POISSONIAN PAIR CORRELATION ON MANIFOLDS
VIA THE HEAT KERNEL

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Abstract. We define a notion of Poissonian pair correlation (PPC) for Riemannian manifolds without boundary and prove that PPC implies uniform distribution in this setting. This extends earlier work by Grepstad and Larcher, Aistleitner, Lachmann, and Pausinger, Steinerberger, and Marklof.

1. Introduction

The concept of Poissonian pair correlation (PPC) for a sequence \((x_k)_{k \in \mathbb{N}}\) in \([0, 1)\) has been introduced by Rudnick and Sarnak \cite{13} and attracted a lot of attention during the last years (see, e. g., \cite{11, 5, 6, 8, 10, 14, 15, 17–20}). Initially this concept was motivated by questions concerning energy-spectra in quantum physics, in particular the Berry-Tabor Conjecture states that discrete energy spectrum of a Hamiltonian operator of a quantum system has PPC. But as it was shown later the concept of PPC has also a strong connection to Diophantine approximation, additive combinatorics, uniform distribution, discrepancy and other areas of mathematics.

The original concept of PPC was one-dimensional, namely a sequence of real numbers \((x_k)_{k \in \mathbb{N}}\) in \([0, 1]\) is said to have PPC, if for all \(s \geq 0\)

\[
\lim_{N \to \infty} \frac{1}{N} \# \left\{ 1 \leq j \neq k \leq N \mid |x_j - x_k| < \frac{s}{N} \right\} = 2s.
\]

Notice that the number pairs of indices \((j, k)\) is \(N^2 - N\), but the condition on the elements of the sequence restricts to a very short interval, so that only a number of pairs of points in the order of \(N\) would satisfy it.

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For higher dimensions the notion obviously generalises, but there is some dependence on the norm chosen as to replace the absolute value. We say that a sequence \((x_k)_{k \in \mathbb{N}}\) of vectors in the \(n\)-dimensional cube \([0, 1)^n\) has PPC, if the multi-dimensional pair correlation statistics for every \(s \geq 0\) satisfies

\[
\lim_{N \to \infty} \frac{1}{N} \# \left\{ 1 \leq k \neq j \leq N : \|x_k - x_j\| < \frac{s}{\sqrt{n}} \right\} = C(\| \cdot \|) s^n,
\]

where

\[C(\| \cdot \|) = \text{vol} \left( \{ x \in \mathbb{R}^n \mid \|x\| \leq 1 \} \right)\]
denotes the volume of the unit ball with respect to the norm \(\| \cdot \|\). The cases of the Euclidean norm \(\| \cdot \|_2\) and the maximum norm \(\| \cdot \|_\infty\) have been investigated especially (see [6, 20]).

It is well-known that for a sequence of independent, identically uniformly distributed (i.i.d.) random points on \([0, 1)^n\), almost surely (1) holds. For \(n = 1\) it was shown in [1, 9] and in the multi-dimensional case in [6, 20].

We say that the sequence \((x_k)_{k \in \mathbb{N}}\) is uniformly distributed or equidistributed, in \([0, 1)^n\) (see, e.g. [7]) if

\[
\lim_{N \to \infty} \frac{1}{N} \# \{ 1 \leq k \leq N : x_k \in [a, b) \} = \prod_{k=1}^{n} (b_k - a_k),
\]

for all \(0 \leq a < b \leq 1\), where we use \(a \leq b\) to mean that \(a_k \leq b_k\), \(1 \leq k \leq n\).

There is an equivalent definition of equidistribution in terms of exponential sums, which is called Weyl’s criterion (see [21]). For more background on uniform distribution theory, see the monograph [7].

It is known that PPC implies uniform distribution of a sequence in \([0, 1)^n\) (for one-dimensional case see, e.g. [15], and for multidimensional case [3]). But on other hand, uniform distribution does not imply PPC. For example, the Kronecker sequence \((\{k\alpha\})_{k \in \mathbb{N}}\), which is uniformly distributed for any irrational \(\alpha\), does not have PPC for any value of \(\alpha\).

However, the sequence \((\{km\alpha\})_{k \in \mathbb{N}}\) with an integer \(m \geq 2\) has PPC for almost all \(\alpha\) (see, e.g. [13]). Another example of sequence with PPC property is \((\{ak\alpha\})_{k \in \mathbb{N}}\), where \((ak)_{k \in \mathbb{N}}\) is a lacunary sequence of positive integers.

