Goodness-of-fit tests in many dimensions

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Abstract

A method is presented to construct goodness-of-fit statistics in many dimensions for which the distribution of all possible test results in the limit of an infinite number of data becomes Gaussian if also the number of dimensions becomes infinite. Furthermore, an explicit example is presented, for which this distribution as good as only depends on the expectation value and the variance of the statistic for any dimension larger than one.

1 Introduction

Goodness-of-fit (GOF) tests are designed to test the hypothesis that a sample of data is distributed following a given probability density function (PDF). The sample could, for example, consist of results of a repeated experiment, and the PDF could represent the theoretical prediction for the distribution of these results. The test consists of the evaluation of a function of the data, the GOF statistic, and the qualification of this result using the probability distribution of all possible results when the hypothesis is true, the test-distribution (TD). Despite the consensus that GOF tests are crucial for the validation of models in the scientific process, their success is mainly restricted to one-dimensional cases, that is, to situations in which the data-points have only one degree of freedom. The quest for GOF tests useful in situations where the number $\dim$ of dimensions is larger than one still continues [1, 2, 3].

In the following, we will see that the difficulty with GOF tests in many dimensions is to keep them distribution-free, that is, to construct them such that the TD is independent of the PDF.\(^1\) We will, however, also see how GOF tests can be constructed such that the asymptotic TD, in the limit of an infinite sample size, has a Gaussian limit for $\dim \to \infty$ for any PDF, so that it only

\(^1\)That is, for binning free tests, which we are considering.
depends on the expectation value and the variance of the GOF statistic this limit. Finally, we will encounter an explicit example for which the asymptotic TD depends, for any PDF, as good as only on the expectation value and the variance of the statistic for any \( \dim > 1 \).

2 The structure of goodness-of-fit tests

A GOF statistic is a function \( T_N \) of the data sample \( \{\omega_i\}_{i=1}^N \) constructed such that, under the hypothesis that the data are distributed in a space \( \Omega \) following the theoretical PDF \( P \), there is a number \( t_\infty \) such that

\[
\lim_{N \to \infty} T_N(\{\omega_i\}_{i=1}^N) = t_\infty .
\]

The initial, naïve trust in its usefulness stems from the idea that, for a sample of finite size, the value of \( T_N \) should be close to \( t_\infty \) if the data are distributed following \( P \), and that the value of \( T_N \) is probably not so close to \( t_\infty \) if the data are not distributed following \( P \). This idea immediately leads to the question what is “close”, which can be answered by the test-distribution (TD)

\[
\mathcal{P}_N(t) = \int \delta( t - T_N(\{\omega_i\}_{i=1}^N) ) \prod_{i=1}^N P(\omega_i) d\omega_i ,
\]

where each integration variable \( \omega_i \) runs over the whole space \( \Omega \), and \( \delta \) denotes the Dirac distribution. \( \mathcal{P}_N \) gives the probability distribution of the value of \( T_N \) under the hypothesis that the data are indeed distributed following \( P \). If it is very low at the value of \( T_N \) for the empirical data, then the hypothesis that these data are distributed following \( P \) has to be rejected; it would under that hypothesis be very improbable to get such a value. In fact, knowledge of the value of the number \( t_\infty \) is not necessary. One only needs to know where the bulk of the TD is.

The evaluation of \( T_N(\{\omega_i\}_{i=1}^N) \) and the qualification of this result with \( \mathcal{P}_N \) constitute a GOF test. Notice that the TD is also necessary to qualify \( T_N \) itself: it should consist of a peak around the expectation value\(^2\)

\[
E(T_N) = \int T_N(\{\omega_i\}_{i=1}^N) \prod_{i=1}^N P(\omega_i) d\omega_i .
\]

If, for example, \( \mathcal{P}_N \) is almost flat, then the test is useless since any data sample will lead to a value of \( T_N \) that is equally probable and the test is not capable of distinguishing them.

