马氏链蒙特卡洛方法

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贝叶斯采样、推理

➢ 有未知归一化常数的目标分布

$$\rho^*(\theta) = \frac{1}{Z} e^{-\Phi_R(\theta)}$$

未知

已知

$$\Phi_R(\theta, y) = \frac{1}{2} \| \Sigma_\eta^{-\frac{1}{2}} (y - \mathcal{G}(\theta)) \|^2 + \frac{1}{2} \| \Sigma_0^{-\frac{1}{2}} (\theta - r_0) \|^2$$

- 计算目标分布的期望、协方差等
- 计算目标函数的期望 $\mathbb{E}[f] = \int f(\theta)\rho^*(\theta)d\theta$
- 生成服从目标分布的样本 $\{\theta_j\} \sim \rho^*(\theta)$

马氏链蒙特卡洛方法

- 马氏链蒙特卡洛(Markov Chain Monte Carlo)方法

暴力网格搜索：假设$N_\theta = 2$,

$$\theta_{i,j} = \left[-L + \frac{2(i-1)}{N-1}L, -L + \frac{2(j-1)}{N-1}L\right] \qquad Z = \sum \rho(\theta_{i,j})$$

随机游走：$\theta_n \to \theta_{n+1}$ 概率分布 $\psi_I(\theta_n, \theta_{n+1})$

不变分布是目标分布

$$\rho^*(\theta) = \int \psi_I(\theta', \theta)\rho^*(\theta')d\theta'$$

遍历性质

$\{\theta_n\}_{n\geq N} \sim \rho^*(\theta)$

马氏链蒙特卡洛方法

➢ 马氏链

马氏核：$p(\cdot,\cdot): R^{N_\theta \times N_\theta} \rightarrow R$

- $(\cdot,\cdot) \geq 0$
- $\int p(\theta,\theta')d\theta' = 1$

不变分布ρ^*：

$$\int \rho^*(\theta')p(\theta',\theta)d\theta' = \rho^*(\theta)$$

马氏链：$\{\theta_n\}\ \ n \in Z^+$

$$\theta_0 \sim \rho_0(\theta)$$

$$\theta_{n+1} \sim p(\theta_n,\theta)$$

当$\rho_0 = \rho^*$, 我们有 $\theta_n \sim \rho^*$

马氏链蒙特卡洛方法

马氏链采样

给定 $f: R^{N_\theta} \to R$, $Var_\rho[f] = 1$，构造不变分布是ρ的马氏链$\{\theta_n\}$，我们定义

$$\rho_{\mathrm{MCMC}}^N(f) = \frac{1}{N}\sum_{n=1}^{N} f(\theta_n)$$

我们有

$$\mathbb{E}^{\theta_0\sim\rho}\left[\rho_{\mathrm{MCMC}}^N(f) - \mathbb{E}_\rho[f]\right] = 0$$

$$\mathbb{E}^{\theta_0\sim\rho}\left[\left(\rho_{\mathrm{MCMC}}^N(f) - \mathbb{E}_\rho[f]\right)^2\right] = \frac{\tau_N^2(f)}{N}$$

其中

$$\tau_N^2(f) = 1 + 2\sum_{n=1}^{N}\frac{N-n}{N} Cov\left[f(\theta^0), f(\theta^n)\right]$$

Metropolis-Hastings 算法

- 马氏链

马氏核：

$$\int p(\theta,\theta')d\theta' = 1$$

不变分布ρ^* ：

$$\int \rho^*(\theta')p(\theta',\theta)d\theta' = \rho^*(\theta)$$

$$\rho^*(\theta) = \int \rho^*(\theta)p(\theta,\theta')d\theta'$$

- 细致平衡

$$\rho^*(\theta')p(\theta',\theta) = \rho^*(\theta)p(\theta,\theta')$$

Metropolis-Hastings 算法

- 细致平衡

$$\rho^*(\theta')p(\theta',\theta) = \rho^*(\theta)p(\theta,\theta')$$

$$\frac{\rho^*(\theta')}{\rho^*(\theta)} = \frac{p(\theta,\theta')}{p(\theta',\theta)}$$

- Metropolis-Hastings 算法

提议核(proposal)：

$$q(\cdot,\cdot):\ R^{N_\theta \times N_\theta} \to R^+ \qquad \int q(\theta,\theta')d\theta' = 1$$

接收概率(acceptance-rejection)：

不需要归一化常数

$$a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')q(\theta',\theta)}{\rho^*(\theta)q(\theta,\theta')},\ 1\right\}$$

Metropolis-Hastings 算法

- Metropolis-Hastings 算法

提议核： $q(\cdot,\cdot): R^{N_\theta \times N_\theta} \to R^+$

修正： $a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')q(\theta',\theta)}{\rho^*(\theta)q(\theta,\theta')}, 1\right\}$

