## Applications of Chatterjee's Correlation in MCMC

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# Introduction

### **Preliminaries**

#### 2.1 Introduction to Markov chain Monte Carlo

**Definition 2.1.** Continuous time markov chain

**Definition 2.2.** markov transition kernel

**Definition 2.3.** time homogeneity

**Definition 2.4.** stationarity

**Definition 2.5.** ergodicity

**Definition 2.6.** time reversibility

**Definition 2.7.** total variation norm

**Definition 2.8.** chapman Kolmogorov

### 2.2 Basic Theorems from Measure Theory

Theorem 2.9. Lebesgue's DCT

# Problems with Pearson correlation coefficent

**Definition 3.1. Pearson correlation coefficient** measures the linear correlation of two sets of data. Given a pair of random variables (X, Y), pearson correlation  $\rho$  is defined as

$$\rho = \frac{\operatorname{Cov}(X, Y)}{\sqrt{\operatorname{Var}[X]} \cdot \sqrt{\operatorname{Var}[Y]}}$$

Pearson's correlation coefficient is very powerful in detecting monotone relations and has a well developed asymptotic theory. The autocorrelation function that we look at in MCMC is also defined using this.

There are two most common problems with this coefficient.

- 1. Firstly, we would like that the correlation would be close to its maximum value if and only if one variable looks like a noiseless function of the other variable. This is not the case for the Pearson's Coefficient as it is close to  $\pm 1$  iff one variable is a noiseless *linear* function.
- 2. Second, we would like the correlation to be close to its minimum value if and only if both the variables are independent of each other. In the case of the Pearson's correlation, it is zero when the variables are independent but the converse is not always true.

# Chatterjee's autocorrelation function

Sourav Chatterjee proposed a new correlation coefficient in [add reference]. This coefficient is (a) as simple as the classical ones, (b) is a consistent estimator of some measure of dependence which is 0 iff the variables are independent, and 1 iff one is a measurable function of the other, and (c) has a simple asymptotic theory under the hypothesis of independence, like the classical coefficients.

**Definition 4.1.** Let (X, Y) be a pair of random variables, where Y is not a constant (for our purposes, both X and Y are continuous). Let  $\{(X_i, Y_i)\}_{i=1}^n$  be i.i.d. pairs following the same distribution as (X, Y).

1. The case when  $X_i's$  and  $Y_i's$  have no ties. Rearrange the data as  $(X_{(1)}, Y_{(1)}), \ldots, (X_{(n)}, Y_{(n)})$  such that  $X_{(1)} < \cdots < X_{(n)}$ . Let  $r_i$  be the rank of  $Y_{(i)}$ , i.e. the number of j such that  $Y_{(j)} \leq Y_{(i)}$ . Then the correlation coefficient  $\xi_n$  is defined to be

$$\xi_n(X,Y) := 1 - \frac{3\sum_{i=1}^{n-1} |r_{i+1} - r_i|}{n^2 - 1}$$

.

2. In the case of ties. If there are ties in  $X_i$ 's, choose an increasing arrangement as follows and break ties uniformly at random. Let  $r_i$  defined as

above, and define  $l_i$  to be the number of j such that  $Y_{(j)} \geq Y_{(i)}$ . Define

$$\xi_n(X,Y) := 1 - \frac{n \sum_{i=1}^{n-1} |r_{i+1} - r_i|}{2 \sum_{i=1}^{n-1} l_i (n - l_i)}$$

. When there are no ties among the  $Y_i's, l_1, \ldots, l_n$  is just a permutation of  $1, \ldots, n$  and the denominator is just  $n(n^2 - 1)/3$ , which reduces to the definition in the no ties case.

The following theorem shows that  $\xi_n$  is a consistent estimator of some measure of dependence between the variables X and Y.

**Theorem 4.2.** If Y is not almost surely a constant, then as  $n \to \infty$ ,  $\xi_n(X, Y)$  converges almost surely to the deterministic limit

$$\xi(X,Y) := \frac{\int Var(\mathbb{E}(1_{\{Y \geq t\}}|X))d\mu(t)}{\int Var(1_{\{Y \geq t\}})d\mu(t)}$$

where  $\mu$  is the pdf of Y. This limit belongs to the interval [0, 1]. It is 0 iff X and Y are independent, and it is 1 iff there is a measurable function  $f: \mathbb{R} \to \mathbb{R}$  such that Y = f(X) almost surely.