2.1 Difficulty in many dimensions

The difficulty with the construction of GOF tests for \( \dim > 1 \) is that it is in general very hard to calculate \( \mathcal{P}_N \). There is a way to avoid this, by using the the distribution from the case that \( P \) is constant. One then needs a mapping \( \varphi \) of the data-points such that the determinant of the Jacobian matrix of this mapping is equal to \( P \):

\[
\left| \det \frac{\partial X_k(\varphi(\omega))}{\partial X_l(\omega)} \right| = P(\omega) ,
\]

\(^2\)If \( E(T_N) \neq t_\infty \) then the statistic is biased.
where $X_k(\omega)$ is the $k$-th coordinate of data-point $\omega$. Under the hypothesis that the original data are distributed following $P$, the mapped data are distributed following the uniform distribution. For $\dim = 1$, this mapping is simply given by the integrated PDF, or probability distribution function
\[
\varphi(\omega) = \int_{-\infty}^{\omega} P(\omega') \, d\omega',
\]
since
\[
\int \delta(\, t - T_N(\{\varphi_i\}_{i=1}^N) \, ) \prod_{i=1}^N P(\omega_i) \, d\omega_i = \int \delta(\, t - T_N(\{\varphi_i\}_{i=1}^N) \, ) \prod_{i=1}^N \, d\varphi_i = P_{\text{uniform}}^N(t),
\]
where each integration variable $\varphi_i$ runs from 0 to 1. $P_{\text{uniform}}^N$ is, for popular tests, known in the limit $N \to \infty$. This asymptotic distribution $P_{\text{uniform}}^\infty$ is assumed not to be too different from $P_{\text{uniform}}^N$. Tests for which this method can be applied are called distribution-free.

### 2.2 Crude solution

For $\dim > 1$, finding the mapping mentioned before is in general even more difficult than finding $P_N$. At least an estimate of $P_N$ can be found using a straightforward Monte Carlo technique: one just has to generate ‘theoretical data samples’ the data-points of which are distributed following $P$ and make a histogram of the values of $T_N$ with these samples. Depending on how accessible the analytic structure of $P$ is, several techniques exist for generating the theoretical samples. In the worst case that $P$ is just given as a ‘black box’, the Metropolis-Hastings method can be used, possibly with its efficiency improved by techniques as suggested in [4]. Notice that one does not need extremely many samples, since one is, for this purpose, interested in the bulk of the distribution, not in the tails.

Even with modern computer power, however, this Monte Carlo method can become very time consuming, especially for large $N$ and large $\dim$. In the next section, we will see how practical GOF statistics for $\dim > 1$ can be constructed for which the asymptotic TD can be obtained in a more efficient way.

### 3 Construction of goodness-of-fit statistics in many dimensions

Several GOF statistics for the uniform distribution in many dimensions exist. They are called discrepancies [5] and intensively studied in the field of Quasi Monte Carlo integration [6, 7], for which one uses low-discrepancy sequences of multi-dimensional integration-points. These sequences give a faster convergence than expected from the common theory of Monte Carlo integration, because they are distributed ‘more uniformly’ than uniformly distributed random sequences; they give a GOF that is ‘unacceptably good’. When $\dim = 1$, discrepancies can be
used directly as GOF tests for general PDFs using the ‘mapping method’ mentioned before, and indeed, the Kolmogorov-Smirnov statistic is equivalent to the ∗-discrepancy, and the Cramér-von Mises statistic is equivalent to the $L^2$-discrepancy.

In the following, we will have a look at the structure of discrepancies, and we will see how they can be deformed into GOF statistics for general PDFs.

