ST451 - Lent term
Bayesian Machine Learning

Kostas Kalogeropoulos

Markov Chain Monte Carlo

Outline

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Motivating Examples

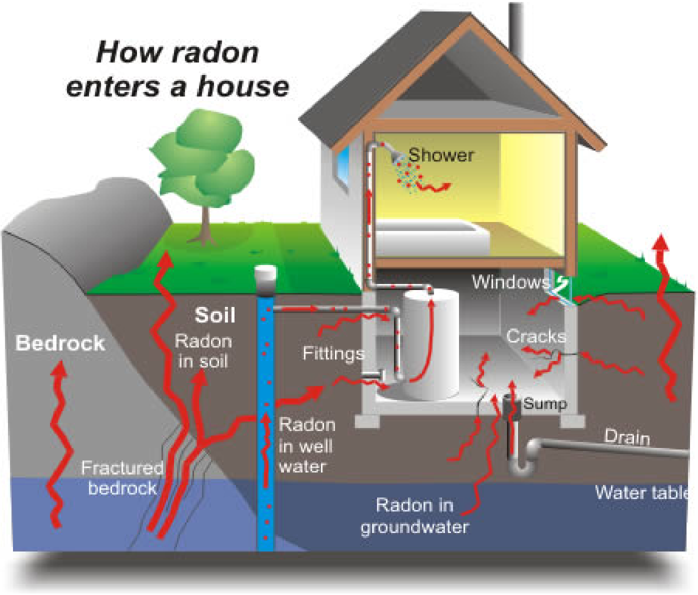
So far we encountered various examples where the posterior was not available in closed form, e.g.

- Logistic regression
- Ising model
- Mixtures

We used approximations such as Variational Bayes and Laplace.

An alternative option is provided by Monte Carlo where the approximation error can be controlled by the user.

Additional Real World Example: Radon

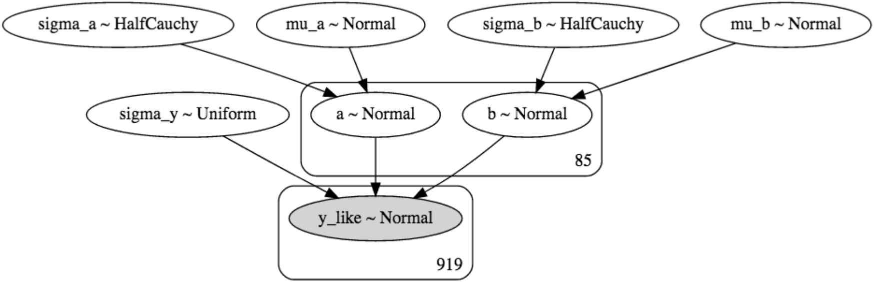


Hierarchical / Multi-level / Panel data

- Radioactive gas measurements from several households taken from different regions.
- An important predictor is whether the measurement is in the basement or first floor or above.
- The region of the household is also important.
- Model:

$$
\begin{aligned}
y_{ij} &= a_i + b_i X_{ij} + \epsilon_{ij}, \\
\epsilon_{ij} &\overset{\text{ind}}{\sim} N(0, \sigma_y^2), \quad a_i \overset{\text{ind}}{\sim} N(\mu_a, \sigma_a^2), \quad b_i \overset{\text{ind}}{\sim} N(\mu_b, \sigma_b^2), \\
\sigma_y &\sim \text{Uniform}(0, 1), \quad \mu_a \sim N(0, 10^6), \quad \mu_b \sim N(0, 10^6), \\
\sigma_a &\sim \text{HalfCauchy}(5), \quad \sigma_b \sim \text{HalfCauchy}(5)
\end{aligned}
$$

DAG of hierarchical model



The model has 175 parameters. Too large for Laplace approximation, Variational Bayes is feasible but still an approximation.

