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On the positivity of Fourier transforms

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Characterizing in a constructive way the set of real functions whose Fourier transforms are positive appears to be yet an open problem. Some sufficient conditions are known but they are far from being exhaustive. We propose two constructive sets of necessary conditions for positivity of the Fourier transforms and test their ability of constraining the positivity domain. One uses analytic continuation and Jensen inequalities and the other deals with Toeplitz determinants and the Bochner theorem. Applications are discussed, including the extension to the two-dimensional Fourier-Bessel transform and the problem of positive reciprocity, i.e. positive functions with positive transforms.

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I. INTRODUCTION

In a previous paper [1], the following questions were asked:

- What are the constraints for an even, real function $\psi(r)$ ensuring that its Fourier transform satisfies,

$$\varphi(s) \equiv \sqrt{\frac{2}{\pi}} \int_0^{+\infty} dr \cos(sr) \psi(r) \geq 0, \quad (1)$$

that is, φ be real and positive?

- What are the constraints on even Fourier partners such that φ and

$$\psi(r) \equiv \sqrt{\frac{2}{\pi}} \int_0^{+\infty} ds \cos(sr) \varphi(s) \geq 0, \quad (2)$$

be *both* positive?

The motivation for such questions came from various areas of mathematics, notably [2], and from physics, for which a good example is the Fourier-Bessel relation [3] between two physically observable quantities which are necessarily positive (for recent references, see *e.g.* [4] for maths, and [5] for various physics domains). In the paper [1] an approach based on a Gaussian times a combination of a few, low order Hermite polynomials, allowing to consider eigenfunctions of the Fourier transforms (1,2), has shown that the structure of the positivity space in the manifold of the components may be quite involved. In the present work we aim at finding results on a more general basis.

Despite the mathematical interest of the problem, one might argue on practical grounds that the power of modern computers legitimates a brute force approach, of the kind, given ψ for instance, numerically calculate φ and “just look at it”. We strongly feel, however, that, despite the existence of subtle methods for the integration of oscillatory integrands, finer analytical methods are in demand. In particular, direct criteria for ψ , for instance, without any numerical estimates for φ , can provide more elegant and more rigorous approaches.

The main optimal issue for finding out the set of functions solutions would be an overall *constructive*, sufficient and necessary condition satisfying the above-mentioned positivity. It seems that one is still far from that goal in the literature, since it appears to be a rather involved mathematical problem [6]. Indeed some general theorems exist on the positivity of Fourier transforms [7], if only the well-known Bochner theorem [8] on the “positive-definiteness” of the function¹ which we will usefully recall later on. They possess a fundamental interest, and will help our studies.

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¹ “Positive-definiteness” of a function f means that for any set of positions $\{r_i, i = 1, \dots, n\}$ the $n \times n$ matrix with elements $f(r_i - r_j)$ is positive definite, i.e. $\sum_{i,j} u_i f(r_i - r_j) u_j \geq 0$ for all test vector \vec{u} .

However, up to our knowledge, they still gave only limited practical tools allowing to get information on the functional set of solutions. Some general useful *sufficient* constructive conditions are known, such as convexity [9] for the function in the integrand (*i.e.* ψ in (2)), but it can be easily shown on specific examples [1] that it gives only a limited part of the space of solutions. Hence *necessary* constructive conditions, namely a set of practical constraints on functions whose Fourier transforms are positive, would be helpful.

In the present work, we derive two separate sets of such constructive and necessary conditions obeyed by a function, say $\psi(r)$, if its Fourier transform $\varphi(s)$ is positive. One method (called in short “matrix method”) is based on the positivity of a hierarchy of determinants of Toeplitz matrices². The second method (called “analytic method”) is based on an analytic continuation onto the imaginary axis associated with Jensen inequalities [11]. They are constructive, meaning that they will be expressed directly (and in a sense “simply”) in terms of $\psi(r)$. They will be formulated as a set of necessary inequalities, for all values of the variable r most often. This we find much constraining, and thus, hopefully, making a step towards a determination of the set of solutions of the positivity condition (1). If starting with positive functions ψ , the same constraints give useful indications on the solution of the condition (2), which is our final goal.

Let us illustrate one typical constraint from the matrix method. Using a generalization of the well-known consequence of Bochner’s theorem, namely

$$\psi(0) \geq \psi(r) , \quad \forall r , \quad (3)$$

coming from the application of positive definiteness to the 2-matrix

$$\begin{pmatrix} \psi(0) & \psi(r) \\ \psi(r) & \psi(0) \end{pmatrix} , \quad (4)$$

one obtains

$$\psi(2r) \geq 2 \frac{\psi(r)^2}{\psi(0)} - \psi(0) , \quad \forall r , \quad (5)$$

with one more dimension of the matrix. Indeed, considering a three-by-three “equidistance” symmetric Toeplitz matrix,

$$\begin{pmatrix} \psi(0) & \psi(r) & \psi(2r) \\ \psi(r) & \psi(0) & \psi(r) \\ \psi(2r) & \psi(r) & \psi(0) \end{pmatrix} , \quad (6)$$

and applying Bochner’s theorem, the positive definiteness of (6) gives (5). Noting that (6) is a symmetric Toeplitz matrix whose generalization to higher dimensions is straightforward, we will take advantage of the hierarchy of inequalities obtained by increasing the dimensionality. Note also that the positive definiteness of the matrix (6) implies that of (4) using test vectors of the form $(a, b, 0)$.

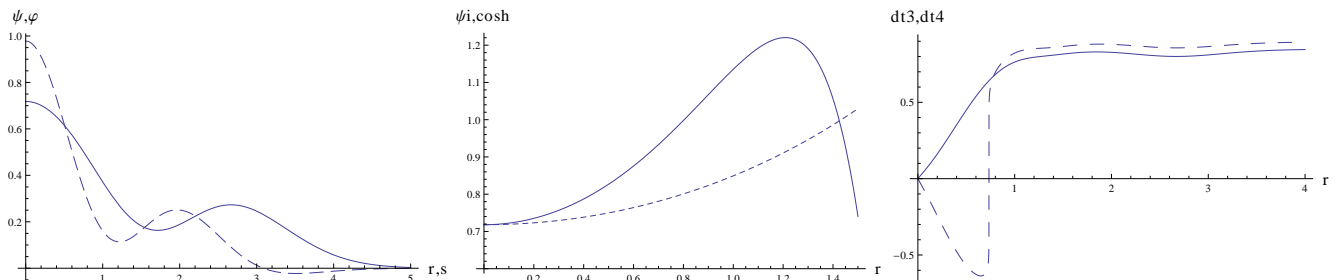


FIG. 1: Left: Full line, positive $\psi(r)$; dashed line, its partly negative transform $\varphi(s)$. Center: Full line, $\psi i \equiv \psi(ir)$; dashed line, its expected cosh lower bound according to (7) fails, thus detecting the non-positivity of φ . Right: Same detection with the matrix method at order 4 (dashed line), while order 3 (full line) is insufficient.

