Markov Chain Monte Carlo

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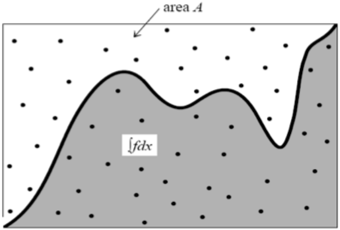
Lecture plan

- Monte Carlo method
- Sampling from a distribution
- Metropolis-Hastings algorithm
- Markov Chain Monte Carlo

Monte Carlo integration

- Numerica method to compute high dimensional integrals $\int \int ... \int f(x_1...x_n)dx_1...dx_n$
- Rectangualr, Trapzoidal, Simpson's rule..
- Numerical integration using random numbers (samples)
- Compute $I = \int_a^b f(x)dx$



Monte Carlo integration

- Expectation value $E_p[z] = \int zp(z)dz = \lim_{n\to\infty} \frac{1}{n}\sum_1^n z_i \approx \frac{1}{n}\sum_1^n z_i$
- Integral $I = \int f(x)dx = \int f(x)\cdot 1\ dx = E_1[f(x)] \approx \frac{1}{n}\sum_1^n f(x_i)$
- Split $f(x) = g(x)p(x)$, where $p(x)$ - PDF, then
  $I = \int f(x)dx = \int g(x)p(x)dx = E_{p(x)}[g(x)] \approx \frac{1}{n}\sum_i^n g(x_i)$
- need to be able to generate random samples
  from complex $p(x)$ distributions

Metropolis-Hastings algorithm

- 1953/1970
- Idea: construct Markov Chain (transition matrix P) with $\pi(x) = p(x)$ stationary distribution $\pi = \pi P$
- Run the chain, generate random samples $x_0, x_1, x_2 ...$

Detailed balance

Ergodic Markov Chain
Sufficient condition for π to be stationary distribution

- reversibility condition
- $\pi_i P_{ij} = \pi_j P_{ji}$
- $\sum_i \pi_i P_{ij} = \sum_i \pi_j P_{ji} = \pi_j \sum_i P_{ji} = \pi_j$
- $\pi P = \pi$ - stationary distribution

Continuous time and space Markov chains

DTDS

- $p_j(n)$
- P_{ij}
- $\sum_j P_{ij} = 1$
- $p_j(n+1) = \sum_i P_{ij} p_i(n)$
- $\pi_j = \sum_i P_{ij} \pi_i$
- $\pi_i P_{ij} = \pi_j P_{ji}$

CTCS

- $x(t)$
- $Q(x, y)$
- $\int Q(x, y) dy = 1$
- $p_{t+1}(x) = \int Q(x, y) p_t(y) dy$
- $\pi(x) = \int Q(x, y) \pi(y) dy$
- $\pi(x) Q(x, y) = \pi(y) Q(y, x)$

Transition matrix construction

Need to find $P(x, y)$ such that $\pi(x)P(x, y) = \pi(y)P(y, x)$
Let Q some "candidate"desity for MC.

1. if $\pi(x)Q(x, y) = \pi(y)Q(y, x)$, done $P \equiv Q$
2. if $\pi(x)Q(x, y) > \pi(y)Q(y, x)$, let $P(x, y) = \alpha(x, y)Q(x, y)$
   where $0 \leq \alpha(x, y) \leq 1$
   $\alpha(x, y)$ - probability of a "forward move"
   $\alpha(y, x)$ - probability of "reverse move";choose $\alpha(y, x) = 1$

   Then $\pi(x)P(x, y) = \pi(x)\alpha(x, y)Q(x, y) =$
   $= \pi(y)\alpha(y, x)\ Q(y, x) = \pi(y)Q(y, x)$

   $$\alpha(x, y) = \frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}$$

3. if $\pi(x)Q(x, y) < \pi(y)Q(y, x)$, let $P(y, x) = \alpha(y, x)Q(y, x)$,

Transition matrix construction

Metropolis-Hastings:

$$\alpha(x, y) = \min\left[\frac{\pi(y)Q(y, x)}{\pi(x)Q(x, y)}, 1\right]$$

Metropolis (symmetric $Q(x, y) = Q(y, x)$)

$$\alpha(x, y) = \min\left[\frac{\pi(y)}{\pi(x)}, 1\right]$$

if $\pi(y) < \pi(x)$, move $x \to y$ with probability $\pi(y)/\pi(x)$
if $\pi(y) > \pi(x)$, move $x \to y$ with probability 1

Metropolis-Hastings algoritm

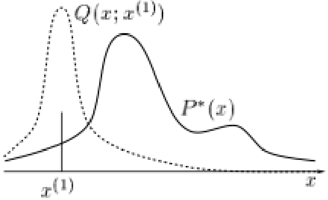
Task: compute N random samples from provability distribution $P(x)$
Select initial $Q(x, y)$

1. select initial value x_0, set $n = 0$
2. generate "canditate"random point $x^* \leftarrow Q(x_n, x^*)$
3. calculate $\alpha(x_n, x^*) = \frac{P(x^*)Q(x^*, x_n)}{P(x_n)Q(x_n, x^*)}$
4. generate uniform random $u \leftarrow U(0, 1)$
5. if $u \leq \alpha(x^*, x_n)$, set $x_{n+1} = x^*$, else set $x_{n+1} = x_n$
6. $n = n + 1$
7. if $n < N$ go to Step 2, else return $\{x_0, x_1, ...x_N\}$

Selection of proposal Q

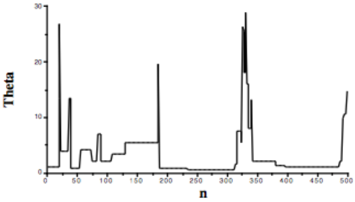
Proposal distribution $Q(x, y)$

- Metropolis - symmetric: $Q(x, y) = Q(y, x) = f(y - x)$, f- Gaussian
- Random walk $y = x + z$, $z \sim \mathcal{N}(0, \sigma^2)$

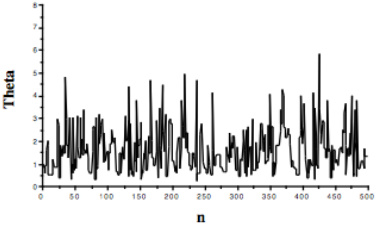


Sample traces

poor mixing chain



well mixing chain



References

- Monte Carlo sampling methods using Markov chains and their applications. W. K. Hastings, Biometrika, 57,1, 1970, p. 97.
- Understanding the Metropolis-Hastings Algorithm. S. Chib, E. Greenberg, The American Statistician, Vol. 49, No. 4. ,1995, pp. 327-335.
- A guided walk Metropolis algorithm. Paul Gustafson, Statistics and computing (1998) 8, 357-364
- Equation of State Calculations by Fast Computing Machines. Metropolis, N.,Rosenbluth, A. W.. Rosenbluth, M. N., Teller. A. H.. and Teller, E, Journal of Chemichal Physics, 21, 1953, p 1087-1092.