Bayesian Variable Selection with sparsity

Recall the linear regression model $y = X\beta + \epsilon$. When most of the X's are not relevant with y it is essential to filter most of them out and come up with sparse model.

Lasso regression achieves that using the prior

$$\begin{aligned} \beta_i &\sim N(0, \tau^2), \\ \tau &\sim \text{Exp}(\lambda), \end{aligned}$$

but only under the posterior mode; the posterior mean is not sparse.

Bayesian sparsity is achieved better by the spike and slab priors

$$\begin{aligned} \beta_i &\sim \gamma_i N(0, \tau^2) + (1 - \gamma_i) N(0, \omega^2), \quad \omega << \tau \\ \gamma_i &\sim \text{Bernoulli}(\pi) \end{aligned}$$

Bayesian Variable Selection with sparsity

Nevertheless, the spike and slab choice often leads to more challenging computational schemes.

A more convenient approach with very similar behaviour is the horseshoe prior. Below is one of its simpler forms

$$\begin{aligned}\beta_i &\sim N(0, \tau^2 \lambda_i),\\ \lambda_i &\sim \text{Cauchy}^+(1),\\ \tau &\sim \text{Cauchy}^+(1),\end{aligned}$$

where Cauchy$^+$ denotes the half-Cauchy distribution (constrained on the positive real line).

Both horseshoe and spike and slab approaches lead to posteriors that are not available in closed form.

Outline

Markov Chains

We will illustrate the theory for discrete RVs but it also holds for continuous RVs.

Let $\{x_t,\ t = 1, \ldots, N\}$ be a sequence of (dependent) random variables. They form a Markov chain or a Markov model if

$$\pi(x_{t+1}|x_1, \ldots, x_t) = P(x_{t+1}|x_t)$$

so, we can then write

$$\pi(x_1, \ldots, x_N) = \pi(x_1) \prod_{t=1}^{N-1} P(x_{t+1}|x_t)$$

Stationary / invariant distribution.

The distributions $P(x_{t+k}|x_t) = T_t(x_t, x_{t+k})$ are called transition probabilities. We will focus on cases where they are independent of time and the chain is called homogeneous

For a homogeneous Markov chain with transition probabilities $T(x', x)$, the distribution $\pi^\star(z)$ is invariant/stationary if

$$\pi^\star(x) = \sum_{x'} T(x', x)\pi^\star(x')$$

The stationary distribution (aka equilibrium) reflects the long term behaviour of the Markov Chain.

Idea 1: Use Markov Chains for simulation

Let x be a Markov Chain with transition probability distribution $P(x_{t+1}|x_t)$.

For a given initial value x_0, we can simulate x in the following way

Markov Chain Simulation

1. Initialise. Set x_0.
2. At each time t, draw the next value, x_{t+1} from $P(x_{t+1}|x_t)$.

After a large t all the values of X_t may be viewed as samples from $\pi(\cdot)$. The samples will be dependent but still ok for Monte Carlo (unless they are 'too dependent').

Numerical example of a Markov chain

Consider the Markov chain that is initial value x_0 and transition probability

$$x_{t+1}|x_t \sim N(0.5x_t, 1)$$

Let's see its trajectories when started at two different starting points. (see file 'MarkovChainExample.ipynb')

The stationary distribution of X is the N$(0, 1.33)$

Existence of a unique stationary distribution

Irreducibility: It is possible to get from any state c ($x_t = c$) to any state d at a finite future time s ($x_s = d$).

Aperiodicity: There shouldn't be any loops for all the states.

Non-null recurrence: From any state it is possible to return in finite time.

Ergodicity: If a chain is non-null recurrent and aperiodic.

Theorem: Every irreducible ergodic Markov chain has a limiting distribution, which is equal to π its unique stationary distribution.

