Markov Chain Monte Carlo

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Bayesian Statistics Explorations

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Contents

Overview

- Monte Carlo simulation: directly sample random numbers from a distribution of interest (e.g. normal distribution).
- There are applications – especially those involving Bayesian inference – where this is not possible.
- Idea of Markov Chain Monte Carlo (MCMC): cleverly choose a Markov chain whose stationary distribution corresponds to the distribution of interest.
- By running simulations of this Markov chain for long enough, construct a sample the approximates the distribution of interest.
- Exposition here uses material from (Lemieux, 2009), (Stachurski, 2016), (Fahrmeir et al., 2009).

Contents

Markov chain

- A standard reference is (Norris, 1998).
- Let λ be a distribution on a countable set I (the state-space).
- A matrix $P = (p_{ij} : i, j \in I)$ is stochastic if every row $(p_{ij} : j \in I)$ is a distribution; this is the so-called transition matrix.

Definition

The process $(X_n)_{n\geq 0}$ is a Markov chain with initial distribution λ and transition matrix P if

(i) X_0 has distribution λ, i.e., $\mathbf{P}(X_0 = j) = \lambda_j$;

(ii) for $n \geq 0$, conditional on $X_n = i$, X_{n+1} has distribution $(p_{ij} : j \in I)$;

(iii) $\mathbf{P}(X_{n+1} = j | X_0 = i_0, X_1 = i_1, \ldots, X_n = i) = \mathbf{P}(X_{n+1} = j | X_n = i)$.

Invariant / stationary distribution

Definition

The distribution λ is invariant (stationary) for P if

$$\lambda P = \lambda.$$

Theorem

Let $(X_n)_{n\geq 0}$ be Markov(λ, P). If λ is invariant for P, then $(X_{m+n})_{n\geq 0}$ is also Markov(λ, P).

Convergence to equilibrium

Definition

A Markov chain is irreducible if it is possible to get to any state from any other state.

Definition

The state $i \in I$ is aperiodic if

$$p_{ii}^{(n)} = \mathbf{P}(X_{n+m} = i | X_m = i) > 0, \qquad \text{for sufficiently large } n.$$

A Markov chain is aperiodic if all states are aperiodic.

Theorem

Let P be irreducible and aperiodic, and suppose that P has an invariant distribution π. Let λ be any distribution. Suppose that $(X_n)_{n \geq 0}$ is Markov(λ, P). Then

$$\mathbf{P}(X_n = j) \to \pi_j \text{ as } n \to \infty \text{ for all } j.$$

Ergodic Markov process

Definition

A Markov chain is ergodic if it is aperiodic, irreducible and if it has an invariant distribution.

Ergodic Theorem

- Ergodic Theorems: limiting behaviour of averages over time.
- Example: Strong law of large numbers.

Theorem (Ergodic Theorem)

Let P be irreducible and let λ be any distribution. If $X = (X_n)_{n\geq 0}$ is Markov(λ, P) and if P has an invariant distribution, then, for any bounded function $f : I \to \mathbb{R}$ we have

$$\mathbf{P}\left(\left(\frac{1}{n}\sum_{k=0}^{n-1} f(X_k) \to \overline{f} \text{ as } n \to \infty\right)\right) = 1,$$

where

$$\overline{f} = \sum_{i\in I} \pi_i f_i,$$

and where $\pi = (\pi_i : i \in I)$ is the unique invariant distribution.

Stochastic kernel

- In the following, we use the notion of a stochastic kernel, which describes the transition behaviour of Markov processes in general.
- A transition matrix is a stochastic kernel for a discrete system.
- A transition density describes the transition behaviour of a Markov chain with state space a subset of $\mathbb{R}^d$.

Definition

Let $\mathcal{B}(S)$ be the Borel subsets of $S \subset \mathbb{R}^K$. A stochastic kernel is a function $Q : S \times \mathcal{B}(S) \to [0, 1]$ such that

(i) $Q(\boldsymbol{s}, \cdot)$ is a probability measure on $\mathcal{B}(S)$ for all $\boldsymbol{s} \in S$ and

(ii) $g_B(\boldsymbol{s}) := Q(\boldsymbol{s}, B)$ is $\mathcal{B}$-measurable for each $B \in \mathcal{B}(S)$.

Contents

Markov Chain Monte Carlo

- MCMC is a way of simulating from a given density π on $S \subset \mathbb{R}^d$. The idea is to construct a stochastic kernel P on S such that
  (i) π is a stationary distribution for P,
  (ii) P is sufficiently ergodic that its sample path averages converge to expectations under π.

MCMC: Metropolis-Hastings algorithm, ideas

- The Metropolis-Hastings algorithm starts with a proposal density $q = q(s, s')$.
- Draws from the proposal density are called proposals.
- Each proposal is
  - either accepted by moving to the new state;
  - or rejected by staying at the existing state.
- The probability of accepting is structured so that the chain tends to stay in regions where π puts most probability mass.
- As a consequence, for a sequence (X_t) generated by this process:

$$\text{fraction of time spent in } B = \frac{1}{T}\sum_{t=1}^{T} \mathbf{1}_{\{X_t \in B\}} \approx \pi(B) \quad \text{for large } T.$$

MCMC: Metropolis-Hastings algorithm

- Assume that the acceptance probability is $\alpha = \alpha(X_t, Y)$, where
  - X_t is the current state,
  - Y is the proposal.
- The algorithm draws Y from $q(X_t, \cdot)$ and $U \sim U(0,1)$ independently.
- If $U \leq \alpha(X_t, Y)$, then $X_{t+1} = Y$, else $X_{t+1} = X_t$.
- It is easily checked that the stochastic kernel of (X_t) has the form

$$P(s, B) = \int_B p(s, s')\,\mathrm{d}s' + (1 - \lambda(s))\mathbf{1}_{\{s \in B\}},$$

where $p(s, s') := q(s, s')\alpha(s, s')$ and $\lambda(s) := \int p(s, s')\,\mathrm{d}s'$.