² Toeplitz matrices are defined, see *e.g.* [10] by coefficients $c_{ij} \equiv c_{i-j}$.

To illustrate the “analyticity method”, one of our results reads,

$$\psi(ir) \geq \psi(0) \cosh \left\{ \frac{2r}{\pi} \int_0^\infty \frac{dr'}{r'^2} \left(1 - \frac{\psi(r')}{\psi(0)} \right) \right\} \quad \forall r \in [0, \infty[, \quad (7)$$

where $\psi(ir)$ is the analytic continuation of $\psi(r)$ onto the imaginary axis. It is a real, convex function, since, by definition (2), $\psi(r)$ is a function of r^2 and it is assumed here that both integrals, $\int_0^\infty ds \cosh(sr)\varphi(s)$, and $\int_0^\infty ds s^2 \cosh(sr)\varphi(s)$, are convergent. As will be shown in the following, the coefficient of r in the cosh seen in formula (3) is the average value of s in Fourier space, but the formula, obviously written in the ψ space, introduces no oscillating cosine term. Figure 1 illustrates a typical case³ where the “cosh test” (7) eliminates a candidate ψ , if only because $\psi(ir)$ is blatantly non convex, and the same detection is obtained provided we use a Toeplitz matrix of order 4 or more.

The plan of the paper is as follows. The next section Sec. II, is devoted to the description of the two sets of constraints, namely those coming from the matrix method, and then from the analyticity method. Section III provides a numerical investigation of the compared efficiency of both methods based on the approach initiated in Ref.[1]. Section IV extends our reasoning and numerical evaluation to the 2-dimensional case of the Fourier-Bessel transform. Section V is a summary and conclusion.

II. NECESSARY CONDITIONS

A. Simple positivity and maximality tests

In the following, $\psi(r)$ is an even function, positive, ($\psi(r) \geq 0, \forall r$), and we further assume that ψ has as many derivatives as might be needed. If its Fourier partner φ is also positive, then, *necessarily*,

i) The function ψ is “positive definite”, hence ψ is *maximum at the origin*, namely $\psi(0) \geq \psi(r), \forall r$, see (3). This may be seen from the Bochner theorem for the pair of points, $x_1 = 0, x_2 = r$, and the test vector, $\vec{u} = (1, -1)$, leading to

$$\sum_{i,j=1,2} u_i \psi(x_i - x_j) u_j = 2[\psi(0) - \psi(r)] \geq 0 . \quad (8)$$

ii) For every positive integer q every product, $\varphi_q \equiv s^q \varphi$, is positive, hence the Fourier partner, $\psi_{2q} \equiv (-)^q d^{2q}\psi/dr^{2q}$, taking into account the change of sign in front of the cosine in formula (2) verifies the same maximality condition *i.e.* ψ_{2q} has its maximum at the origin.

iii) Every moment is positive, $\mu_q \equiv \int_0^\infty ds s^q \varphi(s) > 0$, hence in particular, for *even* moments and thus *from every even derivative of ψ , the condition $\psi_{2q}(0) > 0$* . The somewhat more involved expression for *odd* moments is derived in Subsection C, see further.

iv) *Every average value*, such as μ_q/μ_0 or μ_q/μ_{q-1} , *is positive*. We show in the following how, while even moments, see iii), are easily observed in the r -space, odd average values are also available from the r -space.

v) The positivity, for any width b in momentum space, of a product, $e^{-s^2/(2b^2)} \varphi$, of φ by a Gaussian, induces the “positive-definiteness” of the result of the corresponding convolution,

$$\psi_b(r) \equiv \frac{b}{\sqrt{2\pi}} \int_0^\infty dr' \left[e^{-b^2(r-r')^2/2} + e^{-b^2(r+r')^2/2} \right] \psi(r') , \quad (9)$$

with, for ψ_b and its derivatives, *all the consequences already seen under i)-iv)*.

³ The function and its Fourier transform read, $\psi(r) = e^{-\frac{r^2}{2}} (0.718081 - 0.064879r^2 - 0.0685793r^4 + 0.0269736r^6 + 0.00119983r^8)$, $\varphi(s) = e^{-\frac{s^2}{2}} (0.97805 - 1.24138s^2 + 0.587989s^4 - 0.0605688s^6 + 0.00119983s^8)$; the average of s is $\langle s \rangle = 0.836263$.

B. Matrix method

Elaborating on the positive definiteness of the function ψ following from the Bochner theorem, let us introduce the hierarchy of symmetric real Toeplitz n -matrices T_n

$$\begin{pmatrix} \psi(0) & \psi(r) & \psi(2r) & \dots & \psi[(n-1)r] \\ \psi(r) & \psi(0) & \dots & \dots & \psi[(n-2)r] \\ \dots & \dots & \dots & \dots & \dots \\ \psi[(n-1)r] & \psi[(n-2)r] & \dots & \psi(r) & \psi(0) \end{pmatrix}. \quad (10)$$

Application of the Bochner theorem can be shown to lead to the following set of inequalities on Toeplitz determinants of positive-definite functions (thus whose Fourier transforms are positive):

$$\|T_n\| > 0, \quad \forall n. \quad (11)$$

It is known that the matrices T_{n-1} and T_n have intertwined eigenvalues, Hence the smaller eigenvalue of T_{n-1} is always larger than the one of T_n , which is itself positive from positive definiteness. Hence verifying (11) for any given n , ensures positivity⁴ of all determinants $\|T_k\|$ for $k < n$. Indeed, the matrix method will make a practical use of (11) for finite n . Notice, however, that $\|T_n\|$ vanishes like $\propto r^{n(n-1)}$ when $r \rightarrow 0$, creating numerical accuracy problems for its sign. It may be more efficient to track the first change of sign of the lowest eigenvalue.