Proof of this theorem is presented in Chatterjee's original paper [og paper ref].

Our aim is to create a Markov chain version of this coefficient, i.e. extend this definition to create an analogous of the autocorrelation function defined using the Pearson correlation. Below are some theorems that'll help us in calculating the Chatterjee's autocorrelation function.

Let  $X_1, X_2, ...$  be a stationary, time homogeneous Markov chain with stationary distribution  $\pi$ .

**Theorem 4.3.** Here we present a proof of a well known result about the Pearson Correlation Coefficient.

$$Cov(X_k, X_{k+t})$$
 is independent of  $k$ .

*Proof.* We know that

$$Cov(X_k, X_{k+t}) = \mathbb{E}[X_k X_{k+t}] - \mathbb{E}[X_k] \mathbb{E}[X_{k+t}].$$

Also, as  $X_n$  is a stationary markov chain,  $\mathbb{E}[X_n] = \mu$ , where  $\mu$  is the mean of the distribution  $\pi$ .

And,

$$\mathbb{E}[X_k X_{k+t}] = \int \int xy f_{(X_k, X_{k+t})}(x, y) dx dy$$

where  $f_{(X_k,X_{k+t})}$  is the joint density of  $X_k$  and  $X_{k+t}$ . Now as the markov chain is stationary, this density is dependent only on t, i.e.

$$f_{(X_k, X_{k+t})} = f_{(X_1, X_{1+t})}.$$

As both the terms of  $Cov(X_k, X_{k+t})$  are independent of k,  $Cov(X_k, X_{k+t})$  is independent of k.

The above result is used in estimating the acf using a single Markov chain. The next theorem is the analogous version of the former for the Chatterjee's correlation.

**Theorem 4.4.**  $\xi(X_n, X_{n+k})$  is independent of n, where n and k are in  $\mathbb{N}$ .

Proof.

$$\xi_{(X_n, X_{n+k})} = \frac{\int \operatorname{Var}\left[\mathbb{E}\left[1_{\{X_{n+k} \ge t\}} | X_n = x\right]\right] d\pi(t)}{\int \operatorname{Var}\left[1_{\{X_{n+k} \ge t\}} | d\pi(t)\right]}$$
(4.1)

We'll prove that both the numerator and the denominator are independent of k.

We can write

$$\mathbb{E}[1_{\{X_{n+k} > t\}} | X_n = x] = \Pr(X_{n+k} \ge t | X_n = x)$$

and by time-homogeneity of our Markov chain

$$\Pr(X_{n+k} \ge t | X_n = x) = \int_t^\infty P^k(x, dy)$$

which is independent of n. And hence,

$$\int \operatorname{Var} \left[ \int_{t}^{\infty} P^{k}(x, dy) \right] d\pi(u) \tag{4.2}$$

is also independent of n.

Now for the denominator, we know by stationarity of our Markov chain that  $X_n \sim \pi$ , so for any function  $f, f(X_n) \sim \pi'$  for some distribution  $\pi'$ , and therefore the variance will be same for all n.

Let  $f_t : \mathbb{R} \to \mathbb{R}$  such that  $f_t(X) = 1_{\{X \ge t\}}$ .

We can write the denominator as

$$\int \operatorname{Var}\left[f_t(X_{n+k})\right] d\pi(t)$$

where,

$$\operatorname{Var}\left[f_t(X_{n+k})\right] = \operatorname{Var}\left[f_t(X_1)\right].$$

Therefore,

$$\int \operatorname{Var}\left[f_t(X_{n+k})\right] d\pi(t)$$

is independent of both n and k.

As both the numerator and denominator are independent of n, we can conclude that  $\xi(X_n, X_{n+k})$  is independent of n.

In general,  $\xi$  is not a symmetric in X and Y. This is intentional and useful as we might want to study if Y is a measurable function of X, or X is a measurable function of Y. But for our purposes, it'd be great to have symmetricity as that is required in estimating the variance in the Markov chain version of the Central Limit Theorem.

**Theorem 4.5.**  $\xi(X_n, X_{n+k}) = \xi(X_{n+k}, X_n)$  for time reversal Markov chains for any  $n, k \in \mathbb{N}$ .

*Proof.* By [last theorem ref], we know that the denominator of  $\xi(X_n, X_{n+k})$  is independent of both n and k. So we only have to prove that the numerator is symmetric.