MCMC: Metropolis-Hastings algorithm

- In the Metropolis-Hastings algorithm, the acceptance probability function α is defined as

$$\alpha(s, s') := \min\left\{\frac{\pi(s')q(s', s)}{\pi(s)q(s, s')}, 1\right\},$$

with $\alpha(s, s') = 1$ if $\pi(s)q(s, s') = 0$.

Theorem

In the setting above, π is a stationary distribution for P.

- If $q(s, s') = q(s', s)$, e.g. $q(s, s') = \phi(s - s')$ for some function ϕ, sampling from π boils down to being able to calculate density values of π.

Bayesian estimation

- If π is a posterior density in Bayesian estimation,

$$p(\boldsymbol{\theta}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\boldsymbol{x})},$$

  with $p(\boldsymbol{x}) = \int(p(x|\boldsymbol{\theta}')p(\boldsymbol{\theta}')\,\mathrm{d}\boldsymbol{\theta}'$, then calculation of the integral drops out due to the ratio in α.

- Here,
  - $p(\boldsymbol{\theta})$ is the prior density,
  - $p(\cdot|\boldsymbol{\theta})$ the likelihood (joint density of the data given $\boldsymbol{\theta}$)
  - $p(\cdot|\boldsymbol{x})$ is the posterior density.

Contents

MCMC example

- This follows the example from Section B.5 of (Fahrmeir et al., 2009).
- Let $Y_1, \dots, Y_n$ be a sample of independent, Poisson distributed random variables with parameter λ.
- λ is unknown and to be estimated using Bayesian inference and MCMC.
- The joint distribution of the sample $\boldsymbol{y} = (y_1, \dots, y_n)$ is

$$p(\boldsymbol{y}|\lambda) = \prod_{i=1}^{n} f(y_i; \lambda),$$

where $f(\cdot; \lambda)$ denotes the Poisson probability function with parameter λ.

MCMC example

- Choice of prior: The Gamma distribution is a conjugate prior
  - (i.e., prior and posterior have the same distribution type),

  so we choose $\lambda \sim G(a, b)$.
- Other prior distributions (e.g. uniform, normal, ...) give good results, too.
- The posterior is
$$p(\lambda|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\lambda)p(\lambda)}{\int p(\boldsymbol{y}|\lambda)p(\lambda)\,\mathrm{d}\lambda}.$$
- Using MCMC, the denominator, which is a constant that does not depend on λ, drops out.
- The posterior density is
$$\boldsymbol{y}|\lambda \sim G\left(a + \sum_{i=1}^{n} y_i, b + n\right).$$

MCMC example

- Drawing the sample and setting up likelihood and prior functions:

```
>>> import numpy as np
>>> import scipy as sp
>>> import scipy.stats as scs
>>> import matplotlib.pyplot as plt
>>> plt.style.use('seaborn')  # sets the plotting style
>>> np.random.seed(583920)

>>> a=0.1
>>> y = scs.poisson.rvs(1, size=125) # sample data
>>> y.mean()
0.984

>>> def l(lamb): # likelihood
...     return scs.poisson.pmf(y, lamb).prod()
...
>>> def prior(lamb):
...     return scs.gamma.pdf(lamb, a) # gamma prior
```

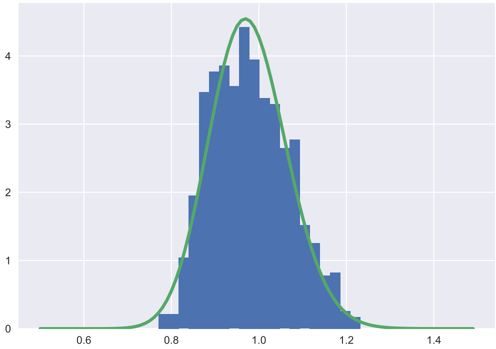
MCMC example

- Running the MCMC algorithm and plotting the posterior density:

```
...
>>> T = 1000
>>> sigma = 0.05
>>> x = np.zeros(T)
>>> z = scs.norm.rvs(size=T) # simulate proposal from normal proposal density
>>> u = scs.uniform.rvs(size=T)
>>> x[0] = 1
>>> for t in range(1,T):
...     s = x[t-1] + sigma * z[t-1] # proposal
...     alpha = l(s) * prior(s) / (l(x[t-1]) * prior(x[t-1])) \
...             if (l(x[t-1]) * prior(x[t-1])) > 0 else 1
...     x[t] = s if u[t] <= alpha else x[t-1]
...
>>> u = np.arange(0.5,1.5,0.01)
>>> _ = plt.hist(x, bins=20, density=True);
>>> alpha = a + y.sum()
>>> beta = 1 + len(y)
>>> _ = plt.plot(u, scs.gamma.pdf(u, alpha) * sp.exp(u * (1-beta)) \
...     * beta**alpha, linewidth=3);
>>> plt.savefig('mcmc_pic.pdf')
>>> print(x.mean())
0.9806439285842388
```

MCMC example

- Output produced:



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Thank you!

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