full conditional: $f_i(x_i \mid x_{-i}) = f_i(x_i \mid x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d)$

The Gibbs sampler algorithm based on the target distribution f is

1. use the full conditional densities $f_1, \dots, f_d$ from f
2. start with the random variable $\mathbf{X} = (X_1, \dots, X_d)^\top$
3. simulate from the conditional densities

$$X_i \mid x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d \sim f_i\left(x_i \mid x_1, x_2, \dots, x_{i-1}, x_{i+1}, \dots, x_d\right)$$

for $i = 1, 2, \dots, d$

Gibbs Sampler

The systematic Gibbs sampler proceeds as follows from initial $x^{(0)} = (x_1^{(0)}, \dots, x_d^{(0)})^\top$:

- **for** $t = 1, 2, \dots$
  - generate $x_1^{(t)}$ from $X_1 \mid X_2 = x_2^{(t-1)}, X_3 = x_3^{(t-1)}, \dots, X_d = x_d^{(t-1)}$
  - generate $x_2^{(t)}$ from $X_2 \mid X_1 = x_1^{(t)}, X_3 = x_3^{(t-1)}, \dots, X_d = x_d^{(t-1)}$
  - ...
  - generate $x_d^{(t)}$ from $X_d \mid X_1 = x_1^{(t)}, X_2 = x_2^{(t)}, \dots, X_{d-1} = x_{d-1}^{(t-1)}$

$\Rightarrow$ full conditionals $f_1, \dots, f_d$ are the only densities used for simulation

The transition kernel is

$$K\left(x^{(t-1)}, x^{(t)}\right) = f_{X_1|X_{-1}}\left(x_1^{(t)} \mid x_2^{(t-1)}, \dots, x_d^{(t-1)}\right) \times f_{X_2|X_{-2}}\left(x_2^{(t)} \mid x_1^{(t)}, x_3^{(t-1)}, \dots, x_d^{(t-1)}\right) \times \cdots \\ \times f_{X_d|X_{-d}}\left(x_d^{(t)} \mid x_1^{(t)}, \dots, x_{d-1}^{(t)}\right)$$

- admits f as stationary distribution (show that $\int k(x, y) f(x) dx = f(y)$)
- does not satisfy the detailed balance condition
- LLN applies if f satisfies positivity condition

Gibbs Sampler and Positivity Condition

Definition:

A distribution with density $f(x_1, x_2, \ldots, x_d)$ and marginal densities $f_{X_i}(x_i)$ is said to satisfy the positivity condition if for all $x_1, \ldots, x_d$ such that $f_{X_i}(x_i) > 0$ we have $f(x_1, x_2, \ldots, x_d) > 0$ (support of joint $= \prod$ support of margins)

Result: If the target distribution f satisfies the positivity condition, then the MC generated by the systematic Gibbs sampler satisfies

$$\lim_{T\to\infty} \frac{1}{T} \sum_{t=1}^{T} h\left(X^{(t)}\right) = \int h(x) df(x)$$

for any integrable function $h : \mathbb{X} \to \mathbb{R}$

Remarks on Gibbs Sampler

Although the systematic Gibbs sampler does not satisfy detailed balance, each of its d components does

$\Rightarrow$ this motivates the *random scan Gibbs sampler*

Algorithm: Random scan Gibbs sampler Let $\left(X_1^{(0)}, \dots, X_d^{(0)}\right)^\top$ be the initial state then iterate for $t = 1, 2, \dots$

1. sample an index j from a distribution on $\{1, \dots, d\}$ (typically uniform)
2. sample $X_j^{(t)} \sim f_{X_j|X_{-j}}\left(\cdot \mid X_1^{(t-1)}, \dots, X_{j-1}^{(t-1)}, X_{j+1}^{(t-1)}, \dots, X_d^{(t-1)}\right)$ and set $X_k^{(t)} := X_k^{(t-1)}$ for $k \neq j$

$\Rightarrow$ Random scan Gibbs is a multi-component Metropolis–Hastings sampler with acceptance probability equal to 1 and transition kernel

$$K\left(x^{(t-1)}, x^{(t)}\right) = \frac{1}{d} \sum_{j=1}^{d} f_{X_j|X_{-j}}\left(x_j^{(t)} \mid x_{-j}^{(t-1)}\right) \delta_{x_{-j}^{(t-1)}}\left(x_{-j}^{(t)}\right)$$