3.1 The structure of discrepancies

Discrepancies anticipate the fact that, if a sequence $\{\omega_i\}_{i=1}^N$ is uniformly distributed in a space $\Omega$ and $N$ becomes large, then the average of a integrable function over the sequence should converge to the integral over $\Omega$ of the function:

$$\langle f \rangle_N \to \langle f \rangle \quad \text{for } N \to \infty,$$

where

$$\langle f \rangle_N = \frac{1}{N} \sum_{i=1}^N f(\omega_i) \quad \text{and} \quad \langle f \rangle = \int_\Omega f(\omega) \, d\omega.$$ 

Thus a class of functions $\mathcal{H}$ and a measure $\mu$ on $\mathcal{H}$ are chosen, and the discrepancy is defined as

$$D_N = \left( \int_{\mathcal{H}} |\langle f \rangle_N - \langle f \rangle|^r \, \mu(df) \right)^{1/r}. \quad (2)$$

So it is the integration error measured in a class of functions. For example, $\mathcal{H}$ could consist of indicator functions of a family $S$ of subsets of $\Omega$ with $\mu$ such that for $r \to \infty$

$$D_N = \sup_{S \subset S} \left| \frac{1}{N} \sum_{\omega_i \in S} 1 - \int_S d\omega \right|.$$

In this case, the discrepancy is the maximum error made, if the volume of each subset is estimated using $\{\omega_i\}_{i=1}^N$. Especially interesting are the quadratic discrepancies [11], for which $r = 2$, so that they are completely determined by the two-point function of $\mu$:

$$D_N = \left( \frac{1}{N^2} \sum_{i,j=1}^N b(\omega_i, \omega_j) \right)^{1/2},$$

with

$$b(\omega_1, \omega_2) = c(\omega_1, \omega_2) - \int_\Omega [c(\omega_1, \omega) + c(\omega_2, \omega)] \, d\omega + \int_\Omega \int_\Omega c(\omega, \eta) \, d\omega \, d\eta,$$

where

$$c(\omega_1, \omega_2) = \int_{\mathcal{H}} f(\omega_1) f(\omega_2) \, \mu(df).$$

So the discrepancy is the sum of the correlations of all pairs of data-points, measured with correlation function $b$. If the measure $\mu$ itself is completely determined by its two-point function, it is called Gaussian.
3.2 From discrepancies to GOF statistics

Discrepancies are usually constructed in order to test the uniformity of sequences in a \( \text{dim} \)-dimensional hyper-cube \([0, 1)^{\text{dim}}\). We are interested in more general cases, in which we want to test whether a sample \( \{\omega_i\}_{i=1}^N \) of data-points is distributed in a space \( \Omega \) following a given PDF \( P \). We will assume that there exists an invertible mapping \( \varphi \) which maps these data-points onto points \( \varphi(\omega_i) \in [0, 1)^{\text{dim}} \) and for which the determinant \( J \) of the Jacobian matrix is known.

The hypothesis dictates that the mapped points are distributed in the hyper-cube following \( (P \circ \varphi^{-1})/(J \circ \varphi^{-1}) \). We will denote this PDF by \( P \) itself from now on, the sample of mapped data-points by \( \{\omega_i\}_{i=1}^N \) and the hyper-cube by \( \Omega \).

We want to use the idea, introduced before, to analyse a data sample \( \{\omega_i\}_{i=1}^N \) by looking at \( \langle f \rangle_N \) for different functions \( f \). We will just have to keep in mind that, if \( \{\omega_i\}_{i=1}^N \) is distributed following \( P \), then

\[
\langle f \rangle_N \to \langle fP \rangle \quad \text{for} \quad N \to \infty ,
\]

where ‘\( fP \)’ denotes point-wise multiplication. This and the definition of the discrepancies lead us to define the statistic

\[
T_N = \left( \int_{\mathcal{H}} |\langle fQ \rangle_N - \langle fQP \rangle| \mu(df) \right)^{1/r} ,
\]

where we inserted the function \( Q \) for flexibility. It could be absorbed in the definition of \( \mu \), but we prefer this formulation, in which we can stick to known examples for \( \mu \). We will see later on that the ideal choice for \( Q \) is

\[
Q = 1/\sqrt{P} . \tag{3}
\]

