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Outline

1. Motivation (Monte Carlo integration; Markov chains)
2. MCMC (Gibbs sampling)
3. Convergence and Monte Carlo standard errors
4. Strengths and weaknesses of MCMC

1. Motivation

Bayesian inference involves expectations, in particular posterior expectations $E(f(\theta) \mid x)$ of functions $f(\theta)$ of unknown parameters θ.

For example,

- $f(\theta) = \theta$: $E(f(\theta) \mid x)$ is the posterior mean of θ.

The posterior expectation of $f(\theta)$ is

$$\begin{aligned} E(f(\theta) \mid x) &= \int f(\theta) p(\theta \mid x) d\theta \\ &= \frac{\int f(\theta) p(x \mid \theta) p(\theta) d\theta}{\int p(x \mid \theta) p(\theta) d\theta} \end{aligned}$$

In practice, integrations for the calculation of $E(f(\theta) \mid x)$ usually are complex, high-dimensional and have no closed form solution.

General problem: How can we evaluate

$$E[f(\theta) \mid x] \;=\; \int f(\theta)\, p(\theta \mid x)\, d\theta \text{ ?}$$

Numerical integration or analytic approximation (e.g. Laplace/saddle-point) can be used, but tends to work poorly if θ is high-dimensional.

A solution: draw samples $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(N)}$ from $p(\theta \mid x)$. Then we can estimate

$$E[f(\theta) \mid x] \approx \frac{1}{N} \sum_{i=1}^{N} f(\theta^{(i)})$$

This is **Monte Carlo integration.**

Problem: Drawing independent samples from $p(\theta \mid x)$ is generally not feasible if $p(\theta \mid x)$ is non-standard.
However, the samples need not necessarily be independent.

Question: How do we draw dependent samples $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(N)}$ from $p(\theta \mid x)$?

Solution: Draw dependent samples using a *Markov chain* having $p(\theta \mid x)$ as its stationary/equilibrium distribution.

Markov chains

A *Markov chain* is a sequence $X^{(0)}, X^{(1)}, \ldots$ of random variables such that, for each $i = 0, 1, \ldots$, the conditional probability distribution of $X^{(i+1)}$ given $X^{(0)}, X^{(1)}, \ldots, X^{(i)}$ depends only on $X^{(i)}$.

That is, $X^{(i+1)}$ is independent of $X^{(0)}, \ldots, X^{(i-1)}$ given $X^{(i)}$, denoted by

$$X^{(i+1)} \perp\!\!\!\perp X^{(0)}, \ldots, X^{(i-1)} \mid X^{(i)}$$

So, in a Markov chain, the future depends on the past only through the present.

Stationary distributions

Subject to regularity conditions, as $i \to \infty$, the Markov chain *converges in distribution* to a unique *stationary/equilibrium* distribution.

This does not depend on $X^{(0)}$.

Example

$$\theta^{(i+1)} \sim \text{Normal}\left(\frac{\theta^{(i)}}{2}, 1\right)$$

$$\theta^{(0)} = -15.0 \qquad \theta^{(0)} = +15.0$$

The stationary distribution is Normal$(0, \frac{4}{3})$.

2. MCMC

If we could construct a Markov chain whose stationary distribution is $p(\theta \mid x)$, then, after M iterations (M is large enough), $\theta^{(M+1)}, \theta^{(M+2)}, \ldots, \theta^{(N)}$ would be dependent samples approximately from $p(\theta \mid x)$ and

$$E[f(\theta) \mid x] \approx \frac{1}{N-M} \sum_{i=M+1}^{N} f(\theta^{(i)})$$

This is *Markov chain Monte Carlo* (MCMC; ie Monte Carlo integration using Markov chains).

How do we construct a Markov chain whose stationary distribution is $p(\theta \mid x)$?

Using the *Metropolis-Hastings algorithm*. (Metropolis et al. 1953; Hastings, 1970)

This algorithm provides a general framework for MCMC. We shall concentrate on one of its special cases: *Gibbs Sampling*.

Gibbs sampling

Split $\boldsymbol{\theta}$ into K components $(\theta_1, \theta_2, \ldots, \theta_K)$ (components can be scalar or vector; eg $\theta_1 = \mu, \theta_2 = \tau, \ldots, \theta_K = \alpha$).

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Choose starting values $\mu^{(0)}$, $\tau^{(0)}$, ..., $\alpha^{(0)}$.
set $i = 0$.
Repeat {
    Sample $\mu^{(i+1)}$ from $p(\mu \mid \tau^{(i)}, \ldots, \alpha^{(i)}, x)$
    Sample $\tau^{(i+1)}$ from $p(\tau \mid \mu^{(i+1)}, \ldots, \alpha^{(i)}, x)$

    $\cdots$
    Sample $\alpha^{(i+1)}$ from $p(\alpha \mid \mu^{(i+1)}, \tau^{(i+1)}, \ldots, x)$

    $i \leftarrow i + 1$
}
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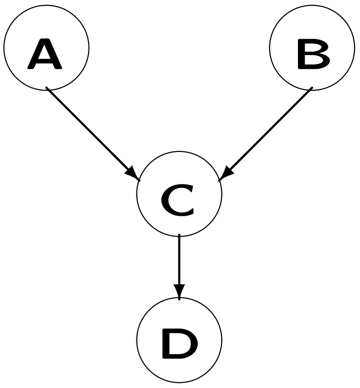
Note:
1. The most up-to-date version of $\boldsymbol{\theta}$ is used at each step.
2. Sampling is from *full-conditional distributions*.