More general analysis of multi-dimensional PPC on compact Riemannian manifolds was done in [10] where a statistical argument was used to show that PPC implies equidistribution on manifolds.

**Definition 1.** Let \(\mathcal{M}\) be a compact Riemannian manifold of dimension \(n\). Then a sequence of point sets \((X_N)_{N \in \mathbb{N}}\) on \(\mathcal{M}\) with \(#X_N = N\) and
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$X_N = \{x_1^{(N)}, \ldots, x_N^{(N)}\}$ has Poissonian pair correlation, if for any $s > 0$

$$\lim_{N \to \infty} \frac{1}{N} \# \left\{ 1 \leq j \neq k \leq N \mid N^{1/n} d(x_j^{(N)}, x_k^{(N)}) < s \right\} = s^n B_n,$$

where $d(\cdot, \cdot)$ denotes the geodesic distance on $\mathcal{M}$ and $B_n$ is the volume of the $n$-dimensional Euclidean unit ball $B_n = \frac{\pi^{n/2}}{\Gamma(n/2 + 1)}$.

**Definition 2.** Let $\mathcal{M}$ be a compact Riemannian manifold of dimension $n$ with normalized surface measure $\mu$. Then a sequence of point sets $(X_N)_{N \in \mathbb{N}}$ on $\mathcal{M}$ with $\#X_N = N$ and $X_N = \{x_1^{(N)}, \ldots, x_N^{(N)}\}$ is uniformly distributed on $\mathcal{M}$, if

$$\lim_{N \to \infty} \frac{1}{N} \# \left\{ 1 \leq k \leq N \mid x_k^{(N)} \in B(x, r) \right\} = \mu(B(x, r))$$

for all geodesic balls $B(x, r) = \{y \in \mathcal{M} \mid d(x, y) < r\}$.

The aim of this paper is to prove the following theorem.

**Theorem 1.** Let $\mathcal{M}$ be a $C^2$ compact Riemannian manifold without boundary and with non-negative Ricci curvature. Then any sequence of point sets $(X_N)_{N \in \mathbb{N}}$ with Poissonian pair correlation is uniformly distributed on $\mathcal{M}$.

2. **The Heat Kernel on a Manifold**

Let $\mathcal{M}$ be a smooth compact $n$-dimensional Riemannian manifold without boundary and non-negative Ricci-curvature. Let $\Delta$ denote the Laplace Beltrami operator. This operator is self–adjoint and densely defined on $L^2(\mathcal{M})$. By general theory it has a sequence of eigenvalues $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \cdots$ and a complete orthonormal system of real eigenfunctions $(\varphi_k(x))_k$, such that

$$\Delta \varphi_k(x) + \lambda_k \varphi_k(x) = 0$$

and

$$\int_{\mathcal{M}} \varphi_k(x) \varphi_j(x) d\mu(x) = \delta_{k,j},$$

where $\mu$ is the normalised surface measure on $\mathcal{M}$. 
Remark 1. By the fact that the functions \((\varphi_k)_{k \in \mathbb{N}_0}\) form a complete orthonormal system their linear combinations are dense in the space of continuous functions. Thus uniform distribution of a sequence of point sets \((X_N)_{N \in \mathbb{N}}\) is equivalent to

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} \varphi_j(x_k) = 0
\]

for all \(j \in \mathbb{N}\) (see \[7\]).

The heat kernel \(H(t, x, y)\) is the fundamental solution of the heat equation

\[
\Delta_x u - \partial_t u = 0
\]

with the property

\[
\lim_{t \to 0^+} \int_{\mathcal{M}} H(t, x, y) f(x) \, d\mu(x) = f(y)
\]

for all test functions \(f\).

The heat kernel can be expressed in terms of the eigenfunctions and eigenvalues of \(\Delta\) by

\[
H(t, x, y) = \sum_{k=0}^{\infty} e^{-\lambda_k t} \varphi_k(x) \varphi_k(y).
\]

The heat kernel satisfies an asymptotic expansion

\[
H(t, x, y) = \exp \left( -\frac{d(x, y)^2}{4t} \right) \left( \sum_{k=0}^{\infty} \frac{u_k(x, y) t^k}{(4\pi t)^{\frac{n}{2}}} \right),
\]

which holds for \(t \to 0^+\) uniformly in \((x, y)\) in some compact neighbourhood of the diagonal of \(\mathcal{M} \times \mathcal{M}\). The functions \(u_k\) can be determined by an iterative process given in \[11\]. For general reference to properties of the heat kernel and this expansion we refer to \[2, 3, 12\].