C. Analyticity method

Recall that $\mu_0 \equiv \int_0^\infty ds \varphi(s) = \sqrt{\pi/2} \psi(0)$. Consider the probability distribution, $\mathcal{P}(s) = \sqrt{2/\pi} \varphi(s)/\psi(0)$. By analytic continuation of (2) in r -space we obtain,

$$\psi(ir) = \psi(0) \int_0^\infty ds \cosh(sr) \mathcal{P}(s) = \psi(0) \langle \cosh(sr) \rangle, \quad (12)$$

where we have already assumed that $\varphi(s)$ decreases fast enough when $s \rightarrow \infty$ to ensure convergence of the integral. Then our key ingredient is to make use of the well-known Jensen inequality [11], $\langle f(X) \rangle_{\mathcal{P}} \geq f(\langle X \rangle_{\mathcal{P}})$, valid for any probability distribution $\mathcal{P}(X)$, and any *convex* function f , the hyperbolic cosine being obviously convex. *The following lower bound holds,*

$$\forall r, \psi(ir) \geq \psi(0) \cosh(\langle s \rangle r). \quad (13)$$

The calculation in r -space of $\langle s \rangle = \mu_1/\mu_0$ is explained in the next subsection D.

An extension of the inequality (13) can be obtained as follows. For notational simplicity, use a short notation σ for $\langle s \rangle$ and, temporarily, set $\psi(0) = 1$, an inessential normalization. More inequalities are easily found if one notices that

$$\psi(r) + \psi(ir) = \langle [\cos(rs) + \cos(irs)] \rangle \geq [\cos(r\sigma) + \cos(i\sigma)], \quad (14)$$

$$\psi(r) - \psi(ir) = \langle [\cos(rs) - \cos(irs)] \rangle \leq [\cos(r\sigma) - \cos(i\sigma)], \quad (15)$$

since the sum, $[\cos x + \cos(ix)]$ and the difference, $[\cos x - \cos(ix)]$, are obviously a convex and a concave real function of x , respectively.

Equivalently, consider now the first complex eighth root ω of unity, $\omega^2 = i$. It is trivial to find that the combinations, $[\cos x + \cos(\omega x) + \cos(\omega^2 x) + \cos(\omega^3 x)]$ and $[\cos x - \cos(\omega x) + \cos(\omega^2 x) - \cos(\omega^3 x)]$ are real convex and that $[\cos x - i \cos(\omega x) - \cos(\omega^2 x) + i \cos(\omega^3 x)]$ and $[\cos x + i \cos(\omega x) - \cos(\omega^2 x) - i \cos(\omega^3 x)]$ are real concave. The following inequalities result,

$$\psi(r) + \psi(\omega r) + \psi(ir) + \psi(\omega ir) \geq \cos(\sigma r) + \cos(\omega \sigma r) + \cos(i\sigma r) + \cos(\omega i\sigma r), \quad (16)$$

$$\psi(r) - \psi(\omega r) + \psi(ir) - \psi(\omega ir) \geq \cos(\sigma r) - \cos(\omega \sigma r) + \cos(i\sigma r) - \cos(\omega i\sigma r), \quad (17)$$

$$\psi(r) - i\psi(\omega r) - \psi(ir) + i\psi(\omega ir) \leq \cos(\sigma r) - i \cos(\omega \sigma r) - \cos(i\sigma r) + i \cos(\omega i\sigma r), \quad (18)$$

$$\psi(r) + i\psi(\omega r) - \psi(ir) - i\psi(\omega ir) \leq \cos(\sigma r) + i \cos(\omega \sigma r) - \cos(i\sigma r) - i \cos(\omega i\sigma r), \quad (19)$$

Further roots of unity clearly give further inequalities.

The bounds found in (13-19) obviously hold, *mutatis mutandis*, for ψ_b and even derivatives of ψ and ψ_b .

⁴ Note also the convergence of $\|T_n\|^{1/n}$, $n \rightarrow \infty$, to a well-defined Fourier series through the Szegő-Kač theorem, see *e.g.* [10].

D. Odd Moments

Odd average values, appearing as inputs in inequalities (13-19), are obviously also required to be positive, as previously noted as condition iii). It is important to obtain them as simply as possible in terms of $\psi(r)$. However, this is less obvious since odd moments of φ cannot be trivially observed from mere derivatives of ψ .

Let us derive them using the Laplace transform of φ ,

$$\chi(r) \equiv \int_0^\infty ds e^{-rs} \varphi(s) \Rightarrow \int_0^\infty ds s \varphi(s) = -\frac{d\chi}{dr}(r=0), \quad (20)$$

which allows a useful expression of the first moment of φ . Indeed, starting with the expression,

$$\chi(r) = \sqrt{\frac{2}{\pi}} \int_0^\infty ds e^{-rs} \int_0^\infty dr' \psi(r') \cos sr', \quad (21)$$

for $r \neq 0$ one can switch the order of integrations in (21) and write,

$$\chi(r) = \sqrt{\frac{2}{\pi}} \int_0^\infty \psi(r') dr' \int_0^\infty ds e^{-rs} \cos sr' = \sqrt{\frac{1}{2\pi}} \int_0^\infty dr' \left\{ \frac{1}{r + ir'} + \frac{1}{r - ir'} \right\} \psi(r'). \quad (22)$$

By integration by part we then obtain,

$$\chi(r) = i\sqrt{\frac{1}{2\pi}} \int_0^\infty dr' \log \left\{ \frac{r + ir'}{r - ir'} \right\} \frac{d\psi(r')}{dr'}, \quad (23)$$

since the boundary term,

$$-i\sqrt{\frac{1}{2\pi}} \left[\log \left\{ \frac{r + ir'}{r - ir'} \right\} \psi(r') \right]_{r'=0}^{r'=\infty}, \quad (24)$$

obviously vanishes for all $r > 0$.

Actually, the expression (23) of the function χ , well defined also at $r=0$ by continuity, is the correct analytic continuation of formula (22) at $r=0$ and thus the representation of the regular Laplace transform (21) for all $r \geq 0$.

