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On the Covariance of Sequences in General Spaces

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On the Covariance of Sequences in General Spaces

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Abstract

We discuss a concept of the covariance of sequences in general spaces. The results are based on the concept of Hilbert spaces with reproducing kernel. We give a probability-free notion of independence of infinite sequences. Also a measure of the dependence of two finite sequences in compact polish spaces is given. The measure of dependence introduced in this paper vanishes asymptotically iff the sequences are independent. Furthermore, we give realistic examples and estimations for pseudo random sequences in the s-dimensional unit cube, including numerical examples.

1 Introduction

Given a probability space with a probability P, the conditional probability $P(A|B)$ is defined as

$$P(A|B) = P(A \cap B)/P(B). \tag{1}$$

The random variables X and Y are independent if for all real x and y holds

$$P(X < x \wedge Y < y) = P(X < x)P(Y < y). \tag{2}$$

In the case of independence of X and Y the following relation holds

$$E(XY) = E(X)E(Y). \tag{3}$$

In general, this condition (3) is not sufficient for the independence of X and Y in the sense of (2). Therefore, in mathematical statistics the concept of covariance

$$\operatorname{cov}(X, Y) = E(XY) - E(X)E(Y) \tag{4}$$

is used. The covariance of X and Y in this sense measures the magnitude of dependence of these random variables. Such concepts deserve a probability measure and an expectation of the random variables under consideration.

In this paper we consider a somewhat different access: Given two spaces E_1 and E_2, let $x_1, x_2, ...x_n, ...$ and $y_1, y_2, ...y_n, ...$ be two arbitrary sequences in E_1 and E_2 respectively. Let $f(x)$ and $g(y)$ be two arbitrary continuous functions over E_1 and E_2. We, now, define the N-covariance C_N of $f(x)$ and $g(y)$ via

$$c_N(f, g) := \frac{1}{N}\sum_{n=1}^{N} f(x_n)\,\overline{g(y_n)} - \frac{1}{N^2}\sum_{n_1 n_2=1}^{N} f(x_{n_1})\,\overline{g(y_{n_2})}. \tag{5}$$

This definition in an obvious way follows paradigm (4), whereas the mathematical expectation is replaced by the mean values of the values of $f(x)$ and $g(y)$, evaluated at the points x_n and y_n, $n = 1, ...N$, respectively.

By means of (5) it is possible to define the concept of asymptotically uncorrelated sequences.

Definition: The sequences $(x_1, x_2, ..., x_n, ...)$ and $(y_1, y_2, ..., y_n, ...)$ are called *asymptotically uncorrelated* if for all continuous functions $f(x)$ and $g(y)$ holds

$$\lim_{N\to\infty} c_N(f, g) = 0. \tag{6}$$

The first question to be answered is the question whether such asymptotically uncorrelated sequences do exist. We give a first

Example: Let (x_1, y_1), $(x_2, y_2), ..., (x_n, y_n)$ be a uniformly distributed sequence in $I \times I = [0, 1) \times [0, 1)$. The famous Weyl's criterion says that for all continuous functions $f(x, y), (x, y) \in I \times I$ holds

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} f(x_n, y_n) = \int_I \int_I f(x, y)\, dxdy \tag{7}$$

Spezializing $f(x, y) = f(x)\, g(y)$ we immediately get relation (6).

Examples for uniformly distributed sequences are the sequences $x_n = \{n\theta_1\}$, $y_n = \{n\theta_2\}$, $n = 1, 2, ...$. ($\{x\}$ denotes the fractional part of x.)

As an application of the classical approximation theorem of Kronecker we get: The sequences $\{n\theta_1\} = x_n$ and $\{n\theta_2\} = y_n$ are asymptotically uncorrelated if and only if the numbers θ_1 and θ_2 are independent over the rational number field. We recall: θ_1 and θ_2 are rational independent if $m_1\theta_1 + m_2\theta_2 = 0$ implies $m_1 = m_2 = 0$. For example, the numbers $\sqrt{2}$ and $\sqrt{3}$ are rationally independent.