We want to focus on the quadratic discrepancies for which \( \mu \) is Gaussian from now on. Like in [11], we shall define the statistic itself as an average case complexity, and not as a square-root of an average:

\[
T_N = \frac{1}{N} \sum_{i,j=1}^N Qc(\omega_i, \omega_j) - 2 \int_{\Omega} \left( \sum_{i=1}^N Qc(\omega, \omega_i) \right) P(\omega) d\omega
\]

\[
- N \int_{\Omega} \int_{\Omega} Qc(\omega, \eta) P(\omega) P(\eta) d\omega d\eta , \tag{5}
\]

where

\[
Qc(\omega_1, \omega_2) = Q(\omega_1)Q(\omega_2) c(\omega_1, \omega_2) . \tag{6}
\]

The reason for the extra factor \( N \) becomes clear when we calculate the expectation value of \( T_N \). Assuming that the data-points are distributed independently following \( P \), it is given by

\[
E(T_N) = \int_{\Omega} Qc(\omega, \omega) P(\omega) d\omega - \int_{\Omega} \int_{\Omega} Qc(\omega_1, \omega_2) P(\omega_1) P(\omega_2) d\omega_1 d\omega_2 .
\]
So it is independent of \( N \) and the statistic is not biased. In order to write down the variance, we shorten the notation such that the expectation value can be written as

\[
E(T_N) = \langle Qc_{1,1}P_1 \rangle - \langle Qc_{1,2}P_1P_2 \rangle ,
\]

and the variance is given by

\[
V(T_N) = \left( 1 - \frac{2}{N} \right) \left( \langle (Qc_{1,2}Qc_{1,2} + Qc_{1,1}Qc_{1,2})P_1P_2 \rangle \\
- \langle (Qc_{1,1}Qc_{2,3} + 4Qc_{1,2}Qc_{2,3})P_1P_2P_3 \rangle \\
+ 3 \langle Qc_{1,2}Qc_{3,4}P_1P_2P_3P_4 \rangle \right) .
\]

Notice that the formulation with Gaussian measures on the function class corresponds to a natural interpretation of the average of a square: given a sequence \( (u_n)_{n=1}^M \) of functions, a sequence \( (\sigma^2_n)_{n=1}^M \) of positive weights and a linear operation \( L \), we have

\[
\sum_{n=1}^M \sigma^2_n L(u_n)^2 = \int L \left( \sum_{n=1}^M x_n u_n \right)^2 \exp \left( - \sum_{n=1}^M \frac{x_n^2}{2\sigma^2_n} \right) \prod_{n=1}^M \frac{dx_i}{\sqrt{2\pi\sigma^2_n}} ,
\]

where the \( x_n \)-integrals run from \(-\infty\) to \( \infty \). So the square averaged over the sequence \( (u_n)_{n=1}^M \) and weighted with \( (\sigma^2_n)_{n=1}^M \) is equal to the square averaged over the class of functions that can be written as linear combination of \( (u_n)_{n=1}^M \) measured with Gaussian weights with widths \( (\sigma_n)_{n=1}^M \). In the formulation of the statistic in terms of the two-point function this means that \( (u_n, \sigma^2_n)_{n=1}^M \) gives its spectral decomposition:

\[
c(\omega_1, \omega_2) = \sum_{n=1}^M \sigma^2_n u_n(\omega_1)u_n(\omega_2) .
\]

The sequence \( (u_n)_{n=1}^M \) usually consists of an orthonormal basis, and several examples of decompositions \( (u_n, \sigma^2_n)_{n=1}^M \) can be found in [11], including cases with \( M = \infty \). One can also find the famous \( \chi^2 \)-statistic interpreted in this way there, with \( (u_n)_{n=1}^M \) a set of indicator functions of non-overlapping subsets of \( \Omega \), and \( \sigma^2_n = 1/\langle u_n \rangle \).

A closer look at formula (5) for the GOF statistic reveals that it is highly impractical for the estimation of the TD with the Monte Carlo method, firstly because it is quadratic in the number of data-points and secondly because a \( dim \)-dimensional integral has to be calculated for each data sample.\(^3\) One such integral evaluation can be performed within acceptable time-scale using Monte Carlo integration techniques, by generating integration-points \( \omega \) distributed following \( P \) and calculating the average of \( \sum_{i=1}^N Qc(\omega_i, \omega) \). In order to make an estimate of the TD with a histogram, however, one would have to calculate in the order of a thousand of such integrals.