Finally, one gets the following formula for the first moment displayed in (20),

$$\int_0^\infty s ds \varphi(s) \equiv -\frac{d\chi}{dr}(r=0) = -\sqrt{\frac{2}{\pi}} \int_0^\infty \frac{dr'}{r'} \frac{d\psi(r')}{dr'}. \quad (25)$$

It is also possible to make a “reverse” integral by part, using an *a priori* arbitrary integration constant C , namely,

$$\int_0^\infty s ds \varphi(s) = -\sqrt{\frac{2}{\pi}} \left\{ \frac{1}{r'} [\psi(r') - C] \right\}_{r'=0}^{r'=\infty} - \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{dr'}{r'^2} [\psi(r') - C]. \quad (26)$$

In fact, the boundary term is nonsingular (and finally zero) only when choosing the constant $C = \psi(0)$, leading to the final formula,

$$\int_0^\infty s ds \varphi(s) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{dr'}{r'^2} [\psi(0) - \psi(r')]. \quad (27)$$

Inserting the result (27) into the inequality (13) gives rise to formula (7), a self-content functional expression depending only on the knowledge of ψ . We stress again that the formula involves no oscillating terms, except those which might be present in ψ .

It will be noticed, incidentally, that any numerical result from Eq. (27) that returns a negative value, $\mu_1 < 0$, for this moment, negates at once the expected positivity of φ . A detailed comparison between $\psi(ir)$, $\psi(r) \pm \psi(ir)$, etc and their respective bounding functions, as detailed above, becomes useless in such a case of negative moment.

Higher order odd moments, μ_{2q+1} are obviously obtained upon substituting ψ_{2q} for ψ in Eq. (27). And the generalization of Eq. (27) to ψ_b and its moments is trivial.

In the following Section III we show numerical, illustrative cases, the existence of so-called “rebels”, where, although φ contains negativity, several among the known criteria described previously are not violated. Then we test and compare in a systematic way the efficiency of both methods in creating an efficient “filter” for positivity.

III. NUMERICAL INVESTIGATIONS

A. 1-d test functions with two parameters; maximality and cosh tests efficiency (Subsecs. II A and C)

We first consider combinations, $\psi = c_0 \xi_0 + c_2 \xi_2 + c_4 \xi_4$, of the following three harmonic oscillator eigenstates,

$$\xi_0 = \pi^{-\frac{1}{4}} e^{-r^2/2}, \quad \xi_2 = \pi^{-\frac{1}{4}} e^{-r^2/2} (2r^2 - 1)/\sqrt{2}, \quad \xi_4 = \pi^{-\frac{1}{4}} e^{-r^2/2} (4r^4 - 12r^2 + 3)/(2\sqrt{6}), \quad (28)$$

with $c_0 = \cos \alpha$, $c_2 = \sin \alpha \cos \beta$, $c_4 = \sin \alpha \sin \beta$, $0 \leq \alpha < \pi/2$ and $0 \leq \beta < 2\pi$. We explored the corresponding half sphere via a grid of parallels and meridians, separated from each other by steps of $\pi/90$ and $\pi/45$ respectively. Only those functions ψ that are positive are retained for further studies. This selects 951 grid points, out of which 520, shown as tiny dots in all parts of Figures 2-4, correspond to simultaneous $\psi > 0$ and $\varphi > 0$. The remaining 431 points, shown with larger dots in the left part of Fig. 2, correspond to those cases where φ has negative parts.

Preselection by conditions of maxima at the origin : As stated in Subsec. II A, it is easy to eliminate 271 out of these 431 cases, via a double maximality condition, namely that $\psi(0)$ and $\psi_2(0)$ be maxima for ψ and ψ_2 , respectively. The 160 remaining “rebels” satisfy this double maximality condition.

The right part of Fig. 2 shows, besides the 520 “fully acceptable cases” (*tiny dots*), 160 cases where the non-positivity of φ is *not* detected by the double maximality condition (*moderate size dots*) and 271 cases where the same condition is efficient for the detection (*big dots*).

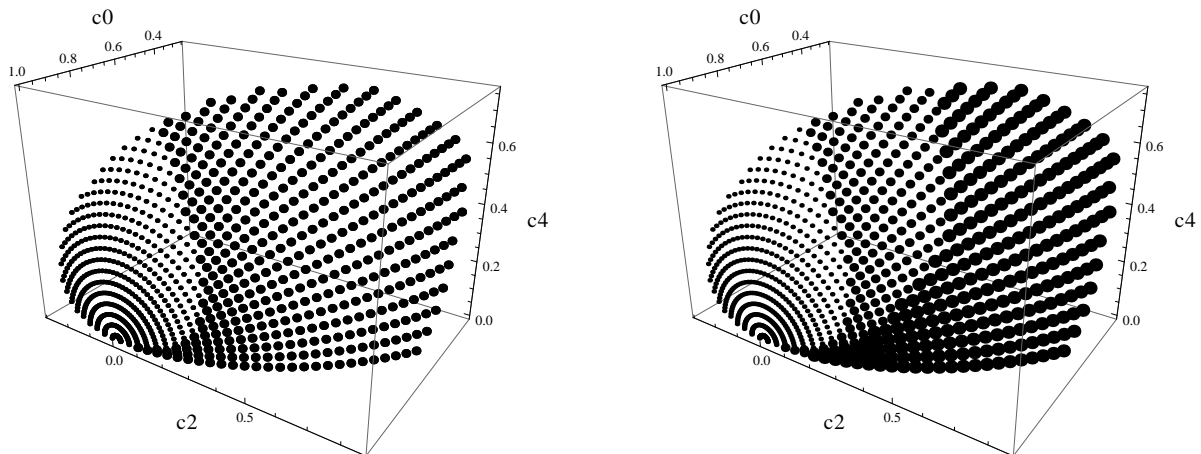


FIG. 2: Left: Tiny dots, simultaneous $\psi > 0$, $\varphi > 0$. Bigger dots, $\psi > 0$, but non-positivity of φ . Right: Same tiny dots. Big dots, cases eliminated by maximality conditions for $\psi(0)$, $\psi_2(0)$. Moderate dots, non-positivity undetected by these conditions.