2 Hilbert Spaces with Reproducing Kernel

Our discussion shows:

1. The definition of the covariance ot two random variables uses the inner product $E(XY)$ which immediately leads to the classical Hilbert space L_2 generally containing functions that essentially are not continuous.
2. The definition of $c_N(f,g)$ implies that $c_N(f,g)$ has all the properties of an inner product. On the other hand the continuous functionals $f \mapsto f(x_n)$, $g \mapsto g(y_n)$ are essentially used whereas the functions f and g are continuous themselves. So we need a Hilbert space of continuous functions. Such Hilbert spaces are called Hilbert spaces with reproducing kernel (H.R.K.).

Definition: A Hilbert space H consisting of continuous functions $f: E \to \mathbb{C}$ is called a *Hilbert spaces with reproducing kernel* (H.R.K.) if there exists a function $K(x,y), K: E \times E \to \mathbb{C}$ such that $\langle f(x), K(x,y)\rangle = f(y)$ holds.

It is well known that such a reproducing kernel is positive definite. Conversely, every positive definite kernel defines a Hilbert space which it reproduces. There are many more and less classical examples of H.R.K. Let us consider the s-dimensional unit cube $I^s = [0,1)^s = E$. Via the second Bernoulli polynomial we introduce the following kernel $K_2(x,y)$:

$$K_2((x_1,...,x_s),(y_1,...,y_s)) := \prod_{i=1}^{s}\left(1-\frac{\pi^2}{6}+\frac{\pi^2}{2}(1-2\{x_i-y_i\})^2\right) \tag{8}$$

That kernel is knowingly positive definite. It plays an important role in the area of number theoretical numerics and in uniform distribution modulo 1.

3 The measure of covariance for compact metric spaces

Let E be a compact metric space. Let $\omega_1 = (x_1, x_2, ..., x_N, ...)$ and $\omega_2 = (y_1, y_2, ..., y_N, ...)$ be infinite sequences in E. After all let (H,K) be a Hilbert space of continuous functions $f: E \to \mathbb{C}$ and $K = K(x,y)$ the reproducing kernel of H. We give the following

Defintion: The sequences ω_1 and ω_2 are *weakly asymptotic uncorrelated with respect to* K (shortly: K-uncorrelated) if for all pairs of functions $f,g \in H$ holds

$$\lim_{N\to\infty}\left[\frac{1}{N}\sum_{n=1}^{N} f(x_n)\overline{g(y_n)} - \frac{1}{N^2}\sum_{n_1,n_2=1}^{N} f(x_{n_1})\overline{g(y_{n_2})}\right] = 0. \tag{9}$$

This definition implies the conditions (5) and (6) exactly. In order to establish the asymptotic uncorrelation properties of the sequences ω_1 and ω_2 one has to check (9) for all pairs of functions. It is the aim of this paper to define a number $C_N(\omega_1, \omega_2)$ in such way that ω_1 and ω_2 are asymptotically uncorrelated if $C_N(\omega_1, \omega_2) \longrightarrow 0$ for $N \longrightarrow \infty$.

On the other hand should $C_N(\omega_1, \omega_2)$ be an estimation for

$$\frac{1}{N} \sum_{n=1}^{N} f(x_n)\overline{g(y_n)} - \frac{1}{N^2} \sum_{n_1,n_2=1}^{N} f(x_{n_1})\overline{g(y_{n_2})} = c_N(f,g)\,. \tag{10}$$

We, now, recall some well-known definitions and properties of the Hilbert space with reproducing kernel: Taking an arbitrary orthonormal base (O.N.B) $(\varphi_n)_{n\geq 1}$ of H one gets the representation

$$K(x,y) = \sum_{m=1}^{\infty} \varphi_m(x)\overline{\varphi_m(y)}. \tag{11}$$

Given a positive definite kernel $K(x,y)$ one gets the reproducing kernel $K^{(2)}$ of $H \times H$ via

$$K^{(2)}((s,t),(u,v)) = K(s,u)\overline{K(t,v)}\ . \tag{12}$$

Given two O.N.B.s $\psi_m(y)$ and $\varphi_m(x)$ in H then the functions $\varphi_{m_1}(x) \cdot \psi_{m_2}(y)$, $m_1, m_1 = 1, 2, ...$ generate an O.N.B. in $H^{(2)} = H \times H$. Doing so one gets the representation

$$K^{(2)}((s,t),(u,v)) = \sum_{m_1,m_2=1}^{\infty} \varphi_{m_1}(s)\overline{\psi_{m_2}(t)}\ \overline{\varphi_{m_1}(u)}\psi_{m_2}(v). \tag{13}$$