Fortunately, the precise definition of the statistic, or more explicitly the spectral decomposition of the two-point function, can be chosen such that the asymptotic TD \( P_\infty \) becomes Gaussian.

\(^3\)The \( 2dim \)-dimensional integral does not depend on the data sample, and has to be calculated only once.
for \( \text{dim} > \infty \), as we will see in the next section. This indicates that, for large \( \text{dim} \), \( \mathcal{P}_\infty \) only depends on the expectation value and the variance of the statistic. In section 5, we will see an explicit example for which \( \mathcal{P} \) influences \( \mathcal{P}_\infty \) as good as only through the expectation value and the variance for any \( \text{dim} > 1 \), even before \( \mathcal{P}_\infty \) looks like a Gaussian. So instead of thousands of \( \text{dim} \)-dimensional integrals for a histogram, one only has to calculate a \( \text{dim} \), two \( 2\text{dim} \), a \( 3\text{dim} \) and a \( 4\text{dim} \)-dimensional integral for the expectation value (7) and the variance (8).

### 4 Calculation of the asymptotic test-distribution

We approach the calculation of \( \mathcal{P}_N \) through its moment generating function

\[
\mathcal{G}_N(z) = E( e^{z T_N} ) .
\]

\( \mathcal{P}_N \) can be recovered from \( \mathcal{G}_N \) by the inverse Laplace transformation

\[
\mathcal{P}_N(t) = \int_{\Gamma} \frac{dz}{2\pi i} \exp( S(t;z) ) , \quad S(t;z) = \log \mathcal{G}_N(z) - tz , \tag{10}
\]

where \( \Gamma \) runs from \(-i\infty \) to \( i\infty \) on the left side of any singularity of \( \mathcal{G}_N \). The analysis of \( \mathcal{G}_N \) can be simplified by the observation that the statistic (4) does not change if we replace

\[
\mu_n \leftarrow \mu_n - \frac{1}{Q} \langle \mu_n Q \rangle
\]

in the spectral decomposition, since \( L(\mu_n) = \langle \mu_n Q \rangle_N - \langle \mu_n Q \rangle \) is invariant (remember that \( \langle P \rangle = 1 \)). In other words, (4) with \( \mu \) Gaussian and two-point function (9) is equivalent to

\[
T_N = N \int_{\mathcal{H}} \langle fQ \rangle_N^2 \mu(df) = \frac{1}{N} \sum_{i,j=1}^N \mathcal{Q}(\omega_i)\mathcal{Q}(\omega_j) c(\omega_i,\omega_j) , \tag{11}
\]

with \( \mu \) Gaussian and two-point function

\[
c(\omega_1,\omega_2) = \sum_{n=1}^M \sigma_n^2 \left( \mu_n(\omega_1) - \frac{\langle \mu_n Q \rangle}{\mathcal{Q}(\omega_1)} \right) \left( \mu_n(\omega_2) - \frac{\langle \mu_n Q \rangle}{\mathcal{Q}(\omega_2)} \right) . \tag{12}
\]

With this decomposition, we can put \( \langle fQP \rangle \) equal to zero under the measure. We continue in the spirit of [9, 11], and write

\[
T_N = \int_{\Omega} \int_{\Omega} c(\omega,\eta) \delta_N(\omega) \delta_N(\eta) \, d\omega d\eta ,
\]

where

\[
\delta_N(\omega) = \frac{\mathcal{Q}(\omega)}{\sqrt{N}} \sum_{i=1}^N \delta(\omega_i - \omega) ,
\]
so that, using Gaussian integration rules, we find that

\[ e^{zT_N} = \int_{\mathcal{H}} e^{\sqrt{2z} \langle f \delta_N \rangle} \mu(df) = \int_{\mathcal{H}} \left( \prod_{i=1}^{N} e^{\sqrt{2z/N} f(\omega_i)Q(\omega_i)} \right) \mu(df) \]

and

\[ G_N(z) = \mathbb{E}(e^{zT_N}) = \int_{\mathcal{H}} e^{z(t^2Q^2P)} \mu(df) \]