For our purposes the first term in the asymptotic expansion \([9]\) suffices. The function \(u_0(x, y)\) is given as (for \(d(x, y) < \text{inj}(\mathcal{M})\), the injectivity radius)

\[
u_0(x, y) = \left( \det(P_{x,y}^{-1} d \exp_{x}(\exp_{x}^{-1}(y))) \right)^{\frac{1}{2}},
\]

where \(\exp_{x} : T_{x}\mathcal{M} \to \mathcal{M}\) denotes the exponential map and \(P_{x,y}\) denotes parallel transport along the unique geodesic joining \(x\) and \(y\). We only need that \(u_0(x, x) = 1\) and that

\[
u_0(x, y) = 1 + \mathcal{O}(d(x, y))
\]

holds by differentiability of \(u_0\).
We will use (9) in the simplified form
\begin{equation}
H(t, x, y) = \exp \left( -\frac{d(x, y)^2}{4t} \right) (1 + O(d(x, y)) + O(t))
\end{equation}
valid for $t \to 0^+$ uniformly in $(x, y)$ with $d(x, y) \leq c$ for some $c > 0$.

We will also need a general upper bound for the heat kernel (see [4,16]). For every $\delta > 0$ there exists a $C_\delta$ such that
\begin{equation}
H(t, x, y) \leq C_\delta \exp \left( -\frac{d(x, y)^2}{4(1+\delta)t} \right) t^{n/2}.
\end{equation}

3. Poissonian pair correlation

We give a simple characterisation of PPC similar to Weyl’s criterion for uniform distribution. This will be needed later in the proof of Theorem 1, but is also of independent interest.

**Proposition 1.** A sequence $(X_N)_N$ of point sets on $\mathcal{M}$ has Poissonian pair correlation, if and only if for every continuous function $f : \mathbb{R}^+ \to \mathbb{R}$ with
\begin{equation}
\int_0^\infty |f(r)| r^{n-1} dr < \infty
\end{equation}
the relation
\begin{equation}
\lim_{N \to \infty} \frac{1}{N} \sum_{\substack{i,j=1\atop i \neq j}}^N f(N^{1/n} d(x_i, x_j)) = nB_n \int_0^\infty f(r)r^{n-1} dr
\end{equation}
holds.

**Proof.** The proof runs along similar lines as the proof of Theorem 1.1 from [7] with the important difference that the underlying measure in our case is infinite. Let $(X_N)_N$ have PPC. This can be rewritten as
\begin{equation}
\lim_{N \to \infty} \frac{1}{N} \sum_{\substack{i,j=1\atop i \neq j}}^N \mathbb{1}_{[0,s]} \left( N^{1/n} d(x_i, x_j) \right) = nB_n \int_0^\infty \mathbb{1}_{[0,s]}(r)r^{n-1} dr,
\end{equation}
for all $s > 0$. From this it follows immediately that for all $0 \leq a < b$
\begin{equation}
\lim_{N \to \infty} \frac{1}{N} \sum_{\substack{i,j=1\atop i \neq j}}^N \mathbb{1}_{[a,b]} \left( N^{1/n} d(x_i, x_j) \right) = nB_n \int_0^\infty \mathbb{1}_{[a,b]}(r)r^{n-1} dr.
\end{equation}

By linearity this implies that (14) holds for every step function $f$ with compact support.
Now let $f$ be a Riemann integrable function with compact support. By the definition of the Riemann integral for any $\varepsilon > 0$ there exist two step functions $f_1$ and $f_2$, such that $f_1(r) \leq f(r) \leq f_2(r)$ for all $r \geq 0$ and $nB_n \int_0^\infty (f_2(r) - f_1(r))r^{n-1}dr < \varepsilon$.

Thus
\[
nB_n \int_0^\infty f(r)r^{n-1}dr - \varepsilon \leq \lim_{N \to \infty} \frac{1}{N} \sum_{i,j=1 \atop i \neq j}^N f_1(N^\frac{1}{n}d(x_i, x_j)) \leq \lim_{N \to \infty} \frac{1}{N} \sum_{i,j=1 \atop i \neq j}^N f(N^\frac{1}{n}d(x_i, x_j)) \leq \lim \sup_{N \to \infty} \frac{1}{N} \sum_{i,j=1 \atop i \neq j}^N f_2(N^\frac{1}{n}d(x_i, x_j)) \leq nB_n \int_0^\infty f(r)r^{n-1}dr + \varepsilon.
\]

This proves the relation (14) for all Riemann integrable functions of compact support.