Assuming the continuity of $K(x,y)$ one receives

$$\max_y \parallel K(x,y) \parallel = \max_y K(y,y)^{1/2} =: C < \infty \tag{14}$$

and furthermore

$$\max_{u,v} \parallel K^{(2)}((s,t),(u,v)) \parallel_2 = \max_{u,v}(K(u,u)K(v,v))^{1/2} = C^2. \tag{15}$$

We are now able to formulate the following

Lemma: Given a reproducing kernel $L(w,z)$ as a function on $D \times D$ where D is compact and metrizable, then for every O.N.B. $(\alpha_m(x))_m$ of the Hilbert space H_L the infinite series

$$L(w,z) = \sum_m \alpha_m(w)\overline{\alpha_m(z)} \tag{16}$$

does converge uniformly.

Proof: Let $L_M(w,z) = \sum\limits_{m=1}^{M} \alpha_m(w)\overline{\alpha_m(z)}$, $L'_M(w,z) = \sum\limits_{m>M} \alpha_m(w)\overline{\alpha_m(z)}$.

According to our preconditions the kernel $L(z,z) = L_M(z,z) + L'_M(z,z)$ is a continuous function on D, whereas $L_M(z,z)$ converges monotonically increasing to $L(z,z)$. According to the famous Dini's theorem the convergence turns out to be uniform. Furthermore, because of the orthonormality of the function system $\alpha_m(x), m \in \mathbb{N}$, and because of the Cauchy-Schwarz inequality we get

$$|L'_M(w,z)|^2 \leq |\langle L'_M(v,z), L'_M(v,w)\rangle|^2 \leq L'_M(z,z)L'_M(z,z). \tag{17}$$

Because of the uniformly vanishing of the $L'_M(z,z)$

$$\lim_{M\to\infty} \max_{s\in D} L'_M(z,z) = 0, \tag{18}$$

the same holds for $L'_M(w,z)$ for all $(w,z) \in D \times D$. This concludes the proof of the lemma.

Using these assumptions we proof the following

Theorem: Given two asymptotically uncorrelated sequences in the support E of the continuous kernel $K(x,y)$, where E is compact and separable then both sequences $\omega_1 = (x_1, x_2, ..., x_N, ...)$ and $\omega_2 = (y_1, y_2, ..., y_N, ...)$ are asymptotically uncorrelated even in the strong sense. Consequently, using

$$C_N := \| \frac{1}{N} \sum_{n=1}^{N} K^{(2)}(s,t), (x_n, y_n) - \frac{1}{N^2} \sum_{n_1,n_2=1} K^{(2)}((s,t), (x_{n_1}, y_{n_2})) \|_2 \tag{19}$$

we get: $\lim_{N\to\infty} c_N(f,g) = 0$ for all $f, g \in H$ if and only if $\lim_{N\to\infty} C_N = 0$.

More precisely, we get the estimation

$$|c_N(f,g)| \leq \| f \| \| g \| C_N .$$

Proof: Because ot the reproducing property of $K^{(2)}$ for all $n_1, n_2 = 1, 2, ..., N, ...$ we get

$$f(x_{n_1})\bar{g}(y_{n_2}) =< f(s).\bar{g}(t), K^{(2)}((s,t), (x_{n_1}, y_{n_2})) > \tag{20}$$

Henceforth holds the representation of $c_N(f,g)$ as an inner product

$$c_N(f,g) = \langle f(s).\bar{g}(t), B_N K^{(2)} \rangle \tag{21}$$

with

$$B_N K^{(2)} = \frac{1}{N} \sum_{n=1}^{N} K^{(2)}((s,t), (x_n, y_n)) - \frac{1}{N^2} \sum_{n_1,n_2=1}^{N} K^{(2)}((s,t), (x_{n_1}, y_{n_2})). \tag{22}$$