We shall restrict ourselves to the asymptotic distribution for \( N \to \infty \) from now on. We find

\[ G_\infty(z) = \lim_{N \to \infty} G_N(z) = \int_{\mathcal{H}} e^{z(t^2Q^2P)} \mu(df) \]

where we used the fact that \( \langle fQ^2P \rangle \) can be taken equal to zero under the measure. Substituting

\[ f(\omega) = \sum_{n=1}^{M} x_n \left( \langle u_n(\omega) - \langle u_nQ^2P \rangle \rangle \right) \quad \text{and} \quad \mu(df) = \prod_{n=1}^{M} e^{-\frac{x_n^2}{2\sigma_n^2}} \frac{d\lambda_n}{\sqrt{2\pi\sigma_n^2}} \]

and applying well known Gaussian integration rules, we find

\[ G_\infty(z) = \det(1 - 2zA)^{-1/2} \]

with

\[ A_{n,m} = \sigma_n \sigma_m \langle u_n u_m Q^2P \rangle - \sigma_n \langle u_n Q^2P \rangle \sigma_m \langle u_m Q^2P \rangle \]

The asymptotic generating function is now determined up to the positions of its singularities, which can directly be written in terms of the eigenvalues \( \lambda_n \) of \( A \), since

\[ G_\infty(z) = \left( \prod_{n=1}^{M} (1 - 2z\lambda_n) \right)^{-1/2} \]

Another way to see how the eigenvalues affect the shape of the TD is by considering the cumulants, which are generated by the logarithm of the generating function:

\[ \frac{d^k}{dz^k} \log G_\infty(z = 0) = 2^{k-1}(k-1)! \sum_{n=1}^{M} \lambda_n^k \]

If \( A \) would consist only of a diagonal term plus a diadic term, then the access to its eigenvalues would be relatively easy. Having in mind that the functions \( u_n \) are orthonormal, this can be achieved by the choice

\[ Q = 1/\sqrt{P} \]

so that

\[ A_{n,m} = \sigma_n^2 \delta_{n,m} - \sigma_n \langle u_n \sqrt{P} \rangle \sigma_m \langle u_m \sqrt{P} \rangle \]
4.1 Gaussian limits

Without loss of generality, we may assume that the weights $\sigma_n$ are ordered from large to small. Then, it is not difficult to see [11] that the eigenvalues $\lambda_n$ of the matrix (15) satisfy

$$\sigma_1 \geq \lambda_1 \geq \sigma_2 \geq \lambda_2 \geq \sigma_3 \geq \lambda_3 \geq \cdots \geq \sigma_{M-1} \geq \lambda_{M-1} \geq \sigma_M \geq \lambda_M.$$  

(16)

It is important to realize that (16) holds whatever $P$ is. The influence $P$ may have on the shape of $P_\infty$ is restricted to the freedom each of the eigenvalues $\lambda_n$ has to change value between $\sigma_n$ and $\sigma_{n+1}$. The smallest eigenvalue is non-negative since the matrix $A$ is positive: for any vector $x$

$$\sum_{n,m=1}^{M} A_{n,m}x_n x_m = \sum_{n=1}^{M} \sigma_n^2 x_n^2 - \left( \sum_{n=1}^{M} \sigma_n \langle u_n \sqrt{P} \rangle x_n \right)^2 \geq 0,$$

where the first inequality is by Schwarz, and the second one is based on the assumption that $(u_n)_{n=1}^{M}$ is an orthonormal (but not necessarily complete) set and $\langle P \rangle = 1$.