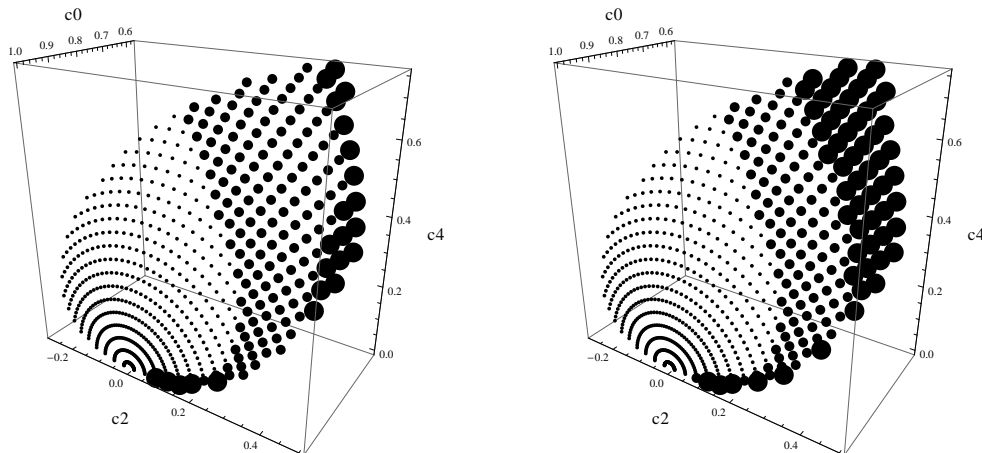


FIG. 3: Tiny dots, simultaneous $\psi > 0$, $\varphi > 0$. Big dots, $\psi > 0$, non-positivity of φ detected with convolution parameter $b = 2$, left, or $b = 1$, right. Moderate dots, $\psi > 0$, non-positive φ_b undetected.

Further screening by a combination of maximality and cosh tests, including convolution : Figure 3 shows, for those 160 functions ψ for which φ is non-positive although $\psi(0)$ and $\psi_2(0)$ are maxima, the result of an analysis of their “convoluted” ψ_b , see Eq. (9), with $b = 2$, then $b=1$, for the left, then right, part of the Figure, respectively. The following eight conditions are used, simultaneously : a) $\psi_b(0) > 0$, $\psi_b(0)$ maximum of ψ_b , b) the same two conditions for $\psi_{b2} \equiv -d^2\psi_b/dr^2$, c) both average moments for ψ_b and ψ_{b2} must be positive, d) both analytic continuations $\psi_b(ir)$ and $\psi_{b2}(ir)$ must be larger than their respective “cosh” lower bound. (Note, incidentally, that preselected functions ψ , so that $\psi(0) > 0$ and $\psi_2(0) > 0$ make maxima, do not extend necessarily such a positivity and maximality to $\psi_b(0)$ and $\psi_{b2}(0)$.) The big dots in Fig. (3) indicate when one, or several violations, eliminate some among the 160 non-positive φ 's. It turns out that the choice, $b = 1$, is here more efficient, with 58 functions rejected out of 160, that the choice, $b = 2$, with only 23 detections. An even better result is obtained if $b = 1/2$, with 83 detections. Clearly, with a more general set of test functions, it will be advisable to use a multiplicity of values of b and more criteria to make the detection very efficient, the price of further calculations following this method having to be paid.

Moderate efficiency of the “cosh bound” criteria (cf.13-19) : The efficiency of the criterion, $\psi(ir) \geq \psi(0) \cosh(\langle s \rangle r)$, even when it is reinforced by its generalizations for ψ_2 , ψ_b and ψ_{b2} , turns out to be slightly disappointing for the present set of 160 “rebel” functions. Most detections can already come from the simpler positivity and maximality criteria for ψ_b , ψ_{b2} and so on. It seems, however, that the criterion is systematically quite useful for somewhat subtle cases where the negative parts of φ are very weak, but extend to high momenta. To attempt an improvement of the criterion, define then the “complement” function, $\psi_c \equiv \psi - \psi_b$. the Fourier transform of which is, obviously, $(1 - \exp[-s^2/(2b^2)])\varphi$. Distinct average momenta, $\langle s \rangle_b$ and $\langle s \rangle_c$ correspond to ψ_b and ψ_c , respectively. A more precise bound results,

$$\psi(ir) \geq \psi_b(0) \cosh[\langle s \rangle_b r] + \psi_c(0) \cosh[\langle s \rangle_c r]. \quad (29)$$

It is then trivial to extend this process to more components for the bound. For instance one could use two values b and b' simultaneously for the convolution parameter, hence test functions ψ_b and $\psi_{b'}$, and set a combination, $\psi_c = \psi - w\psi_b - w'\psi_{b'}$, with positive weights w, w' such that $w + w' \leq 1$, to retain the assumed positivity of the respective Fourier images $\varphi_b, \varphi_{b'}, \varphi_c$. The corresponding bound,

$$\psi(ir) \geq w\psi_b(0) \cosh[\langle s \rangle_b r] + w'\psi_{b'}(0) \cosh[\langle s \rangle_{b'} r] + \psi_c(0) \cosh[\langle s \rangle_c r]. \quad (30)$$

obviously samples the “probability distribution” $\mathcal{P}(s)$ better.

Criteria from convolution and even derivatives : Alternately, a multiplication of φ by a product of the form, $s^{2q} \exp[-s^2/(2b^2)]$, obviously combines derivatives and convolution, to provide further probes of φ in adjustable domains, and better detect possible defects of positivity.

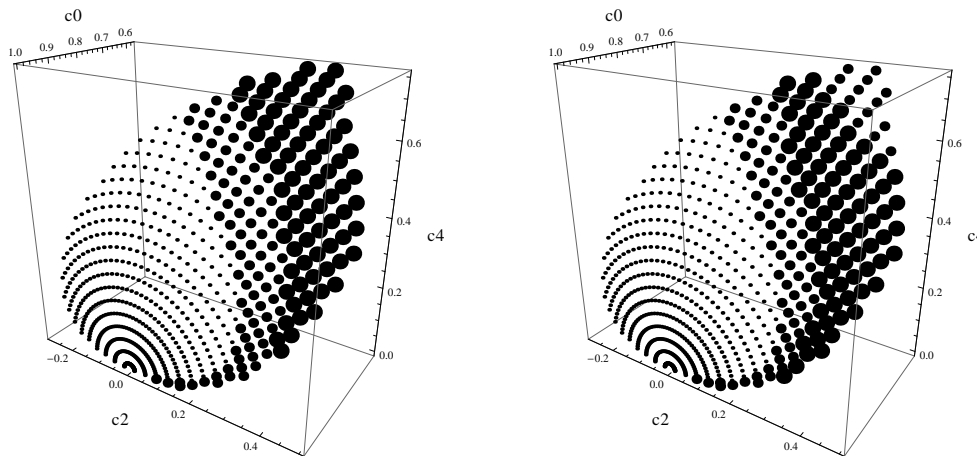


FIG. 4: Tiny dots, simultaneous $\psi > 0$, $\varphi > 0$. Big dots, $\psi > 0$, non-positivity of φ detected with $b = 1/2$ and just the hyperbolic cosine bound for ψ_{b2} , left, or for ψ_{b4} , right. Moderate dots, $\psi > 0$, non-positive φ undetected by such a bound alone.