Cauchy-Schwarz's inequality immediately delivers the estimation asserted in the theorem:

$$|c_N(f,g)| \leq \parallel f \parallel \parallel g \parallel C_N \ . \tag{23}$$

Now we assume that the sequences $\omega_1 = (x_1, x_2, ...x_N, ...)$ and $\omega_2 = (y_1, y_2, ...y_N, ...)$ are asymptotically uncorrelated. We show now $\lim_{N\to\infty} C_N = 0$. After a short computation one gets

$$\begin{aligned}
C_N^2 = \frac{1}{N^2} \sum_{n_1,n_2=1}^{N} K^{(2)}((x_{n_1}, y_{n_1}), (y_{n_2}, y_{n_2}))- \\
- \frac{1}{N^3} \sum_{n=1}^{N} \sum_{n_1,n_2=1}^{N} K^{(2)}((x_{n_1}, y_{n_2}), (x_n, y_n))- \\
- \frac{1}{N^3} \sum_{n=1}^{N} \sum_{n_1,n_2=1}^{N} K^{(2)}((x_n, y_n), (x_{n_1}, y_{n_2}))+ \\
+ \frac{1}{N^4} \sum_{n_1,n_2,n_3,n_4} K^{(2)}((x_{n_1}, y_{n_2}), (x_{n_3}, y_{n_4})).
\end{aligned} \tag{24}$$

Because of the representation (13) of the kernel $K^{(2)}((s,t),(u,v))$ after some calculations one gets

$$C_N^2 = \sum_{\max(m_1,m_2)\leq M} |c_N(\varphi_{m_1}, \varphi_{m_2})|^2 + \sum_{\max(m_1,m_2)>M} |c_N(\varphi_{m_1}, \varphi_{m_2})|^2.$$

In accordance with the above lemma we choose a natural number M in such a way that

$$\sum_{\max(m_1,m_2)>M} |c_N(\varphi_{m_1}, \varphi_{m_2})|^2 < \frac{\varepsilon^2}{2} \ . \tag{25}$$

is fulfilled. Because of the assumption that the sequences ω_1 and ω_2 are weakly asymptotically uncorrelated there exists a natural $N_0(\varepsilon)$ such that

for all $N > N_0(\varepsilon)$ holds

$$\sum_{\max(m_1,m_2)\leq M} |c_N(\varphi_{m_1}, \varphi_{m_2})|^2 < \frac{\varepsilon^2}{2} \ . \tag{26}$$

Therefore, for all $N > N_0(\varepsilon)$ holds

$$C_N < \varepsilon, \tag{27}$$

which means

$$\lim_{N\to\infty} C_N = 0. \tag{28}$$

On the contrary, given (28) from (23) immediately follows that for all $f, g \in H$ the relation

$$\lim_{N\to\infty} c_N(f,g) = 0.$$

holds. This completes the proof.

Remark: The complexity of computation of the estimation C_N according to (24) is of order $5N^2$. In general this estimation of complexity of computation cannot be improved in an essential manner: all pairs (x_{n_1}, y_{n_2}), $n_1, n_2 = 1, ..., N$ are to be used computing our measure of correlation.

From the practical point of view the use ot the s-dimensional unit cube is one of the most important cases. Therfore, we give an application for $E = I^s = [0,1]^s$:

Let ω_1 and ω_2 be sequences from I^s, $\omega_1 = (x_1, x_2, ...x_N, ...)$, $\omega_2 = (y_1, y_2, ...y_N, ...)$ where $x_N = \left(x_N^{(1)}, ..., x_N^{(s)}\right)$, $y_N = \left(y_N^{(1)}, ..., y_N^{(s)}\right)$, $0 \le x_N^{(i)}, y_N^{(i)} \le 1$, $i = 1, ..., s$, $N \in \mathbb{N}$. According to (8) the kernel $K(x,y)$ consists of the second Bernoulli polynomial. We set $K_2\left((x^{(1)},, ..., x^{(s)}), \left(y^{(1)},, ..., y^{(s)}\right)\right) = K_2(x,y)$. We, then, get