We have to show that

$$\int \operatorname{Var}\left[\Pr(X_{n+k} \ge t | X_n)\right] d\pi(t) = \int \operatorname{Var}\left[\Pr(X_n \ge t | X_{n+k})\right] d\pi(t).$$

**Lemma 1.** For a time reversible Markov chain,  $X_n$  and  $X_{n+k}$  are exchangable, i.e.

$$f_{(X_n, X_{n+k})}(x, y) = f_{(X_{n+k}, X_n)}(x, y) \ \forall (x, y) \in \mathbb{R}^2.$$

*Proof.* It is enough to show that for any two  $A, B \in \mathcal{B}(\mathbb{R})$ 

$$\Pr(X_n \in A, X_{n+k} \in B) = \Pr(X_{n+k} \in A, X_n \in B)$$

which is same as

$$\int_{A} \pi(dx) P^{k}(x, B) = \int_{B} \pi(dy) P^{k}(y, A)$$

$$\iff \int_{A} \int_{B} \pi(dx) P^{k}(x, dy) = \int_{B} \int_{A} \pi(dy) P^{k}(y, dx).$$

To prove the above statement, it is enough to show that for any  $x \in A$  and  $y \in B$ ,

$$\pi(dx)P^k(x, dy) = \pi(dy)P^k(y, dx).$$

We proceed by strong induction on k. For k = 1, it is true by definition of reversibility of Markov chains.

Assume that it is true for all  $1 \le m < k$ . We want to prove it for k. By the Chapman-Kolmogorov equation, we have

$$\pi(dx)P^{k}(x,dy) = \pi(dx) \int_{\mathcal{X}} P^{m}(x,dz) \cdot P^{k-m}(z,dy)$$
$$= \int_{\mathcal{X}} \pi(dx)P^{m}(x,dz)P^{k-m}(z,dy)$$

by the inductive hypothesis, we get

$$= \int_{\mathcal{X}} \pi(dz) P^{m}(z, dx) P^{k-m}(z, dy)$$

$$= \int_{\mathcal{X}} P^{m}(z, dx) \pi(dz) P^{k-m}(z, dy)$$

$$= \int_{\mathcal{X}} P^{m}(z, dx) \pi(dy) P^{k-m}(y, dz)$$

$$= \pi(dy) \int_{\mathcal{X}} P^{k-m}(y, dz) P^{m}(z, dx)$$

again by the Chapman-Kolmogorov equation, we get that

$$= \pi(dy) \cdot P^k(y, dx).$$

By this **Lemma 1**, it is clear that

$$\Pr(X_{n+k} \ge t | X_n) = \Pr(X_n \ge t | X_{n+k}) \ \forall t \in \mathbb{R}$$

which implies the result above.

The next theorem states that as the time difference approaches  $\infty$ , the correlation approaches 0.

**Theorem 4.6.**  $\lim_{n\to\infty} \xi(X_1,X_n)=0$  for an Ergodic Markov chain

*Proof.* We have

$$\xi(X_1, X_n) = \frac{\int \operatorname{Var}\left[\mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x]\right] d\pi(t)}{\int \operatorname{Var}\left[1_{\{X_n \ge t\}}\right] d\pi(t)}.$$

The denominator is independent of n as proven in [last to last theorem ref], so we only need to show that the numerator goes to 0 as  $n \to \infty$ .

#### Lemma 2.

$$\lim_{n\to\infty} \int Var\left[\mathbb{E}[1_{\{X_n\geq t\}}|X_1=x]\right] d\pi(t) = \int \lim_{n\to\infty} Var\left[\mathbb{E}[1_{\{X_n\geq t\}}|X_1=x]\right] d\pi(t)$$

*Proof.* Define  $f_n(t) := \operatorname{Var}\left[\Pr(X_n \geq t | X_1 = x)\right] \cdot \pi(t)$ . Assume for the time being that  $f_n$  is measurable,  $\int_{-\infty}^{\infty} f_n < \infty$  and  $f_n$  is continuous.