Reversible Markov chains

A chain is reversible if it satisfies the detailed balance equation:

$$\pi(x_t)P(x_{t+1}|x_t) = \pi(x_{t+1})P(x_t|x_{t+1})$$

Summing over x_t satisfies the stationarity condition

$$\sum_{x_t} \pi(x_t)P(x_{t+1}|x_t) = \sum_{x_t} \pi(x_{t+1})P(x_t|x_{t+1}) = \pi(x_{t+1})$$

For continuous Markov chains replace sums with integrals

$$\int \pi(x_t)P(x_{t+1}|x_t)dx_t = \int \pi(x_{t+1})P(x_t|x_{t+1})dx_t = \pi(x_{t+1})$$

Outline

Markov Chain Monte Carlo: A tale of rediscovery

- First discovered during world war II by Physicists in Los Alamos.
- Mainly in Physics but first published in a Chemistry journal by Metropolis (1953).
- A publication in Statistics by Hastings (1970) was largely unnoticed.
- A special case (Gibbs algorithm) was re-invented for the case of the Ising model by Geman and Geman (1984).
- Gelfand and Smith (1990) make the algorithm well-known and Bayesian inference becomes mainstream.
- `https://cs.gmu.edu/~henryh/483/top-10.html`

Main ideas of MCMC

- Construct Markov Chains with the posterior as stationary.

  Note: Possible even if we only know the likelihood and the prior.

- Use Markov Chains to sample from their stationary distribution.

Main MCMC algorithms:

- Metropolis Hastings
- Gibbs Sampler
- Hamiltonian MCMC

Metropolis-Hastings algorithm

From now on switch from x to θ (y denotes data)

Metropolis Hastings algorithm

The following algorithm will provide samples from the $\pi(\theta|y)$

1. Initialise θ_0 at t=0
2. Repeat for t=0:T-1
   - Sample a point θ^* from q$(\theta^*|\theta_t)$.
   - Set $\theta_{t+1} = \theta^*$ with probability $\alpha(\theta_t, \theta^*)$

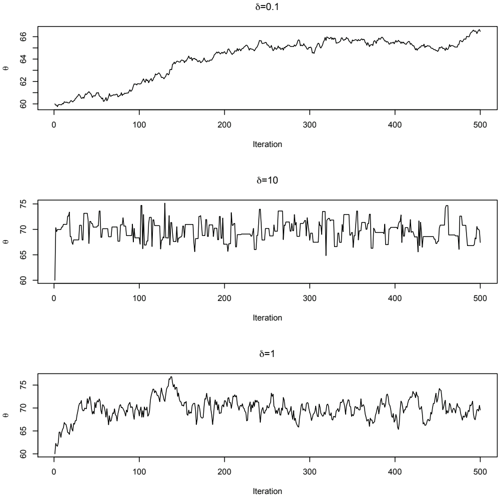
$$\alpha(\theta_t, \theta^*) = \min\left(1, \frac{\pi(\theta^*|y)q(\theta_t|\theta^*)}{\pi(\theta_t|y)q(\theta^*|\theta_t)}\right)$$

otherwise set $\theta_{t+1} = \theta_t$.

Note that $\frac{\pi(\theta^*|y)}{\pi(\theta_t|y)} = \frac{f(y|\theta^*)\pi(\theta^*)}{f(y|\theta_t)\pi(\theta_t)}$. Suffices to know $\pi(\theta_t|y)$ up to proportionality.

Traceplots of Metropolis-Hastings Markov Chains

Convergence and mixing (dependence of the samples) are typically assessed with traceplots. Below we see examples of bad (top), good(middle) and medium (down) cases.



Special cases of Metropolis-Hastings

If we set $q(\theta^*|\theta_t) = q(\theta^*)$ we get the Independence sampler.

$$\alpha(\theta_t, \theta^*) = \min\left(1,\ \frac{\pi(\theta^*|y)q(\theta_t)}{\pi(\theta_t|y)q(\theta^*)}\right) = \min\left(1,\ \frac{f(y|\theta^*)\pi(\theta^*)q(\theta_t)}{f(y|\theta_t)\pi(\theta_t)q(\theta^*)}\right)$$

Can either perform very well but also poorly.