For the case that $P = 1$, it has been shown in [8] that $P_\infty$ becomes Gaussian if and only if there is a limit for the statistic such that

$$\frac{\lambda_1^2}{\sum_{n=1}^{M} \lambda_n^2} \rightarrow 0.$$  

(17)

Typically, this limit may be $\text{dim} \rightarrow \infty$, as is shown in various examples. For simplicity, we assume that $\sigma_1 = \sigma_2$, which is actually the case in most examples in [8]. Using this and (16), it is easy to see that, if (17) holds, then also $\lambda_1^2/(\sum_{n=1}^{M} \sigma_n^2) \rightarrow 0$ and $\lambda_1^2/(\sum_{n=2}^{M} \sigma_n^2) \rightarrow 0$, and that the limit holds for any $P$. So we may conclude that whenever the spectral decomposition is chosen such that $\sigma_1 = \sigma_2$ and there is a limit such that

$$\frac{\sigma_1^2}{\sum_{n=1}^{M} \sigma_n^2} \rightarrow 0,$$

then $P_\infty$ becomes Gaussian in this limit.

5 Example

The following example of a GOF statistic in many dimensions is based on the diaphony [10, 11], and has the following spectral decomposition. The basis is the Fourier basis in $\text{dim}$ dimensions:

$$u_{\vec{n}}(\omega) = \prod_{k=1}^{\text{dim}} u_{n_k}(X_k(\omega)) \quad , \quad n_k = 0, 1, 2, \ldots \quad , \quad k = 1, 2, \ldots, \text{dim}$$
with
\[ u_0(x) = 1 , \quad u_{2n-1}(x) = \sqrt{2} \sin(2\pi nx) , \quad u_{2n}(x) = \sqrt{2} \cos(2\pi nx) , \]
for \( n \) from 1 to \( \infty \). The corresponding weights are given by
\[ \sigma_{\vec{n}} = \prod_{k=1}^{\text{dim}} \sigma_{n_k} \quad \text{with} \quad \sigma_0 = 1 , \quad \sigma_{2n} = \sigma_{2n-1} = \frac{1}{n} . \]

The two-point function is equal to
\[ c(\omega_1, \omega_2) = \sum_{\vec{n}} \sigma_{\vec{n}}^2 u_{\vec{n}}(\omega_1) u_{\vec{n}}(\omega_2) = \prod_{k=1}^{\text{dim}} c_1( X_k(\omega_1) - X_k(\omega_2) ) , \]
where \( \sum_{\vec{n}} = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \sum_{n_{\text{dim}}=0}^{\infty} \) and
\[ c_1(x) = 1 + \frac{\pi^2}{3} - 2\pi^2(x \mod 1)(1 - x \mod 1) . \]

The only important difference with the two-point function of the diaphony is that there the constant mode, the \( \text{dim} \)-dimensional basis function which is equal to 1, is missing. This makes sense since the diaphony is constructed in order to test the uniform distribution and the contribution of the constant mode cancels in (2). The advantage is that the diaphony is directly given by the sum of all two-point correlations between the data-points and no integrals of two-point functions have to be calculated. Notice that this cancellation also appears in (15): the first row and column of the matrix \( A \) consist of only zeros if \( P = 1 \), since all modes except the constant mode have zero integral. For a general PDF these cancellations also exist, but not for a single mode, and hence are not of practical use. For example, \( f = 1/Q \) cancels in (4).

It is useful to introduce the function \( \rho \) which counts the number of weights with the same value:
\[ \rho(s) = \sum_{\vec{n}} \delta_{s,1/\sigma_\vec{n}} . \]

The numbers \( \rho(s) \) increase as function of \( \text{dim} \). Using \( \rho \), (14) and (16), the generating function can be written as
\[ G_\infty(z) = \left( \prod_{s=1}^{\infty} (1 - 2z/s^2)^{\rho(s)-1}(1 - 2z\lambda_s) \right)^{-1/2} , \]
where the numbers \( \lambda_s \) depend on the PDF under consideration, but are, following (16), restricted by the relation
\[ 1/s^2 > \lambda_s \geq 1/(s + 1)^2 . \]