$\Rightarrow$ satisfies detailed balance and admits f as stationary distribution

Toy Example

Using the systematic Gibbs sampler, calculate $P(X_1 \geq 0, X_2 \geq 0)$ for

$$X = (X_1, X_2)^\top \sim \mathcal{N}\left(\begin{pmatrix}\mu_1 \\ \mu_2\end{pmatrix}, \begin{pmatrix}\sigma_1^2 & \rho \\ \rho & \sigma_2^2\end{pmatrix}\right)$$

Easy, since Gaussian conditionals are Gaussian:

$$X_i \mid X_j = x_j \sim \mathcal{N}\left(\mu_i + \frac{\rho}{\sigma_j^2}(x_j - \mu_j), \sigma_i^2 - \frac{\rho^2}{\sigma_j^2}\right)$$

E.g., for $\mu_1 = \mu_2 = 0$, $\sigma_1 = \sigma_2 = 1$ and $\rho = 0.3$, we have...

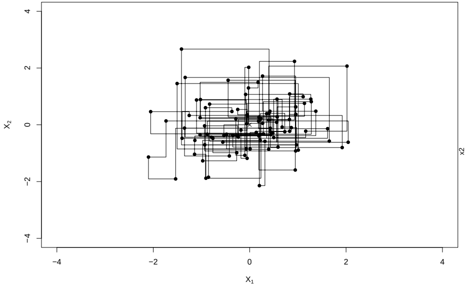
Toy Example

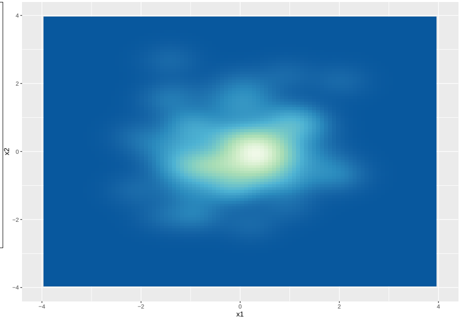
```r
set.seed(123)
burnin <- 1000
TT  <- 2000
X1  <- rep(0, burnin+TT)
X2  <- rep(0, burnin+TT)
rho <- 0.3
X1[1] <- 0
X2[1] <- 0
for(t in 2:(burnin+TT)){
  X1[t] <- rnorm(1,0+rho/1*(X2[t-1]-0), sqrt(1-rho^2/1))
  X2[t] <- rnorm(1,0+rho/1*(X1[t]-0), sqrt(1-rho^2/1))
}
X1 <- X1[-(1:burnin)]
X2 <- X2[-(1:burnin)]

sum(I(X1 >= 0 & X2 >= 0 ))/TT # empirical P(X1 >= 0, X2 >= 0)
```

Toy Example

Markov chain $X^{(t)}$ has correlated successive samples

First 100 steps (with $\rho = 0.3$)

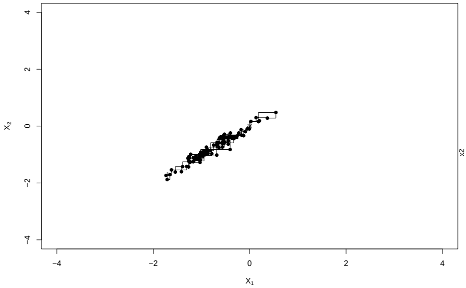


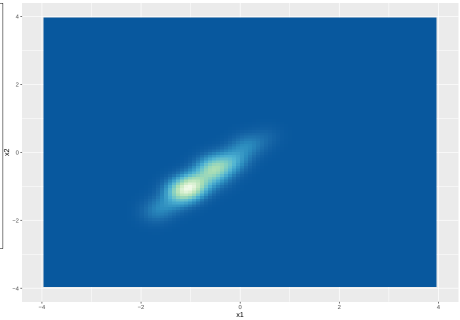


$P(X_1 \geq 0, X_2 \geq 0)$ is estimated at 0.298

Markov chain $X^{(t)}$ has strongly correlated successive samples $\Rightarrow$ chain mixes slowly

First 100 steps (with $\rho = 0.99$)