$$F_N(w_1) = \left(\frac{1}{N^2}\sum_{n_1,n_2=1}^{N} K_2(x_{n_1}, x_{n_2}) - 1\right)^{1/2} \tag{29}$$

which is the diaphony of ω_1 introduced by Zinterhof [9] and investigated by various other authors. The kernel K_2 is interesting because of the fact that ω_1 is uniformly distributed if and only if $\lim_{N\to\infty} F_N = 0$. For the kernel K_2 on I^s the estimator $C_N\left(\omega_1, \omega_1\right)$ writes as

$$\begin{aligned}
C_N^2 = &\frac{1}{N^2}\sum_{n_1,n_2=1}^{N} K_2(x_{n_1}, x_{n_2})K_2(y_{n_1}, y_{n_2}) - \\
&- \frac{2}{N^3}\sum_{n=1}^{N}\sum_{n_1,n_2=1}^{N} K_2(x_{n_1}, x_n)K_2(y_{n_2}, y_n) + \\
&+ \frac{1}{N^4}\left(\sum_{n_1,n_3=1}^{N} K_2(x_{n_1}, x_{n_3})\right)\left(\sum_{n_2,n_4=1}^{N} K_2(y_{n_2}, y_{n_4}\right).
\end{aligned} \tag{30}$$

In the case of number theoretical numerics different well-distributed sequences of nodes $x_1, x_2, ...x_N, ... \in I^s = [0,1]^s$ are available. These Quasi Monte Carlo sequences in general share very good properties with respect to high dimensional numerics. They are used for simulation purposes as well, whereas some statistical properties such as correlation properties play an important role. We restrict us to one of the most important examples:

The integer vector $a = (a_1, ..., a_s)$ is, after Hlawka, called a *good lattice point* or, after Korobow, an *optimal coefficient* if for $a = a(N)$ holds

$$\frac{1}{N}\sum_{n=1}^{N} K_2\left(a \cdot \frac{n}{N}, 0\right) - 1 \leq C_s \frac{\ln^{2\beta(s)} N}{N^2} \quad . \tag{31}$$

This definition of an optimal coefficient is different from the definitions given by Korobow, Bachwalow and Hlawka, however, it is equivalent. Small indexes $\beta(s) \leq s$ are more favourable, of course. An index $\beta(s) \leq s$ is possible, as is well known.

Theorem: Let K_2 be the Bernoulli kernel according to (8), and let $(a_1, ..., a_s, b_1, ..., b_s)$ be optimal coefficients for the modulus N and the dimension $2s$, $\beta(2s)$ being the index. In this case the following estimation holds

$$C_N = O\left(\frac{(\ln N)^{\beta(2s)}}{N}\right). \tag{32}$$

Proof: For $N \in \mathbb{N}$ and $m \in \mathbb{Z}$ we set

$$\delta_N(m) = \begin{cases} 0 & , \quad N \nmid m \\ 1 & , \quad N \mid m \end{cases} . \tag{33}$$

So, for integer vectors $(m_1, ..., m_s)$ and $(d_1, ..., d_s)$ holds

$$\delta_N(d_1 m_1 + \ldots + d_t m_t) = \frac{1}{N}\sum_{n=1}^{N} e^{2\pi i (d_1 m_1 + \ldots + d_s m_s)\cdot n/N}. \tag{34}$$

From the general case (30) we deduce:

$$\begin{aligned}
C_N^2 &= \frac{1}{N^2}\sum_{n_1,n_2=1}^{N} K_2(x_{n_1}, x_{n_2}) K_2(y_{n_1}, y_{n_2}) - \\
&- \frac{2}{N^3}\sum_{n=1}^{N}\sum_{n_1,n_2=1}^{N} K_2(x_{n_1}, x_n) K_2(y_{n_2}, y_n) + \\
&+ \frac{1}{N^4}\left(\sum_{n_1,n_3=1}^{N} K_2(x_{n_1}, x_{n_3})\right)\left(\sum_{n_2,n_4=1}^{N} K_2(y_{n_2}, y_{n_4})\right) =: \\
&=: I - II + III\,.
\end{aligned} \tag{35}$$