In order to find the probability density \( P_\infty \), the inverse Laplace transformation (10) has to be performed on \( G_\infty \). The logarithm of the product can best be evaluated as described in [12], by extracting the first and the second order terms in \( z \):
\[ \log G_\infty(z) = Ez + \frac{1}{2} Vz^2 + \sum_{s=1}^{\infty} \left( g_s(z) - g_s'(0)z - \frac{1}{2} g_s''(0)z^2 \right) , \quad (18) \]
where \( g_s(z) = -\frac{\rho(s) - 1}{2} \log(1 - 2z/s^2) - \frac{1}{2} \log(1 - 2z\lambda_s), \) and \( E \) and \( V \) are the expectation value and the variance of the statistic. For the case that \( P = 1 \), so that \( \lambda_s = 1/(s + 1)^2 \), they can be calculated directly and are given by

\[
E_{\text{uniform}} = \left(1 + \frac{\pi^2}{3}\right)^{\text{dim}} - 1, \quad V_{\text{uniform}} = 2\left(1 + \frac{\pi^4}{45}\right)^{\text{dim}} - 2.
\]

We want to study the influence of \( P \) on \( P_\infty \) by generating the eigenvalues \( \lambda_s \) at random, uniformly distributed within their borders, and plotting the result. First, however, we need to find out how many terms in the infinite sum of (18) have to be taken into account in order to obtain a trustworthy result. This can be done at \( \text{dim} = 1 \), since we know already that \( P_\infty \) will tend to look like a Gaussian for larger values of \( \text{dim} \) so that the sum must become less important. Furthermore, there is the advantage that at \( \text{dim} = 1 \) and \( P = 1 \) there exists a simple formula for the generating function:

\[
G_{\text{uniform}}(z) = \frac{\sqrt{2\pi^2 z}}{\sin \sqrt{2\pi^2 z}}. \tag{19}
\]

In Figure 1, we present the result with this formula and with (18) using only one term. With 10 terms, the difference between the curves is invisible and this is the number we further use. Results for \( \text{dim} = 2 \) are depicted in Figure 2. As expected, the curves look more ‘Gaussian’ than the 1-dimensional curve. The crosses represent the case \( P = 1 \), and the two continuous curves represent two cases with ‘typical’ sets of random eigenvalues. The curves are clearly different, but if we go over to standardized variables, that is, if we plot

\[
\sqrt{V} P_\infty(\sqrt{V} (t + E) \),
\]

Figure 1: \( P_\infty(t) \) for \( \text{dim} = 1 \) and \( P = 1 \) using (19) and (18) with one term.
so that the expectation value is equal to 0 and the variance is equal to 1, we find Figure 3, and we may conclude that the curves almost only depend on the expectation value and the variance. Again, we know that this behavior becomes only stronger for higher values of dim because of the Gaussian limit. We conclude that $P_\infty$ for general $P$ can, to satisfying accuracy, be approximated by

$$P_\infty(t) \approx \sqrt{V_{\text{uniform}}/V} \left( \sqrt{V_{\text{uniform}}/V} (t - E_{\text{uniform}}) + E_{\text{uniform}} \right),$$

where $P_{\text{uniform}}$, $E_{\text{uniform}}$, and $V_{\text{uniform}}$ are the asymptotic test-distribution, the expectation value and the variance for the case that $P = 1$.

6 Conclusion

We have seen how to construct practical GOF statistics to test the hypothesis that a sample of data is distributed following a given PDF in many dimensions, for which the asymptotic test-distribution in the limit of an infinite sample size becomes Gaussian in the limit of an infinite number of dimensions. Furthermore, we have seen an explicit example of such a statistic, for which the asymptotic test-distribution depends on the PDF as good as only through the expectation value and the variance of the statistic for any number of dimensions larger than one.

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Figure 3: $\sqrt{V} P_\infty (\sqrt{V} t + E)$ for the same situations as in Figure 2.

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