Toy Example

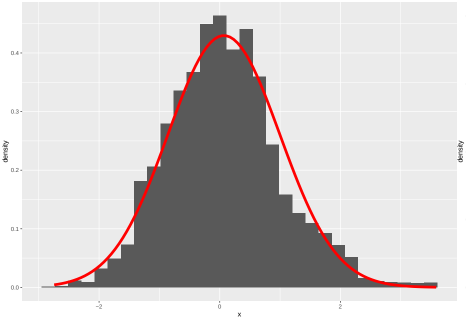


Figure 1: large correlation

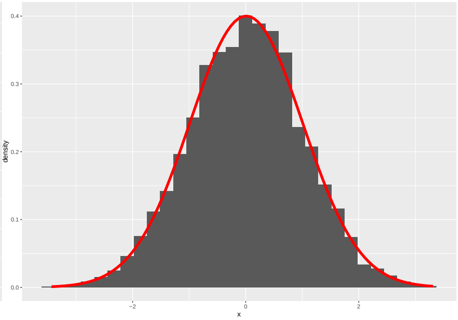


Figure 2: small correlation

Histogram of first component after
4000 iterations

Toy Example

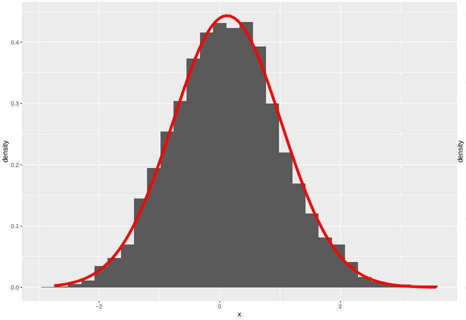


Figure 3: large correlation

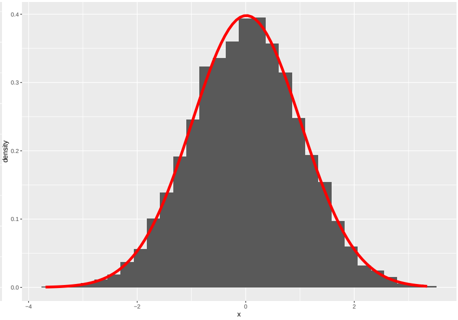


Figure 4: small correlation

Histogram of first component after
10000 iterations

Metropolis-within-Gibbs

What if sampling from full conditionals isn't easy for Gibbs?

- do a single Metropolis–Hastings step instead

What if parameters are naturally grouped in a real application?

- e.g., some parameters correspond to location and others to scale
- location parameters can usually be sampled at once, conditionally on all the other parameters
    - *blocked Gibbs sampler*: blocks of variables are updated by sampling from their joint conditional on all other variables
    - potentially via a M–H step

Limitations of the Gibbs sampler

- limits the choice of target distributions
- requires some knowledge of f
- is multi-dimensional, by construction

Output Analysis

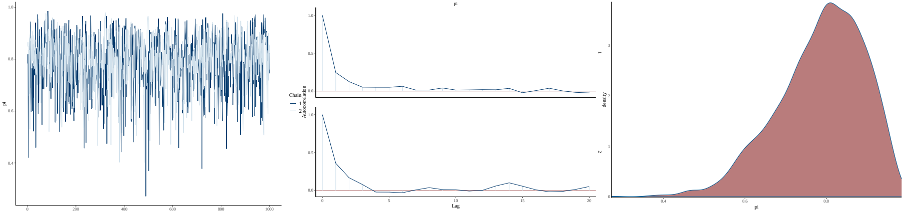
MCMC compared to MC:

- sacrifices independence for more versatility
  - ergodic theory: independence not really needed in the long run
- in practice, the question is: what is a long enough run?
- just inspect the samples drawn (after discarding burnin)
  - check whether the acceptance rate is reasonable
  - visualize graphical outputs (to follow)
  - calculate diagnostic statistics (to follow)
- in reality, we can never know
  - silent failure?! E.g., careless use of Gibbs (conditional distributions are well defined but their combination does not correspond to any joint distribution...), or positivity condition violated

Output Analysis

- simple ideas such as running multiple chains and checking that they are converging to similar distributions are often employed in practice
- shrink factor of Gelman–Rubin: variance between chains relative to variance within chains (if multiple chains reached the target then this factor should be 1)
  - > 1 indicates instability, with variability in the combined chains exceeding that within the chains
  - rule of thumb: red flag if > 1.05
- trace plots are often used to informally assess stochastic convergence
  - if MCMC is working, they should look like a "fat, hairy caterpillar"
- ACF (autocorrelation function) plots display the autocorrelation within a chain as a function of the lag
  - if the ACF takes too long to decay to 0, the chain exhibits a high degree of dependence and will tend to get stuck