The Fourier expansion of $K_2(x, y)$ is well known:

$$K_2(x, y) = \sum_{m \in \mathbb{Z}^s} e^{2\pi i m(x-y)}/R^2(m), \tag{36}$$

Here denotes $R(m) = \max(1, |m_1|) \cdot \max(1, |m_2|) \cdots \max(1, |m_s|)$. So, from (31) we get the expression

$$I = \frac{1}{N^2} \sum_{n_1,n_2} \sum_{m_1,m_1 \in \mathbb{Z}^s} e^{2\pi i (m_1 a + m_2 b)(n_1 - n_2)/N} / (R^2(m_1).R^2(m_2)) =$$
$$= \sum_{m_1,m_2 \in \mathbb{Z}^s} \delta_N(m_1 a + m_2 b)/(R^2(m_1).R^2(m_2)) =$$
$$= 1 + O\left(\frac{\ln N)^{2\beta(2s)}}{N^2}\right). \tag{37}$$

Analogously, one gets

$$II = 2 + O\left(\frac{(\ln N)^{2\beta(2s)}}{N^2}\right) \tag{38}$$

and

$$III = 1 + O\left(\frac{(\ln N)^{2\beta(2s)}}{N^2}\right). \tag{39}$$

This leads to the result stated above:

$$C_N^2 = 1 - 2 + 1 + O\left(\frac{(\ln N)^{2\beta(2s)}}{N^2}\right). \tag{40}$$

Without proof we state a similar theorem for the so-called Kronecker sequences.

Theorem: The sequences $n\theta_1$ and $n\theta_2$ are modulo 1 asymptotically uncorrelated if the $2s$-dimensional vector (θ_1, θ_2) is independent over $\mathbb{Z}^{2s}$. Furthermore, for almost all vectors and every $\varepsilon > 0$ holds

$$C_N((n\theta_1), (n\theta_2)) = O\left(\frac{1}{N^{1-\varepsilon}}\right). \tag{41}$$

In particular one can choose $\theta = (e^{r_1}, e^{r_2}, ..., e^{r_s}, e^{r_{s+1}}, ...e^{r_{2s}})$, $r_i \neq r_k, 0 \neq r_i \in \mathbb{Q}$.

The proof is based on methods of Zinterhof [10] which follows from a famous result from A. Baker.

Finally, we give some few numerical experiments which are performed only in one dimension $s = 1$. in row RND we used sequences which are generated by our built-in random generator. In row EXP we used sequences of the type $n \cdot \exp(1) = x_n$ and $n \cdot \exp(1/2) = y_n$, respectively.

N	10	50	100	1000	2000	5000
RND	1.0735	0.4677	0.2736	0.1005	0.0658	0.0407
EXP	1.0693	0.30608	0.2022	0.0328	0.0164	0.0069

All of the numerical experiments show that the standard random generators provide unnecessarily bad results. The type of the built-in random generator is not known to us.

Final remarks: We introduced the measure of correlation C_N for sequences $x_1, x_2, ...x_N, ... \in E$ and $y_1, y_2, ...y_N, ... \in E$ using a reproducing kernel $K(x, y)$ as a main tool. It is possible to generalize the results by introducing two compact and metrizable spaces E_1 and E_2 equipped with kernels $K_1(x, y) : E_1 \times E_1 \to \mathbb{C}$ and $K_2(x, y) : E_2 \times E_2 \to \mathbb{C}$ resulting in a measure of correlation for sequences $x_1, x_2, ...x_N, ... \in E_1$ and $y_1, y_2, ...y_N, ... \in E_2$. Such a generalization is interesting form the practical point of view, and for theoretical reasons as well.

Literature

The definition of the statistical independence of sequences traces back to Rauzy [1]. In the sequel Grabner and Tichy [2], Grabner, Tichy and Strauch [3, 4] obtained forthcoming results for the special case $E = [0, 1)^s$. Amstler and Zinterhof introduced discrepancies and diaphony in the framework of Hilbert spaces with reproducing kernel [5]. A comprehensive exposition of the theory of uniformly distributed sequences containing two thousand quotations gave Drmota and Tichy [6]. Still one of the best references for Hilbert spaces with reproducing kernel is Aronszajn [7]. Also Saitoh [8] has many merits.

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