If $q(\theta^*|\theta_t) = q(\theta_t|\theta^*)$, e.g. N($\theta_t$,$S_\theta$) , we get the Random-walk Metropolis

$$\alpha(\theta_t, \theta^*) = \min\left(1,\ \frac{\pi(\theta^*|y)}{\pi(\theta_t|y)}\right) = \min\left(1,\ \frac{f(y|\theta^*)\pi(\theta^*)}{f(y|\theta_t)\pi(\theta_t)}\right)$$

The optimal choice for S_θ is a value such that the acceptance rate is 0.234.

Gibbs sampler

Suppose that $\theta = (\theta_1, \theta_2, \ldots, \theta_p)$.

Consider a M-H algorithm where at each iteration we update θ as follows: Update only θ_1 first, then only θ_2 and keep going until θ_p.

Suppose also that we know $\pi(\theta_i|\theta_{-i}, y)$ for each θ_i, where

$$\theta_{-1} = (\theta_1, \ldots \theta_{i-1}, \theta_{i+1}, \ldots \theta_p).$$

We can then use $\pi(\theta_i|\theta_{-i}, y)$, aka full conditionals, as proposals distributions $q(\theta)$.

The acceptance probability will be 1 in all steps (see exercise 1).

Gibbs Sampler (cont'd)

The Gibbs sampler provides samples from the posterior $\pi(\theta_1, \dots \theta_p | y)$

Gibbs Sampler

1. Initialise $\theta^0 = (\theta_1^{(0)}, \theta_2^{(0)}, \dots, \theta_p^{(0)})$
2. Repeat for t=1:n
   - Draw $\theta_1^{(t)}$ from $\pi(\theta_1 | \theta_2^{(t-1)}, \dots \theta_p^{(t-1)}, y)$
   - Draw $\theta_2^{(t)}$ from $\pi(\theta_2 | \theta_1^{(t)}, \theta_3^{(t-1)} \dots \theta_p^{(t-1)}, y)$
   - Draw $\theta_3^{(t)}$ from $\pi(\theta_3 | \theta_1^{(t)}, \theta_2^{(t)} \dots \theta_p^{(t-1)}, y)$

   $$\dots$$

   - Draw $\theta_p^{(t)}$ from $\pi(\theta_p | \theta_1^{(t)}, \theta_2^{(t)} \dots \theta_{p-1}^{(t)}, y)$

Example: Normal with θ and σ^2 unknown

Given random sample $y = (y_1, \ldots, y_n)$ from N(θ,σ^2) with N(μ,τ^2) and IGamma(α,β) as priors. The posterior is proportional to

$$\begin{aligned}\pi(\theta, \sigma^2 | y) \quad &\propto (\sigma^2)^{-n/2} \exp\left(-\frac{\sum_{i=1}^{n}(y_i - \theta)^2}{2\sigma^2}\right) \exp\left(-\frac{(\theta-\mu)^2}{2\tau^2}\right) \\ &\qquad (\sigma^2)^{-\alpha-1} \exp\left(-\frac{\beta}{\sigma^2}\right)\end{aligned}$$

For $\pi(\theta | y, \sigma^2)$ gather all the terms involving θ and see if you can identify the distribution.

$$\begin{aligned}\pi(\theta | y, \sigma^2) \quad &\propto \quad \exp\left(-\frac{\sum_{i=1}^{n}(y_i - \theta)^2}{2\sigma^2}\right) \exp\left(-\frac{(\theta - \mu)^2}{2\tau^2}\right) \\ \ldots \quad &\stackrel{D}{=} \mathrm{N}\left(\frac{\frac{\sigma^2}{n}\mu + \tau^2 \bar{x}}{\tau^2 + \frac{\sigma^2}{n}}, \frac{\tau^2 \frac{\sigma^2}{n}}{\tau^2 + \frac{\sigma^2}{n}}\right)\end{aligned}$$