Now, as  $f_n$  is a product of two bounded functions, it is also bounded. Set

$$C := \sup_{n \in \mathbb{N}} (\sup_{t \in \mathbb{R}} (\operatorname{Var} \left[ \Pr(X_n \ge t | X_1 = x) \right]))$$

then

$$\int_{-\infty}^{\infty} f_n(t)dt \le \int_{-\infty}^{\infty} C\pi(t)dt = C < \infty$$

As  $f_n$  is dominated by g (where  $g(t) := C \cdot \pi(t) \forall t \in \mathbb{R}$ ), by Lebesgue's Dominated Convergence Theorem,

$$\lim_{n \to \infty} \int f_n(t)dt = \int (\lim_{n \to \infty} f_n(t))dt.$$

#### Lemma 3.

 $\lim_{n \to \infty} Var \left[ \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right] = Var \left[ \lim_{n \to \infty} \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right]$ 

*Proof.* We can write

$$\operatorname{Var}\left[\mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x]\right] = \mathbb{E}[\mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x]^2] - \mathbb{E}[\mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x]]^2$$
$$= \mathbb{E}[\Pr(X_n \ge t | X_1 = x)^2] - \mathbb{E}[\Pr(X_n \ge t | X_1 = x)]^2.$$

Assuming that both  $\lim_n \mathbb{E}[\Pr(X_n \ge t | X_1 = x)^2]$  and  $\lim_n \mathbb{E}[\Pr(X_n \ge t | X_1 = x)]^2$  exist,

$$\lim_{n \to \infty} \operatorname{Var} \left[ \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right] = \lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)^2]$$

$$- \lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)]^2$$

$$= \lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)^2]$$

$$- \left(\lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)]\right)^2.$$

For any  $n \in \mathbb{N}$ , we can write

$$\mathbb{E}[\Pr(X_n \ge t | X_1 = x)^n] = \int_{-\infty}^{\infty} \Pr(X_n \ge t | X_1 = x)^n \cdot \pi(t) dt.$$

#### Lemma 4.

$$\lim_{n \to \infty} \int \Pr(X_n \ge t | X_1 = x)^n \cdot \pi(t) dt = \int \lim_{n \to \infty} \Pr(X_n \ge t | X_1 = x)^n \cdot \pi(t) dt.$$

*Proof.* Define  $f_n(t) := \Pr(X_n \ge t | X_1 = x)^n \cdot \pi(t)$ .

Assume for the time being that  $f_n$  is measurable,  $\int_{-\infty}^{\infty} f_n < \infty$  and  $f_n$  is continuous.

Now, as  $f_n$  is a product of two bounded functions, it is also bounded. Now,

$$\int_{-\infty}^{\infty} f_n(t)dt \le \int_{-\infty}^{\infty} \pi(t)dt = 1 < \infty.$$

As  $f_n$  is dominated by  $\pi$ ,

by Lebesgue's Dominated Convergence Theorem,

$$\lim_{n \to \infty} \int f_n(t)dt = \int (\lim_{n \to \infty} f_n(t))dt.$$

Using the **Lemma 4** for n = 1 and 2, we can take limit in both the terms inside, i.e.

$$\lim_{n \to \infty} \operatorname{Var} \left[ \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right] = \lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)^2]$$

$$- \left( \lim_{n \to \infty} \mathbb{E}[\Pr(X_n \ge t | X_1 = x)] \right)^2$$

$$= \mathbb{E}[\lim_{n \to \infty} \Pr(X_n \ge t | X_1 = x)^2]$$

$$- \left( \mathbb{E}[\lim_{n \to \infty} \Pr(X_n \ge t | X_1 = x)] \right)^2$$

$$= \operatorname{Var} \left[ \lim_{n \to \infty} \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right]$$

Now, by (2.4), we know that

$$\mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] = \int_t^\infty P^{n-1}(x, dy)$$

For an Ergodic Markov chain, under the Total Variation Norm, we know that

$$||P^k(x,\cdot) - F(\cdot)|| \to 0 \text{ as } k \to \infty$$

This implies

$$\lim_{n \to \infty} \int \operatorname{Var} \left[ \mathbb{E}[1_{\{X_n \ge t\}} | X_1 = x] \right] d\pi(t) = \lim_{n \to \infty} \int \operatorname{Var} \left[ \int_t^{\infty} P^{n-1}(x, dy) \right] d\pi(t)$$

$$= \int \operatorname{Var} \left[ \int_t^{\infty} \lim_{n \to \infty} P^{n-1}(x, dy) \right] d\pi(t)$$

$$= \int \operatorname{Var} \left[ \int_t^{\infty} F(dy) \right] d\pi(t)$$

$$= \int \operatorname{Var} \left[ 1 - F(t) \right] d\pi(t)$$

$$= \int 0 \cdot d\pi(t)$$

$$= 0$$

under the Total Variation Norm.

Chapter 5
Sketch of Proof of consistency

Some simulation plots and conclusion