Output Analysis: Beta-Binomial Model



- the chains mix quickly (move quickly around plausible values of the posterior
- the autocorrelation quickly drops off
- shrink factor ≈ 1 (stability across parallel chains)

$\Rightarrow$ if not try different prior parameters or different scaling of proposal (if M–H)

Simple but Real Example

- the height of college students has $\mathcal{N}(\mu, \sigma^2)$
  - we work with σ, i.e., the standard deviation instead of variance
- only binned data available

```
X
(-Inf,60]    (60,62]    (62,64]    (64,66]    (66,68]    (68,70]    (70,72]    (72,74] (74, Inf]
       32         77        110        108        107         78         81         34        20
```

- multinomial data, probabilities depend on μ and σ
  - e.g. prob. of an observation falling into $(60, 62]$ is $\Phi_{\mu,\sigma}(62) - \Phi_{\mu,\sigma}(60)$
- likelihood:

$$f(d \mid \mu, \sigma) \propto \prod_{j=1}^{9} \{\Phi_{\mu,\sigma}(a_j) - \Phi_{\mu,\sigma}(a_{j-1})\}^{d_j} =: \ell(\mu, \sigma)$$

- prior: $f(\mu, \sigma) = 1/\sigma$
  - improper prior (Jeffrey's prior)
  - changing variable $\lambda = \log(\sigma)$ removes $1/\sigma$ from the posterior

Posterior:

$$f(\mu, \sigma \mid D = d) \propto \ell\{\mu, \exp(\lambda)\}$$

Real but Simple Example

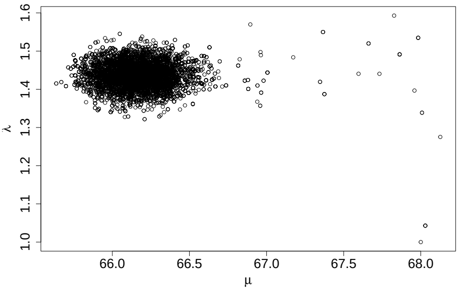
- **Aim**: sample from posterior using normal random walk M–H

$$U^{(t+1)} = X^{(t)} + sZ$$

  where $Z \sim \mathcal{N}(0, \Sigma)$ and $s > 0$ is a scale parameter
  - overparametrization for the sake of convenience (debatable)
- for MH we have to choose
  - starting point $(\mu^{(0)}, \lambda^{(0)})^\top$
  - scale s
  - covariance Σ

Real but Simple Example

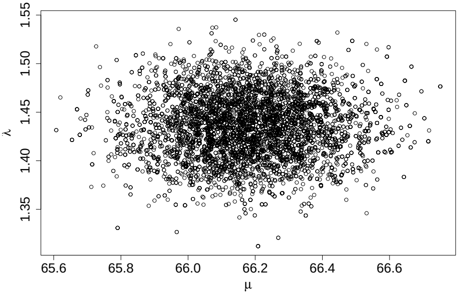
- Looking at the binned data, why not take
  - $(\mu^{(0)}, \lambda^{(0)})^\top = (68, 1)^\top$
  - scale $s = 1 \Rightarrow$ acceptance too low, so let's take $s = 0.1$
  - covariance $\Sigma = I_{2\times 2}$



Acceptance rate: 0.3134

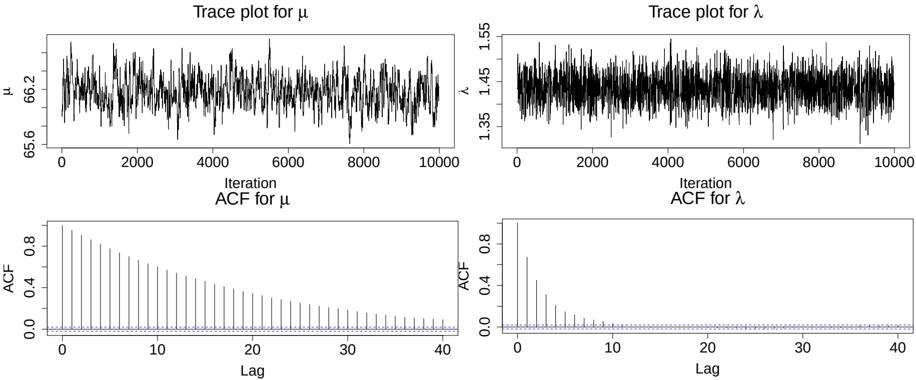
Real but Simple Example

- above starting point chosen badly
- normally taken care of by burnin, here let's re-run
  - $(\mu^{(0)}, \lambda^{(0)})^\top = (66, 1.4)^\top$