Example: Normal with θ and σ^2 unknown (cont'd)

Similarly for $\pi(|y,\theta)$ we get

$$
\begin{aligned}
\pi(\sigma^2|y,\theta) &\propto (\sigma^2)^{-n/2}\exp\left(-\frac{\sum_{i=1}^n (y_i-\theta)^2}{2\sigma^2}\right)(\sigma^2)^{-\alpha-1}\exp\left(-\frac{\beta}{\sigma^2}\right)\\
&= (\sigma^2)^{-(n/2+\alpha)-1}\exp\left(-\frac{\beta+\frac{1}{2}\sum_{i=1}^n (y_i-\theta)^2}{\sigma^2}\right)\\
&\overset{D}{=} \text{IGamma}\left(n/2+\alpha, \beta+\frac{1}{2}\sum_{i=1}^n (y_i-\theta)^2\right)
\end{aligned}
$$

A Gibbs Sampler initiates θ and σ^2 and then alternates between drawing from the two full conditionals at each iteration.

Metropolis-Hastings vs Gibbs

Gibbs is generally preferred when it is possible to implement (not available in most cases) as it is automatic. It will perform poorly only when θ_i's are highly dependent a-posteriori.

Metropolis-Hastings is black box and could perform better than Gibbs in cases of high posterior correlation. But it needs to be tuned; some adaptive methods are available.

Metropolis within Gibbs: Metropolis-Hastings and Gibbs sampler can be combined by updating each $\theta_i|\theta_{-i}, y$ with proposals and accept/reject steps.

Metropolis within Gibbs can be used when Gibbs is not available and is hard to tune Metropolis-Hastings.

Hamiltonian Markov Chain Monte Carlo

Let $\Phi(\theta) = -\log f(y|\theta) - \log \pi(\theta)$ so that $\pi(\theta|y) \propto \exp\{-\Phi(\theta)\}$

Extend the location $\theta \in \mathbb{R}^d$ via an auxiliary velocity $v \sim N(0, S)$, $v \perp \theta$, and consider the total energy based on a user-specified covariance S

$$H(\theta) = \Phi(\theta) + \frac{1}{2} v^T S^{-1} v$$

$H(\theta)$ consists of the potential $\Phi(x)$ and the kinetic energy $\frac{1}{2} v^T S^{-1} v$.

We define the distribution on the (θ, v)-space:

$$\pi(\theta, v|y) \propto \exp\{-H(\theta)\} = \exp\{-\Phi(\theta) - \frac{1}{2} v^T S^{-1} v\}$$

Hamiltonian Dynamics

The Hamiltonian dynamics defined on $\mathbb{R}^{2d}$, involve gradients and express preservation of energy

$$\begin{aligned}\frac{d\theta}{dt} &= v \\ \frac{dv}{dt} &= -S\nabla\Phi(x)\end{aligned}$$

Exact solution of the above equation returns exact samples from $\pi(\theta, v|y)$. However only numerical integrators are available.

The standard option is the following leapfrog scheme (L and h need to be specified)

$$\begin{aligned}v_{h/2} &= v_0 - \tfrac{h}{2}\, S\,\nabla\Phi(\theta_0)\ , \\ \theta_h &= \theta_0 + h\, v_{h/2} \\ v_h &= v_{h/2} - \tfrac{h}{2}\ S\,\nabla\,\Phi(\theta_h)\ ,\end{aligned}$$

The Hamiltonian MCMC algorithm

The leapfrog scheme is symmetric and volume preserving but not energy preserving. Hence, a correction is required, via the following algorithm, to obtain exact samples from $\pi(\theta|y)$

Hamiltonian MCMC

(i) Start with an initial value $(\theta^{(0)}, v^{(0)}) \sim \otimes_{i=1}^{d} N(0,1) \times \pi(\theta)$

(ii) Given $\theta^{(k)}$ sample $v^{(k)} \sim N(0, S)$ and propose and apply L leapfrog steps to obtain $(\theta^{(\star)}, v^{(\star)})$ from $(\theta^{(k)}, v^{(k)})$

(iii) Consider

$$a = \min\left(1, \exp\left\{-H(x^{(\star)}, v^{(\star)}) + H(x^{(k)}, v^{(k)})\right\}\right)$$

(iv) Set $\theta^{(k+1)} = x^{\star}$ with probability a; otherwise set $\theta^{(k+1)} = \theta^{(k)}$.