Recall that $\psi_{b2}(r) = -b/\sqrt{2\pi} d^2/(dr^2) \int_0^\infty dr' [e^{-b^2(r-r')^2/2} + e^{-b^2(r+r')^2/2}] \psi(r')$, with a similar formula for ψ_{b4} . The left part of Figure 4 shows, with $b = 1/2$, how the bound, $\psi_{b2}(ir) \geq \psi_{b2}(0) \cosh[\langle s \rangle_{b2} r]$, taken alone, converts 79 among the 160 “moderate size” dots into “big dots”. Its right part shows the same, with 80 detections, for the bound, $\psi_{b4}(ir) \geq \psi_{b4}(0) \cosh(\langle s \rangle_{b4} r)$. These two sets of big dots, while much overlapping, show significant differences. If both criteria are used simultaneously, the detection rate increases to $94/160 \simeq 59\%$.

Returning to combining criteria already used in this numerical study, most of them positivity and maximality criteria, and taking into account those earlier 271 cases where elimination was very easy, a typical best detection rate reads, $(98 + 271)/(160 + 271) \simeq 85\%$.

B. 1-d test functions with four parameters; more statistics; efficiency of the matrix method (Subsec.II B)

We now consider normalized combinations of the first five even eigenstates of the harmonic oscillator. Components c_0, c_2, \dots, c_8 are random and we have a set of 4388 cases with both ψ and φ positive and, as a test set for our criteria, 21988 cases where φ is partly negative while ψ remains positive.

For our statistics, we consider in the following ten “associated functions”, namely ψ , its sign weighted derivatives, $(-)^q d^{2q}/dr^{2q}\psi$, $q = 1, 2, 3, 4$, then, with $b = 1$, its convoluted form (9) and its sign weighted derivatives, $(-)^q d^{2q}/dr^{2q}\psi_b$, $q = 1, 2, 3, 4$, to be simultaneously tested. Recall that any of these associated functions is just a candidate for a positive Fourier transform related to the same φ .

Bochner test with the 3-matrix : A first test consists in the positiveness of the spectrum of the three equidistant point Toeplitz matrix (6). Typically, we let r run with steps .025 until $r = 3.5$; this is sufficient in the present case. As soon as any of the found eigenvalues for any of the associated functions is negative, the non positivity of φ is exposed. This detects 19653 among the 21988 cases of interest, hence an efficiency of $\simeq 89\%$. If one looks at the remaining 2335 “rebel” cases to see whether the the bound, $\psi(r) \geq \psi(0) \cosh(\langle s \rangle r)$, holds, only 14 more cases show their violation.

Weaker efficiency of the “cosh test” : A second test consists in omitting the “Bochner test” and rather starting by seeing whether the same bound, $\psi(r) \geq \psi(0) \cosh(\langle s \rangle r)$, is violated by any among the ten associated functions. Out of 21988 cases, we find 15887 violations, hence an efficiency of $\simeq 72\%$ for this mode of negativity detection. This leaves 6101 “rebel” cases, to be filtered, in turn, by the Bochner test. We find 3780 additional eliminations. As expected, $19653 + 14 = 15887 + 3780 = 19667$, the latter number being the number of detections when both test modes are used.

Sensitivity to the convolution parameter : We also considered different values of the parameter b , ranging from $b = 1/5$ to $b = 5$. Detections rates are sensitive to b . Best rates correspond to b values between $\simeq 1/2$ and $\simeq 1$, and the choice, $b = 1$, guided by the exponential decrease in our harmonic oscillator basis, is quite acceptable.

Weak efficiency of the “cosh \pm cos” test : For the sake of completeness, the remaining, undetected 2321 cases when $b = 1$ were submitted to the test described by Eqs. (14-15). No new detection was brought by such bounds.

Further Bochner tests : Then, for the same 2321 cases, the function ψ alone, without its nine associates, was submitted to the Bochner test, by an “equidistance” matrix again, of order 5 now. A gain of 20 more detections was obtained.

Returning to the initial basis of 21988 cases, this test of ψ alone by the 5th order Bochner matrix yields 18003 detections, to be compared with the 19653 results obtained with the third order matrix applied to all ten associates. A simultaneous test of ψ and ψ_2 reaches 18687 detections and a simultaneous test of ψ and ψ_b , with again $b = 1$, returns 19247 detections. This seems to show that a Bochner test on the convoluted ψ_b is more useful than a test on the derivative ψ_2, ψ_2, \dots provided that b is well chosen. The same fifth order Bochner test applied to ψ, ψ_2, ψ_b and ψ_{b2} yields 19941 detections. When all ten associates are involved, the result reaches 20468, *i.e.* $\simeq 93\%$. Combining this 5th order Bochner test for the ten associates with a convexity bound test for the same hardly gives $\simeq 10$ more detections.

Preliminary conclusions on the efficiency of criteria : At this stage with this basis of test functions three conclusions stand, namely i) Bochner tests are more efficient than the cosh tests and similar ones obtained from the Jensen inequality, ii) “associate functions”, by derivations and convolutions, do improve results and iii) good detection rates, of order 90% at least, are rather easily available.

IV. TWO-DIMENSIONAL GENERALIZATION

We are interested in the same problematics described in the introduction, applied to the 2-dimensional Fourier case, in the form of the Fourier-Bessel transform. Indeed, one consider here rotationally invariant partners $\psi(x)$ and $\varphi(k)$, where x and k are the lengths of two-dimensional vectors \vec{x} and \vec{k} , respectively. Typically [3], in particle physics, $\varphi(k)$ corresponds to a gluon distribution in transverse momentum space $k \equiv |\vec{k}|$ and $\psi(x)$ is the quark-antiquark dipole distribution in transverse size $x \equiv |\vec{x}|$, both distributions being physically required to be positive real functions.