Constructing full-conditional distributions

- Suppose we have a DAG



- By *factorisation of joint distribution*

$$p(\mathbf{V}) = \prod_{v \epsilon \mathbf{V}} p(v \mid \text{parents}[v]), \quad \text{we have}$$

$$p(A, B, C, D) = p(A)\, p(B)\, p(C \mid A, B)\, p(D \mid C) \quad (*)$$

- *Two ways to get the full-conditional distribution for C.*

1. Either

$$\begin{aligned} p(C \mid A, B, D) &\propto \text{terms on RHS of } (*) \text{ containing } C \\ &= p(C \mid A, B)\, p(D \mid C) \end{aligned}$$

2. Or

$$\begin{aligned} p(C \mid \mathbf{V} \backslash C) &\propto p(C \mid \text{parents}\,[C]) \\ &\quad \times \prod_{w \,\in\, \text{children}[C]} p(w \mid \text{parents}\,[w]) \end{aligned}$$

ie, $p(C \mid A, B, D) \propto p(C \mid A, B)\, p(D \mid C)$

Sampling from full-conditional distributions

We must be able to sample from

$$p(\theta_k \mid \theta_1, \ldots, \theta_{k-1}, \theta_{k+1}, \ldots, \theta_K)$$

to do Gibbs sampling.

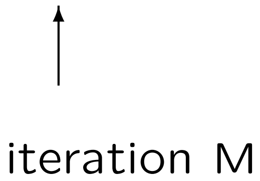
In simple problems, the full-conditional distributions have closed forms.

Otherwise, a range of algorithms is available. E.g.

- rejection sampling
- adaptive rejection sampling
- ratio-of-uniforms method

(see Chapter 5 of MCMC in Practice (Gilks et al., 1996) for more information).

3. Convergence and Monte Carlo standard errors



Early iterations $\theta^{(1)}, \ldots, \theta^{(M)}$ reflect starting value $\theta^{(0)}$.
These iterations are called the *burn-in*.

After burn-in we say the chain has ‘converged’.
$\Rightarrow \theta^{(M+1)}, \ldots, \theta^{(N)}$ are samples approximately from $p(\theta \mid x)$.

Omit the burn-in, we estimate $E[f(\theta) \mid x]$ by using sample average,

$$\bar{f}_{MN} = \frac{1}{N-M} \sum_{i=M+1}^{N} f(\theta^{(i)})$$

Determining M

Problem: strictly speaking, convergence is only achieved for $M = \infty$.

In practice: We can only make a reasonable effort to detect *lack of convergence*.
If no evidence of lack of convergence is found, we are more confident that the chain has 'converged'.

- Using *trace plots*. Once convergence has been reached, samples should look like a random scatter about a stable value.
- Using *convergence diagnostics* to determine M for the 'burn-in'.
  Many convergence diagnostics have been proposed.

The Gelman-Rubin diagnostic (1992)

A single chain can be misleading. So, run several chains, with widely differing starting values. After burn-in, the behavior of all chains should be approximately the same.

Specifically, for a certain parameter θ_k, the variance within the chains should be the same as the variance across the chains.

Determining N

Q: After burn-in, how long should we run the chain?

A: It is reasonable to run the chain until the **Monte Carlo standard error** (MCSE), SE($\bar{f}_{MN}$), is sufficiently small.

Q: How small should MCSE be?

A: We want MCSE small in relation to posterior standard deviation of $f(\theta)$.
Rule of thumb: run the chain until the MCSE of each parameter is less than 5% of the parameter's posterior standard deviation.

4. Strengths and weaknesses of MCMC

Strengths

- Can offer freedom in modelling
  - in principle, no limits
- Can offer freedom in inference
  - in principle, no limits
  - can estimate arbitrary functions of model parameters (e.g. ranks, probabilities of threshold exceedence, etc)
- Can coherently integrate uncertainty
- Is the only available method for complex problems

Weaknesses and dangers

- Can be slow: may need to generate very long chains to
  - achieve convergence
  - reduce MCSE to acceptable level
- May fail to diagnose lack of convergence
- May be difficult to validate the computer code written for the implementation of the MCMC

My MCMC has converged because

- *I ran it for 10,000 iterations;*
- *my wife called out 'coffee's ready';*
- *WinBUGS crashed;*
- *the plots were still going down. . . . . .*

— T. O'Hagan

Outline revisited

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