Notes on Hamiltonian MCMC

- Also known as Hybrid Monte Carlo.
- It used information from the gradient and results in more ‘targeted’ proposals.
- It is black-box, i.e. can be applied to any model.
- The parameters h, L and S need to be specified. This can be done by looking at the history of the chain, but it is not always and easy task.
- Can be implemented via Python and R packages like Stan.

Today's lecture - Reading

Bishop: 11.1.4 11.2, 11.3 11.5

Murphy: 24.2.1-3 24.3.1-4 24.4.1 24.5.4

Outline

Metropolis Hastings Markov Chains are stationary

Proposition: A Markov chain from a Metropolis-Hastings algorithm is reversible. In other words (suppressing the dependency on y)

$$\pi(\theta_t)P(\theta_{t+1}|\theta_t) = \pi(\theta_{t+1})P(\theta_t|\theta_{t+1})$$

Proof: Note that $P(\theta_{t+1}|\theta_t) = q(\theta_{t+1}|\theta_t)\alpha(\theta_t, \theta_{t+1})$.

We will consider the three possible cases for $\pi(\theta_t)q(\theta_{t+1}|\theta_t)$ and $\pi(\theta_{t+1})q(\theta_t|\theta_{t+1})$ separately.

Case 1: If $\pi(\theta_t)q(\theta_{t+1}|\theta_t) = \pi(\theta_{t+1})q(\theta_t|\theta_{t+1})$, then

$$\alpha(\theta_t, \theta_{t+1}) = \frac{\pi(\theta_{t+1})q(\theta_t|\theta_{t+1})}{\pi(\theta_t)q(\theta_{t+1}|\theta_t)} = 1 = \alpha(\theta_{t+1}, \theta_t),$$

so the detailed balance is satisfied with

$$P(\theta_{t+1}|\theta_t) = q(\theta_{t+1}|\theta_t) \text{ and } P(\theta_t|\theta_{t+1}) = q(\theta_t|\theta_{t+1})$$

Proof of reversibility of Metropolis-Hastings

Case 2: If $\pi(\theta_t)q(\theta_{t+1}|\theta_t) > \pi(\theta_{t+1})q(\theta_t|\theta_{t+1})$, then $\alpha(\theta_{t+1}, \theta_t) = 1$ so $\pi(\theta_{t+1})P(\theta_t|\theta_{t+1}) = \pi(\theta_{t+1})q(\theta_t|\theta_{t+1})$. But

$$\alpha(\theta_t, \theta_{t+1}) = \frac{\pi(\theta_{t+1})q(\theta_t|\theta_{t+1})}{\pi(\theta_t)q(\theta_{t+1}|\theta_t)}.$$

Hence

$$\begin{aligned}
\pi(\theta_t)P(\theta_{t+1}|\theta_t) &= \pi(\theta_t)q(\theta_{t+1}|\theta_t)\alpha(\theta_t, \theta_{t+1}) \\
&= \pi(\theta_t)q(\theta_{t+1}|\theta_t)\frac{\pi(\theta_{t+1})q(\theta_t|\theta_{t+1})}{\pi(\theta_t)q(\theta_{t+1}|\theta_t)} \\
&= \pi(\theta_{t+1})q(\theta_t|\theta_{t+1}) \\
&= \pi(\theta_{t+1})P(\theta_t|\theta_{t+1})
\end{aligned}$$

Case 3: Similar to Case 2.