The Bessel-Fourier transforms analogous to formulas (1,2) read,

$$\varphi(k) = \int_0^{+\infty} x dx J_0(kx) \psi(x), \quad (31)$$

$$\psi(x) = \int_0^{+\infty} k dk J_0(kx) \varphi(k) \quad (32)$$

Conditions i)-v) extend without difficulty, *mutatis mutandis*, to this two-dimensional, and more precisely radial, situation. The following Subsections are therefore restricted to only those considerations which reflect the change of dimensionality.

A. Matrix method

The Bochner theorem is known to apply to higher dimensional Fourier transforms. Hence, applying it on the abscissa axis $\vec{x} = (x, 0)$ for the rotational invariant function $\psi(x)$, one is led to consider the matrix method applied to the following set of Toeplitz matrices

$$\begin{pmatrix} \psi(0) & \psi(x) & \psi(2x) & \dots & \psi[(n-1)x] \\ \psi(x) & \psi(0) & \dots & \dots & \psi[(n-2)x] \\ \dots & \dots & \dots & \dots & \dots \\ \psi[(n-1)x] & \psi[(n-2)x] & \dots & \psi(x) & \psi(0) \end{pmatrix}. \quad (33)$$

Looking for positive definiteness of matrices (33), or its failure, then follows the same path as in the one-dimensional case.

B. Analyticity method

Basic lower bound

Following the same method as for the one-dimensional Fourier transform, one defines the probabilistic formulation of a positive Fourier-Bessel transform as

$$k dk \mathcal{P}(k) \equiv k dk \varphi(k)/\psi(0) \Rightarrow \psi(x) = \psi(0) \langle J_0(kx) \rangle, \quad (34)$$

where $\psi(0) = \int_0^\infty k dk \varphi(k)$ provides the normalization.

For the same reasons as for the 1-d case, the analytic continuation $x \rightarrow ix$ leads to the following Jensen inequality,

$$\psi(ix) = \psi(0) \langle I_0(kx) \rangle \geq \psi(0) I_0(x \langle k \rangle) = \psi(0) I_0 \left[x \int_0^\infty k dk k \varphi(k)/\psi(0) \right], \quad \forall x \in [0, \infty[, \quad (35)$$

where the convex function $I_0(u) \equiv J_0(iu)$ is the Bessel function of the second kind.

As in the previous section, the next step is to make from Eq. (35) a self-content equation in terms of ψ . For this sake, one introduces the Laplace transform,

$$\chi(x) = \int_0^\infty k dk e^{-kx} \varphi(k) = \int_0^\infty k dk e^{-kx} \int_0^\infty x' dx' \psi(x') J_0(kx'). \quad (36)$$

Exchanging the integrals, while keeping $x > 0$, strictly positive in order to preserve the convergence of the integration first over k which can be done analytically, one finds,

$$\chi(x) = \int_0^\infty x' dx' \psi(x') \int_0^\infty k dk e^{-kx} J_0(kx') = x \int_0^\infty \frac{x' dx'}{(x^2 + x'^2)^{3/2}} \psi(x'). \quad (37)$$

An integration by part, similar to that used in subsection II C, returns the derivative of χ for all strictly positive x ,

$$\frac{d\chi}{dx}(x) = \int_0^\infty x' dx' \frac{2x^2 - x'^2}{(x^2 + x'^2)^{5/2}} \psi(x') = - \int_0^\infty dx' \frac{d\psi}{dx'}(x') \frac{x'^2}{(x^2 + x'^2)^{3/2}}, \quad (38)$$

where the last expression, obtained by another integration by part, is now regular at $x = 0$ and thus a faithful representation of the function $d\chi/dx$ for all $x \geq 0$. One then gets for the required moment,

$$\int_0^\infty k dk k \varphi(k) = -\frac{d\chi}{dx}(x=0) = -\int_0^\infty \frac{dx'}{x'} \frac{d\psi}{dx'}(x') = \int_0^\infty \frac{dx'}{x'^2} (\psi(0) - \psi(x')) . \quad (39)$$

Interestingly enough, this is the same expressions, except for a coefficient, as (27) obtained in the 1-d case. Inserting the result (39) into the inequality (35) yields,

$$\psi(ix) \geq \psi(0) I_0 \left[x \int_0^\infty \frac{dx'}{x'^2} \left(1 - \frac{\psi(x')}{\psi(0)} \right) \right], \quad \forall x \in [0, \infty] . \quad (40)$$

Hierarchy of further bounds

Let us introduce the hierarchy of positive functions,

$$\varphi_p(k) \equiv k^p \varphi(k) ; \quad \varphi_0(k) \equiv \varphi(k) . \quad (41)$$

Following the same approach as in section II, we introduce the probability distributions,

$$k dk \mathcal{P}_p(k) \equiv k dk \frac{\varphi_p(k)}{\int_0^\infty k dk \varphi_p(k)} . \quad (42)$$

We also introduce the 2-dimensional radial Laplacian operator Δ_2 acting on $\psi(x)$. It leaves the Bessel functions $J_0(kx)$, $I_0(kx)$ invariant up to factors, namely,

$$\Delta_2 [\psi(x)] \equiv -\frac{1}{x} \frac{d}{dx} \left(x \frac{d}{dx} \right) [\psi(x)] \Rightarrow \Delta_2 [J_0(kx)] = k^2 J_0(kx) . \quad (43)$$

This operator Δ_2 plays in our 2-dimensional problem the role of the ordinary double derivative in 1-d. Then, for even $p = 2q$, we now define a new function $\psi_{2q}(x)$ from the multiple Δ_2 -derivatives of $\psi(x)$,

$$\psi_{2q}(x) \equiv [\Delta_2]^q \psi(x) = \int_0^{+\infty} k dk J_0(kx) k^{2q} \varphi(k) = \int_0^{+\infty} k dk J_0(kx) \varphi_{2q}(k) , \quad (44)$$

by acting on the Bessel-Fourier transform formula (32). In particular, we get for an even moment of φ , of order $2q$, namely the zeroth order moment of φ_{2q} ,

$$\psi_{2q}(0) = [\Delta_2]^q \psi(x)|_{x=0} = \int_0^{+\infty} k dk \varphi_{2q}(k) . \quad (45)$$

Now, extending the Jensen inequality (13) to the probability distributions (42), we get for the positive functions $\psi_{2q}(ix)$ the following hierarchy of inequalities,

$$\psi_{2q}(ix) = \psi_{2q}(0) \langle I_0(xk) \rangle_{\mathcal{P}_{2q}} \geq \psi_{2q}(0) I_0 \left\{ \langle xk \rangle_{\mathcal{P}_{2q}} \right\} = \psi_{2q}(0) I_0 \left\{ x \frac{\int_0^\infty k dk \varphi_{2q+1}(k)}{\int_0^\infty k dk \varphi_{2q}(k)} \right\} , \quad (46)$$

where,

$$\psi_{2q}(ix) = \int_0^{+\infty} k dk I_0(xk) \varphi_{2q}(k) , \quad (47)$$

is the analytic continuation of $\psi(x)$ onto the imaginary axis.