给定 θ_n

- 采样 $\theta' \sim q(\theta_n, \theta')$
- 计算$a(\theta_n, \theta')$

$$\theta_{n+1} = \begin{cases} \theta' & \text{以 } a(\theta_n,\theta') \text{的概率} \\ \theta_n & \text{以 } 1 - a(\theta_n,\theta') \text{的概率} \end{cases}$$

$$p_{\mathrm{MH}}(\theta,\theta') = a(\theta,\theta')q(\theta,\theta')$$
$$p_{\mathrm{MH}}(\theta,\theta) = q(\theta,\theta) + \int \big(1 - a(\theta,\theta')\big)q(\theta,\theta')\mathrm{d}\theta'\delta(\theta)$$

Metropolis-Hastings 算法

- Metropolis-Hastings 算法

提议核： $q(\cdot,\cdot): R^{N_\theta \times N_\theta} \to R^+$

修正： $a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')q(\theta',\theta)}{\rho^*(\theta)q(\theta,\theta')}, 1\right\}$

- 随机游走的Metropolis-Hastings 算法

$$q(\theta,\theta') = \mathcal{N}(\theta';\theta,\delta^2 I)$$

$$q(\theta,\theta') = q(\theta',\theta) \qquad a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')}{\rho^*(\theta)}, 1\right\}$$

希望 $a(\theta,\theta')$尽量大，以更大概率接收、移动

Metropolis-Hastings 算法

- Metropolis-Hastings 算法

提议核：$q(\cdot,\cdot): R^{N_\theta \times N_\theta} \rightarrow R^+$

修正：$a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')q(\theta',\theta)}{\rho^*(\theta)q(\theta,\theta')}, 1\right\}$

- 重要性采样的Metropolis-Hastings 算法

$$q(\theta,\theta') = f(\theta')$$

$$a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')f(\theta)}{\rho^*(\theta)f(\theta')}, 1\right\}$$

目标 $f(\theta') \sim \rho^*(\theta')$，比如: $f = \rho_{\text{prior}}$

Metropolis-Hastings 算法

- Metropolis-Hastings 算法

  提议核：　$q(\cdot,\cdot): R^{N_\theta \times N_\theta} \to R^+$

  修正：　$a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')q(\theta',\theta)}{\rho^*(\theta)q(\theta,\theta')}, 1\right\}$

- Metropolis-Adjusted Langevin (MALA) 算法

  $\rho^*(\theta) \propto e^{-\Phi_R(\theta)}$

  梯度下降方法：　$\theta \to \theta - \epsilon\nabla_\theta\Phi_R(\theta)$

  $\Phi_R\big(\theta - \epsilon\nabla_\theta\Phi_R(\theta)\big) < \Phi_R(\theta) \qquad \rho^*\big(\theta - \epsilon\nabla_\theta\Phi_R(\theta)\big) > \rho^*(\theta)$

  $q(\theta,\theta') = \mathcal{N}(\theta';\theta - \epsilon\nabla_\theta\Phi_R(\theta), \delta^2 I) \qquad \delta^2 = 2\epsilon$

  $a(\theta,\theta') = \min\left\{\frac{\rho^*(\theta')\mathcal{N}(\theta;\ \theta' - \epsilon\nabla_\theta\Phi_R(\theta'), \delta^2 I)}{\rho^*(\theta)\mathcal{N}(\theta';\theta - \epsilon\nabla_\theta\Phi_R(\theta), \delta^2 I)}, 1\right\}$

随机过程

Fokker Planck方程

$(\theta_t)_{t\geq 0} \in R^d$满足$d\theta_t = b(\theta_t, t)dt + \sigma(\theta_t, t)dB_t$， 若

$\theta_t \sim \rho_t$，那么

$$\dot{\rho}_t = -\nabla_\theta \cdot (b_t \rho_t) + \sum_i \sum_j \frac{\partial^2}{\partial_i \partial_j} [D_{ij}\, \rho_t]$$

