STAT0008: Stochastic Processes

Lecture 13 - Markov Chain Monte Carlo

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Key concepts:

- *Gibbs sampling;*
- *Metropolis-Hastings algorithm.*

13.1 Gibbs sampling

Theorem 13.1 (Hammersley-Clifford)
设概率密度 $\pi(x_1, x_2, ..., x_d)$满足正定性条件*(positivity condition)*，即如果对于所有$x_1, ..., x_d$，边缘密度$\pi_{X_i}(x_i) > 0$，就有

$$\pi(x_1, x_2, ..., x_d) > 0$$

成立，那么对于所有$(z_1, ..., z_d) \in supp(\pi)$，即$\pi(z_1, ..., z_d) > 0$，

$$\pi(x_1, x_2, ..., x_d) \propto \prod_{j=1}^{d} \frac{\pi_{X_j|X_{-j}}(x_j|x_1, ..., x_{j-1}, z_{j+1}, ..., z_d)}{\pi_{X_j|X_{-j}}(z_j|x_1, ..., x_{j-1}, z_{j+1}, ..., z_d)}$$

Proof: 由条件概率的定义

$$\pi(x_1, x_2, ..., x_d) = \pi_{X_d|X_{-d}}(x_d|x_1, ..., x_{d-1})\, \pi(x_1, x_2, ..., x_{d-1})$$

对于z_d，同样有

$$\pi(x_1, x_2, ..., x_{d-1}, z_d) = \pi_{X_d|X_{-d}}(z_d|x_1, ..., x_{d-1})\, \pi(x_1, x_2, ..., x_{d-1}).$$

那么

$$
\begin{aligned}
\pi\left(x_1,x_2,...,x_d\right) &= \pi\left(x_1,x_2,...,x_{d-1},z_d\right)\frac{\pi_{X_d|X_{-d}}\left(x_d|x_1,...,x_{d-1}\right)}{\pi_{X_d|X_{-d}}\left(z_d|x_1,...,x_{d-1}\right)}\\
&= \dots\\
&= \pi\left(z_1,...,z_d\right)\frac{\pi_{X_1|X_{-1}}\left(x_1|z_2,...,z_d\right)}{\pi_{X_1|X_{-1}}\left(z_1|z_2,...,z_d\right)}\cdots\frac{\pi_{X_d|X_{-d}}\left(x_d|x_1,...,x_{d-1}\right)}{\pi_{X_d|X_{-d}}\left(z_d|x_1,...,x_{d-1}\right)}
\end{aligned}
$$

正定性条件保证了我们引入的条件概率是大于0的。 ■

Proposition 13.2 *Systematic scan Gibbs sampler* 的不变分布为 π.

Proof: 只证明$d=2$的情形，$d>2$类似。要证π是Systematic scan Gibbs sampler 的不变分布，即证：

$$\int_S \pi\left(x^{(t-1)}\right)P\left(x^{(t-1)},x^{(t)}\right)dx^{(t-1)}=\pi\left(x^{(t)}\right)$$

其中

$$P\left(x^{(t-1)},x^{(t)}\right)=\pi_{X_1|X_{-1}}\left(x_1^{(t)}\middle|x_2^{(t-1)}\right)\cdot\pi_{X_2|X_{-2}}\left(x_2^{(t)}\middle|x_1^{(t)}\right)$$

那么

$$
\begin{aligned}
&\int \pi\left(x^{(t-1)}\right)P\left(x^{(t-1)},x^{(t)}\right)dx^{(t-1)}\\
&=\int \pi\left(x^{(t-1)}\right)\pi_{X_1|X_{-1}}\left(x_1^{(t)}\middle|x_2^{(t-1)}\right)\cdot\pi_{X_2|X_{-2}}\left(x_2^{(t)}\middle|x_1^{(t)}\right)dx_1^{(t-1)}dx_2^{(t-1)}\\
&=\int \pi_{X_2}\left(x_2^{(t-1)}\right)\pi_{X_1|X_{-1}}\left(x_1^{(t)}\middle|x_2^{(t-1)}\right)\cdot\pi_{X_2|X_{-2}}\left(x_2^{(t)}\middle|x_1^{(t)}\right)dx_2^{(t-1)}\\
&=\int \pi\left(x_1^{(t)},x_2^{(t-1)}\right)\cdot\pi_{X_2|X_{-2}}\left(x_2^{(t)}\middle|x_1^{(t)}\right)dx_2^{(t-1)}\\
&=\pi_{X_1}\left(x_1^{(t)}\right)\cdot\pi_{X_2|X_{-2}}\left(x_2^{(t)}|x_1^{(t)}\right)\\
&=\pi\left(x_1^{(t)},x_2^{(t)}\right).
\end{aligned}
$$

■

13.2 Metropolis-Hastings 算法

Proposition 13.3 *MH* 算法的转移概率为

$$P\left(x^{(t-1)},x^{(t)}\right)=\alpha\left(x^{(t)}\middle|x^{(t-1)}\right)q\left(x^{(t)}\middle|x^{(t-1)}\right)+\left(1-a\left(x^{(t-1)}\right)\right)\delta_{x^{(t-1)}}\left(x^{(t)}\right)$$