Since ψ_{2q} is just another function assumed to have a positive Fourier transform, we can at once take advantage of Eq. (40) and obtain,

$$\psi_{2q}(ix) \geq \psi_{2q}(0) I_0 \left\{ x \int_0^\infty \frac{dx'}{x'^2} \left(1 - \frac{\psi_{2q}(x')}{\psi_{2q}(0)} \right) \right\} . \quad (48)$$

Convolution

For any width b the product, $\exp[-k^2/(2b^2)] \varphi(k)$, retains the assumed positivity of φ and converts the partner ψ into the result of a convolution,

$$\psi_b(x) = b^2/(2\pi) \int_0^{2\pi} d\theta \int_0^\infty x' dx' \exp[-(x^2 + x'^2 - 2xx' \cos \theta) b^2/2] \psi(x'), \quad (49)$$

an obvious generalization of Eq. (9). The angle θ is that between \vec{r} and \vec{r}' and the angular integration yields,

$$\psi_b(x) = b^2 \exp[-b^2 x^2/2] \int_0^\infty x' dx' I_0(b^2 x x') \exp[-b^2 x'^2/2] \psi(x'). \quad (50)$$

Additional inequalities are easily obtained because the Taylor series of J_0 has the same alternating sign structure as that of \cos . The combinations, $J_0(x) + J_0(ix)$ and $J_0(x) - J_0(ix)$, therefore, are convex and concave, respectively. Generalizations of inequalities (14)-(19) to the present radial, 2-d situation are obvious. An extension of relations (14)-(19) to this hierarchy of functions ψ_{2q} , and to the corresponding functions associated with ψ_b , is trivial.

C. Numerical investigations for the Bessel transform

We generated 10127 test functions $\psi(x)$ by randomly mixing the following 5 functions, $\sqrt{2}e^{-x^2/2}$, $\sqrt{2}e^{-x^2/2}(1-x^2)$, $e^{-x^2/2}(2-4x^2+x^4)/\sqrt{2}$, $e^{-x^2/2}(6-18x^2+9x^4-x^6)/(3\sqrt{2})$, $e^{-x^2/2}(24-96x^2+72x^4-16x^6+x^8)/(12\sqrt{2})$. This is an orthonormal basis with the measure $x dx$, $0 \leq x < +\infty$, using Laguerre polynomials. The basis states are eigenstates of the Fourier-Bessel transform, with eigenvalues $\{1, -1, 1, -1, 1\}$, respectively. Then our random mixtures were screened so that each ψ be square normalized, positive, with its maximum at the origin, while φ has some negativity, to be detected.

We implemented the “matrix test” at orders 5, 8, 9 and 10 for ψ alone, for simplicity, neglecting its associated derivative and convoluted functions. Detection rates were $\simeq 29\%$, 39% , 41% , 43% , respectively, compared to $\simeq 69\%$, 82% , 84% , 86% , for the 1-dimensional case again for ψ alone. These 2-d detection rates are less satisfactory than the detection rates obtained with our 1-d test set, but still acceptable, because of our screening for cases with a maximum at the origin only.

The analyticity test for ψ alone returned hardly a $\simeq 3\%$ detection rate, which is weak and similar to $\simeq 5\%$ for the 1-dimensional case. This is confirmed by combining the matrix test at order 10 with this analyticity test. Except for one case, those 14% functions undetected by the matrix test also escape the analyticity test.

V. CONCLUSION AND OUTLOOK

The constructive characterization of real functions with positive Fourier transforms in one and two-dimensional (radial) dimensions has been analyzed here with two different methods. One, the “analyticity method”, makes use of analytic continuation combined with convexity properties (Jensen inequalities). The other, the “matrix method”, deals with finite Toeplitz matrices testing the Bochner theorem through tests of positive definiteness.

We test these methods on a set of random mixtures of functions combining a Gaussian with polynomials forming a finite, but of sizable dimension, orthogonal basis. We estimate and compare the efficiencies of both methods.

In one dimension, the matrix method reaches a 86% efficiency for the test on the function ψ alone, and reaches easily more than 93% for the combined test including derivatives. This is to be compared with 43% for the analyticity method and 85% at most, after combining with suitable convolutions and differentiation preserving the positivity of the Fourier transform. All in all the matrix method seems at present quite successful and more directly efficient than the analyticity one.

In the two-dimensional (radial) case, the situation is less satisfactory for the matrix method. It reaches a 43% efficiency under the same conditions, but is still probably not too difficult to improve quantitatively. The analyticity method, by contrast, is at the present stage much ineffective, with only $\simeq 3\%$ detection for the same set of non positive Fourier-Bessel transforms. This method requires a qualitative improvement to be competitive; a good subject for future research.

By way of an outlook, there are possible directions for improvement.

Although our sets of test functions are reasonably big (10^4 typically) and diversified, we feel that our conclusions should be strengthened by the consideration of a larger basis and not necessarily weighted by Gaussians, with more allowed configuration mixing. However, we may already define quite a few new research directions on the same line, namely:

- In two dimensions, it is clear that a vectorial version of the matrix model is to be investigated, by comparison with the one-dimensional projection used in section IV.
- The analyticity method, despite its mathematical simplicity based on generalized convexity properties, seems at its present stage suffering from a deficit of efficiency. The question remains of improved convexity tests.
- Considering the matrix method and its growing accuracy with matrix dimension, it is tempting to consider the possibility of using Toeplitz matrices of large rank.
- At last but not least, the full constructive characterization of positive positive-definite functions is yet to be reached, hoping that the steps made in the present paper may lead to this goal.

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