其中 $D = \frac{1}{2} \sigma_t \sigma_t^T$

马氏链蒙特卡洛方法

- 有限状态空间

考虑有限状态空间 $S=\{1,2,\cdots,d\}$ 上的马氏链

马氏核对应了转移概率矩阵 $P\in R^{d\times d}$

$$P(i,j)\geq 0$$

$$\sum_j P(i,j)=1$$

不变分布对应向量 $\rho^*\in R^d$，满足

$${\rho^*}^T P={\rho^*}^T$$

对于马氏链 $\theta_0\sim\rho_0^T$，我们有

$$\theta_n\sim\rho_n^T=\rho_0^T P^n$$

$$\rho_{n+1}^T=\rho_n^T P$$

马氏链收敛性

有限状态马氏链的收敛性

对于有限状态空间 $S=\{1,2,\cdots,d\}$ 上的马氏链，假设转移概率矩阵 $P\in R^{d\times d}$ 满足

$$\min_{(i,j)\in S\times S} P(i,j) \geq \frac{\epsilon}{d}$$

那么存在唯一不变分布 $\rho\in R^d$，满足

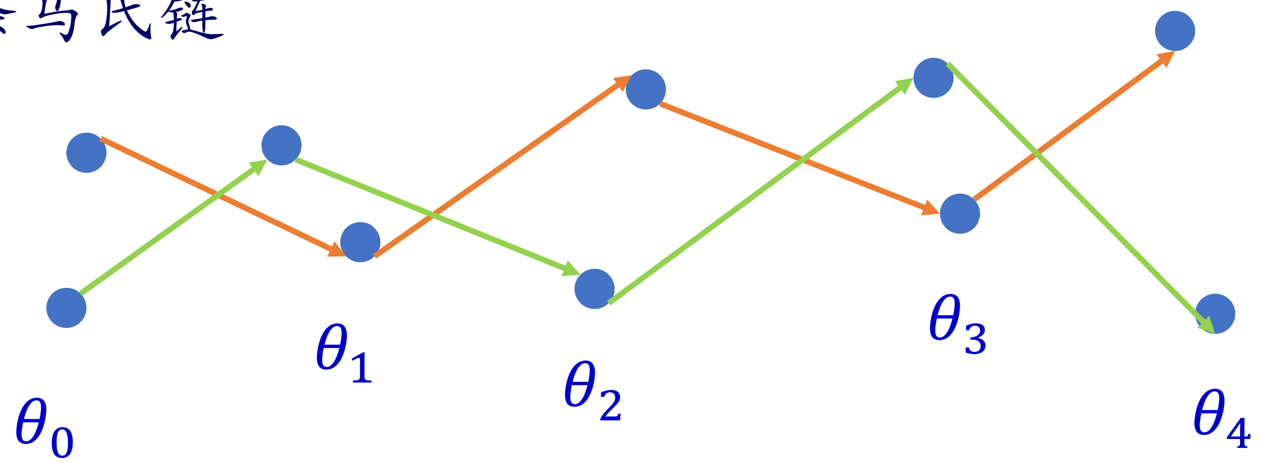
$$\rho^T P = \rho^T$$

对于马氏链 $\{\theta_n\}$，$\theta_n \sim \rho_n$，我们有

$$\mathcal{D}_{TV}(\rho_n,\rho) \leq (1-\epsilon)^n$$

马氏链蒙特卡洛方法

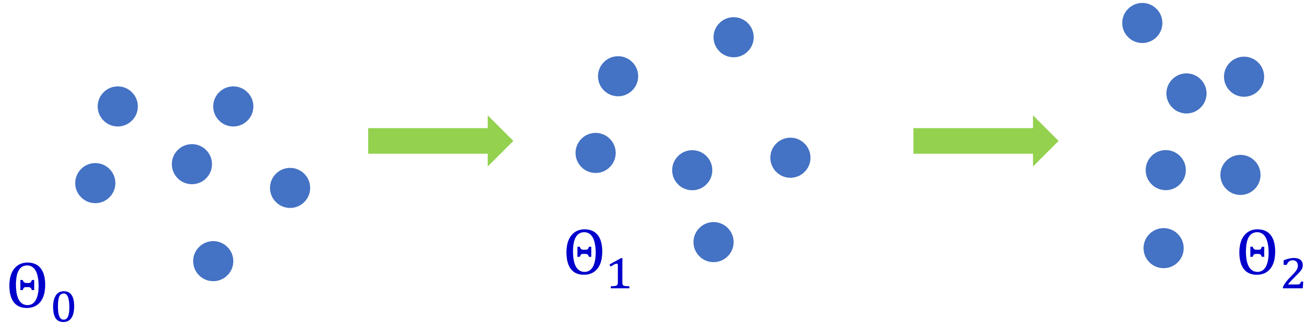
- 两条马氏链



- 交互粒子系统

$$\Theta_n = [\theta_n^1; \theta_n^2; \cdots \theta_n^J] \in R^{N_\theta} \otimes R^{N_\theta} \cdots \otimes R^{N_\theta}$$

$$P^* = \rho^* \otimes \rho^* \cdots \otimes \rho^*$$



马氏链蒙特卡洛方法

➢ 仿射不变马尔可夫链蒙特卡洛集合采样器

https://emcee.readthedocs.io/en/stable/index.html

emcee

emcee is an MIT licensed pure-Python implementation of Goodman & Weare's Affine Invariant Markov chain Monte Carlo (MCMC) Ensemble sampler and these pages will show you how to use it.

This documentation won't teach you too much about MCMC but there are a lot of resources available for that (try this one). We also published a paper explaining the emcee algorithm and implementation in detail.

emcee has been used in quite a few projects in the astrophysical literature and it is being actively developed on GitHub.

GitHub dfm/emcee | Tests passing | license MIT | arXiv 1202.3665 | coverage 96%

Basic Usage

If you wanted to draw samples from a 5 dimensional Gaussian, you would do something like:

```
import numpy as np
import emcee

def log_prob(x, ivar):
    return -0.5 * np.sum(ivar * x ** 2)

ndim, nwalkers = 5, 100
ivar = 1. / np.random.rand(ndim)
p0 = np.random.randn(nwalkers, ndim)

sampler = emcee.EnsembleSampler(nwalkers, ndim, log_prob, args=[ivar])
sampler.run_mcmc(p0, 10000)
```