其中$\delta_{x^{(t-1)}}$是在$x^{(t-1)}$处的$Dirac$测度，

$$a\left(x^{(t-1)}\right)=\int_S \alpha\left(x\middle|\, x^{(t-1)}\right) q\left(x\middle|\, x^{(t-1)}\right) dx.$$

Proof: 对任意$A\subset S$,

$$\begin{aligned}
& P\left(X^{(t)}\in A|X^{(t-1)}=x^{(t-1)}\right)\\
={}& P\left(X^{(t)}\in A,\ \text{accepted}|X^{(t-1)}=x^{(t-1)}\right)+P\left(X^{(t)}\in A,\ \text{rejected}\middle|\, X^{(t-1)}=x^{(t-1)}\right)\\
={}& P\left(X^{(t)}\in A,\ \text{accepted}|X^{(t-1)}=x^{(t-1)}\right)\\
& +P\left(X^{(t)}\in A|X^{(t-1)}=x^{(t-1)},\ \text{rejected}\right)P\left(\text{ rejected}|X^{(t-1)}=x^{(t-1)}\right)\\
={}& \int_A \underbrace{\int_S \delta_x\left(x^{(t)}\right)\alpha\left(x|x^{(t-1)}\right)q\left(x|x^{(t-1)}\right)dx}_{=\alpha\left(x^{(t)}|x^{(t-1)}\right)q\left(x^{(t)}|x^{(t-1)}\right)}\,dx^{(t)}+\underbrace{\int_A \delta_{x^{(t-1)}}\left(x^{(t)}\right)dx^{(t)}}_{=\mathrm{I}_A\left(x^{(t)}\right)}\cdot\left(1-a\left(x^{(t-1)}\right)\right).
\end{aligned}$$

由于

$$P\left(X^{(t)}\in A\middle|\, X^{(t-1)}=x^{(t-1)}\right)=\int_A P\left(x^{(t-1)},x^{(t)}\right)dx^{(t)}$$

所以

$$P\left(x^{(t-1)},x^{(t)}\right)=\alpha\left(x^{(t)}\middle|\, x^{(t-1)}\right)q\left(x^{(t)}\middle|\, x^{(t-1)}\right)+\left(1-a\left(x^{(t-1)}\right)\right)\delta_{x^{(t-1)}}\left(x^{(t)}\right)$$

■

Proposition 13.4 *MH*算法是关于π可逆的，即

$$\pi\left(x^{(t-1)}\right)P\left(x^{(t-1)},x^{(t)}\right)=\pi\left(x^{(t)}\right)P\left(x^{(t)},x^{(t-1)}\right)$$

因此π也是MH算法的不变分布。

Proof:

$$\begin{aligned}
& \pi\left(x^{(t-1)}\right)q\left(x^{(t)}|x^{(t-1)}\right)\alpha\left(x^{(t)}\middle|\, x^{(t-1)}\right)\\
={}& \pi\left(x^{(t-1)}\right)q\left(x^{(t)}\middle|\, x^{(t-1)}\right)\min\left(1,\frac{\pi\left(x^{(t)}\right)q\left(x^{(t-1)}\middle|\, x^{(t)}\right)}{\pi\left(x^{(t-1)}\right)q\left(x^{(t)}\middle|\, x^{(t-1)}\right)}\right)\\
={}& \min\left(\pi\left(x^{(t-1)}\right)q\left(x^{(t)}\middle|\, x^{(t-1)}\right),\pi\left(x^{(t)}\right)q\left(x^{(t-1)}\middle|\, x^{(t)}\right)\right)\\
={}& \pi\left(x^{(t)}\right)q\left(x^{(t-1)}\middle|\, x^{(t)}\right)\min\left(1,\frac{\pi\left(x^{(t-1)}\right)q\left(x^{(t)}\middle|\, x^{(t-1)}\right)}{\pi\left(x^{(t)}\right)q\left(x^{(t-1)}\middle|\, x^{(t)}\right)}\right)\\
={}& \pi\left(x^{(t)}\right)q\left(x^{(t-1)}|x^{(t)}\right)\alpha\left(x^{(t-1)}|x^{(t)}\right)
\end{aligned}$$

那么

$$
\begin{aligned}
&\pi\left(x^{(t-1)}\right) P\left(x^{(t-1)}, x^{(t)}\right) \\
=&\underbrace{\pi\left(x^{(t-1)}\right) q\left(x^{(t)} \middle| x^{(t-1)}\right) \alpha\left(x^{(t)} \middle| x^{(t-1)}\right)}_{=\pi\left(x^{(t)}\right) q\left(x^{(t-1)} \middle| x^{(t)}\right) \alpha\left(x^{(t-1)} \middle| x^{(t)}\right)} + \pi\left(x^{(t-1)}\right) \underbrace{\left(1-a\left(x^{(t-1)}\right)\right) \underbrace{\delta_{x^{(t-1)}}\left(x^{(t)}\right)}_{=0 \text{ if } x^{(t)} \neq x^{(t-1)}}}_{\left(1-a\left(x^{(t)}\right)\right) \delta_{x^{(t)}}\left(x^{(t-1)}\right)} \\
=&\pi\left(x^{(t)}\right) P\left(x^{(t)}, x^{(t-1)}\right).
\end{aligned}
$$

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