Now let $f$ be a non-negative Riemann integrable function with (13). Then for every $R > 0$ we have
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i,j=1 \atop i \neq j}^N f(N^\frac{1}{n}d(x_i, x_j)) = nB_n \int_0^R f(r)r^{n-1}dr.
\]

This relation is monotonic with respect to $R$. We let $R$ tend to infinity to obtain (14) for all non-negative Riemann integrable functions $f$ satisfying (13). Splitting $f$ into its positive and negative part, this gives (14) for all Riemann integrable function satisfying (13). From this we get (14) for all continuous functions satisfying (13).

Assume now that (14) holds for all continuous functions $f$ satisfying (13). For any $s > 0$ and every $\varepsilon > 0$ there exist continuous functions $f_1$ and $f_2$ such that
\[
f_1(r) \leq 1_{[0,s]}(r) \leq f_2(r)
\]
and
\[
\int_0^\infty (f_2(r) - f_1(r))r^{n-1}dr < \varepsilon.
\]

Repeating the arguments above this gives that (14) implies (3). □
4. Proof of the theorem

We compute

\[
\frac{1}{N^2} \sum_{i,j=1}^{N} H(CN^{-\frac{2}{n}}, x_i, x_j) = \frac{1}{(4\pi C)^{\frac{n}{2}}} \left( 1 + O(N^{-\frac{2}{n}}) \right)
\]

\[
+ \frac{1}{N} \sum_{i,j=1 \atop i \neq j}^{N} \frac{1}{(4\pi C)^{\frac{n}{2}}} \exp \left( -\frac{(N^{\frac{1}{n}} d(x_i, x_j))^2}{4C} \right) \left( 1 + O(N^{-\frac{2}{n}}) + O(N^{-\alpha}) \right)
\]

\[
+ \frac{1}{N^2} \sum_{i,j=1 \atop d(x_i, x_j) > N^{-\alpha}}^{N} H(CN^{-\frac{2}{n}}, x_i, x_j)
\]

for some $0 < \alpha < \frac{1}{n}$. Here we have used (11) to replace the heat kernel in the first sum. By (12) the second sum can be estimated by

\[
\frac{1}{N^2} \sum_{i,j=1 \atop d(x_i, x_j) > N^{-\alpha}}^{N} H(CN^{-\frac{2}{n}}, x_i, x_j) \leq C_\delta C^{\frac{n}{2}} N \exp \left( -\frac{N^{\frac{2}{n}} - 2\alpha}{4(1 + \delta)C} \right),
\]

which tends to 0 for $N \to \infty$.

Applying Proposition 1 we have that

\[
\lim_{N \to \infty} \frac{1}{N^2} \sum_{i,j=1 \atop i \neq j}^{N} \frac{1}{(4\pi C)^{\frac{n}{2}}} \exp \left( -\frac{(N^{\frac{1}{n}} d(x_i, x_j))^2}{4C} \right) = \frac{nB_n}{(4\pi C)^{\frac{n}{2}}} \int_0^\infty \exp \left( -\frac{r^2}{4C} \right) r^{n-1} dr = 1.
\]

This gives

\[
\lim_{N \to \infty} \frac{1}{N^2} \sum_{i,j=1}^{N} H(CN^{-\frac{2}{n}}, x_i, x_j) = (4\pi C)^{-\frac{n}{2}} + 1
\]

and by positive definiteness we have

\[
\sum_{0 < \ell < L} e^{-\lambda_\ell CN^{-\frac{2}{n}}} \left( \frac{1}{N} \sum_{i=1}^{N} \varphi_\ell(x_i) \right)^2 \leq \frac{1}{N^2} \sum_{i,j=1}^{N} H(CN^{-\frac{2}{n}}, x_i, x_j) - 1.
\]
Applying lim sup to this last inequality we derive
\[
\limsup_{N \to \infty} \sum_{0 < \ell < L} e^{-\lambda_{CN}^N} \left( \frac{1}{N} \sum_{i=1}^{N} \varphi_{\ell}(x_i) \right)^2 \leq (4\pi C)^{-\frac{n}{2}}.
\]
Since this holds for every $C > 0$ and every $L > 0$ this implies that
\[
\lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \varphi_{\ell}(x_i) = 0
\]
for every $\ell > 0$, which is equivalent to uniform distribution of the sequence of point sets $(X_N)_N$ by Remark [1].

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