Acceptance rate: 0.3196

Real but Simple Example - Ouput Check



Real but Simple Example - Ouput Check

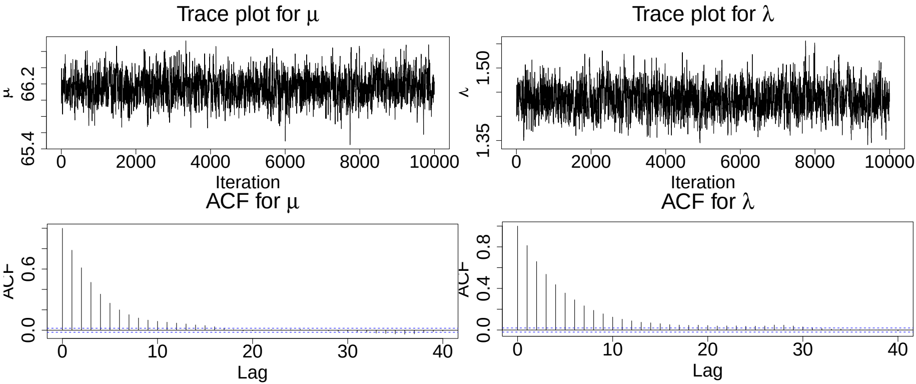
- the plots above look good, but values of μ are correlated for too long
- their correlation can be reduced by taking Σ diagonal with the variance for μ higher than that for λ
- actually, why not take Σ estimated from our previous run

```
             [,1]         [,2]
[1,] 3.035891e-02 7.329492e-05
[2,] 7.329492e-05 9.306388e-04
```

- acceptance too high with our $s = 0.1$ now, let's increase s
  - $s = 1$ gives 58%
  - let's take $s = 2$

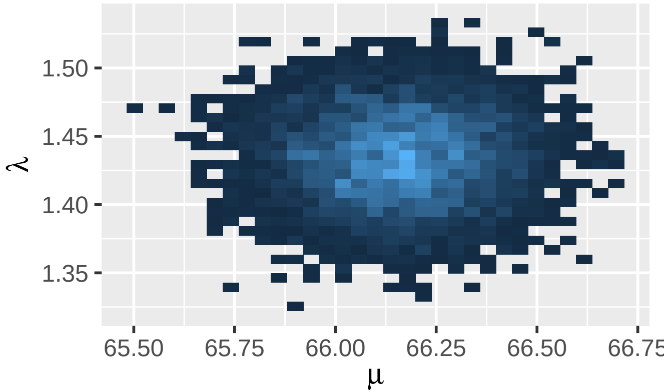
Real but Simple Example - Final Run

Lets analyze the output again



Acceptance rate: 0.5386

Real but Simple Example - Estimated Posterior



The posterior mean estimates are $\hat{\mu} = 66.159$ and $\hat{\lambda} = 1.435$

Final Thoughts

- Bayesianism is a different way of thinking about problems
  - e.g., hierarchical models
- prior versus no prior
- MLE versus MAP
- sampling not the only way to be Bayesian
  - *variational* methods (back to optimization)
  - *empirical* Bayes (back to frequentism)
- Hamiltonian MC and NUTS
  - explore the space in an adaptive way
- BUGS & JAGS
  - packages for Bayesian computations (JAGS has R interface `rjags`)
  - uses model structure and Gibbs sampling whenever possible
- STAN
  - a package with R interface `rstan`
  - uses NUTS
- silent failure!?
  - multimodal distributions problematic for sampling
  - plateau regions problematic for optimization

Final Thoughts

- as sample size $|D|$ grows:
  - at first, we are going away from the prior, and the posterior is getting complicated
  - then, the posterior becomes more and more regular (courtesy of CLT) and the prior serves as a bit of regularization
  - eventually, the prior stops mattering
    - back to frequentism in the large sample limit
- in every statistical task, there are three sources of error:
  - data is random (vanishes with increasing data set)
  - my model is wrong (never goes away)
  - inference is inexact (vanishes with investing more computational resources)

> *Far better an approximate answer to the right question, than the exact answer to the wrong question.*
>
> – John W. Tukey