From Herglotz-Nevanlinna functions to completely monotonic functions

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Herglotz-Nevanlinna Functions and their Applications to Dispersive Systems and Composite Materials
CIRM, Luminy, May 23-27, 2022

Partially based on joint work with
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Overview

Part 1

Introduction to Herglotz-Nevanlinna functions and related classes of functions

1. Holomorphic functions in a domain with non-negative real or imaginary part
2. Completely monotonic functions and Stieltjes functions

Part 2

3. A study of the family of functions

$$f_\alpha(z) = \exp(\alpha) - (1 + 1/z)^{\alpha z}, \alpha \in \mathbb{C}$$

4. The entire functions φ_α such that

$$f_\alpha(z) = \int_0^\infty \exp(-sz)\varphi_\alpha(s)\, ds, \quad \operatorname{Re} z > 0$$

5. Graphs of $f_\alpha, \alpha > 0$

Gustav Herglotz (1881-1953), Czech born German mathematician

Theorem (Herglotz, 1911)

The holomorphic functions f defined in the unit disc $\mathbb{D}$ and having non-negative real part are characterized by the following formula

$$f(z) = i\beta + \int_{\mathbb{T}} \frac{t+z}{t-z}\, d\mu(t), \quad z \in \mathbb{D},$$

where $\beta \in \mathbb{R}$ and μ is a positive measure on the unit circle $\mathbb{T}$.

Rolf Nevanlinna (1895-1980), Finnish
Georg Pick (1859-1942), Austrian

Via a conformal mapping of the unit disc onto the upper half-plane, Herglotz' representation is equivalent with the following integral representation of holomorphic functions f, defined in the upper half-plane $\mathbb{H} := \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}$, such that $\operatorname{Im} f(z) \geq 0$ for all $z \in \mathbb{H}$. The class $\mathcal{N}$ of these functions carry many names: At this meeting Herglotz-Nevanlinna functions, but they are also called Pick functions and R-functions. They are the functions

$$f(z) = \alpha z + \beta + \int_{-\infty}^{\infty} \frac{tz+1}{t-z}\, d\tau(t), \quad z \in \mathbb{H},$$

where $\alpha \geq 0, \beta \in \mathbb{R}$ and τ is a positive finite measure on $\mathbb{R}$.

Nevanlinna

Pick

More on Pick functions

Using the identity

$$(1+t^2)\left(\frac{1}{t-z}-\frac{t}{1+t^2}\right)=\frac{tz+1}{t-z}$$

the representation can be written

$$f(z)=\alpha z+\beta+\int_{-\infty}^{\infty}\left(\frac{1}{t-z}-\frac{t}{1+t^2}\right)\,d\sigma(t), \quad (*)$$

where $\sigma=(1+t^2)\tau$ satisfies $\int(1+t^2)^{-1}d\sigma(t)<\infty$. This gives

$$\operatorname{Im} f(x+iy)=\alpha y+\int_{-\infty}^{\infty}\frac{y}{(t-x)^2+y^2}\,d\sigma(t)\geq 0, \quad y>0,$$

and it is easily seen that

$$\alpha=\lim_{y\to\infty}\frac{f(iy)}{iy},\ \beta=\operatorname{Re} f(i),\ \sigma=\lim_{y\to 0^+}\frac{1}{\pi}\operatorname{Im} f(x+iy)\,dx \text{ vaguely.}$$

More about the representing measure

This means

$$\int \varphi(x)\, d\sigma(x) = \lim_{y\to 0^+} \frac{1}{\pi} \int_{-\infty}^{\infty} \operatorname{Im} f(x+iy)\varphi(x)\, dx, \quad \varphi \in C_c(\mathbb{R}).$$

Corollary

Let $f \in \mathcal{N}$ have the representation $(*)$ and assume that

$$s(x) = \lim_{y\to 0^+} \frac{1}{\pi} \operatorname{Im} f(x+iy)$$

exists for x in an open set $I \subset \mathbb{R}$ and that the convergence is uniform on compact subsets of I. The the restriction of σ to I has the density s with respect to Lebesgue measure.

Note that by $(*)$ a Pick function f automatically extends to a holomorphic function in $\mathbb{C} \setminus \mathbb{R}$ satisfying $f(\overline{z}) = \overline{f(z)}$.

Stability properties of the class $\mathcal{N}$. Examples

a) $\mathcal{N}$ is a convex cone.
b) A Pick function f is either a real constant function (the degenerate case) or satisfies $\operatorname{Im} f(z) > 0$ for all $z \in \mathbb{H}$ (the non-degenerate case), i.e. $f(\mathbb{H}) \subseteq \mathbb{H}$.
c) If f, g are non-degenerate Pick functions, then $f \circ g$ is a non-degenerate Pick function.
d) If $f \in \mathcal{N} \setminus \{0\}$ then $-1/f \in \mathcal{N}$.

Examples 1. The principle logarithm $\operatorname{Log} z = \ln |z| + i \operatorname{Arg} z$ is a Pick function and

$$\operatorname{Log} z = \int_{-\infty}^{0} \left(\frac{1}{t - z} - \frac{t}{1 + t^2} \right) dt.$$

2. Any linear fractional transformation of the form

$$f(z) = \frac{az + b}{cz + d}, \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL_2(\mathbb{R})$$

is a Pick function. In fact, $\operatorname{Im} f(x + iy) = y/|cz + d|^2$.

Further examples of Pick functions

3. $f(z) = z^\alpha = \exp(\alpha \operatorname{Log} z)$, $0 \le \alpha \le 1$.
4. $\tan z$, since

$$\operatorname{Im} \tan(x + iy) = \frac{\sinh y \cosh y}{\cos^2 x + \sinh^2 y}.$$

5.

$$\frac{\log \Gamma(z+1)}{z \operatorname{Log} z}; \quad \frac{\log \Gamma(z+1)}{z}.$$

Berg and Henrik L. Pedersen, Rocky Mountain J. Math. **32** (2002), motivated by a study of the asymptotic behaviour of $V_n^{1/n \log n}$ where $V_n = \pi^{n/2}/\Gamma(1 + n/2)$ is the volume of the unit ball in $\mathbb{R}^n$.

6. Various extensions to multiple Gamma functions by Pedersen and coauthors.

Stieltjes transforms, Thomas Jan Stieltjes (1856-1894), Dutch born French

The Stieltjes transform of a positive finite measure σ on $\mathbb{R}$ is the special Pick function

$$I_\sigma(z) = \int \frac{1}{t - z}\, d\sigma(t), \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

The following result is easy but important:

Proposition

The special Pick functions I_σ are characterized as the Pick functions f for which $f(iy) = O(1/y)$, $y \to \infty$

Indeterminate moment problems

An indeterminate Hamburger moment sequence is a real sequence $(s_n)_{n\geq 0}$ for which there are infinitely many probability measures σ on $\mathbb{R}$ with moments s_n, i.e.,

$$s_n = \int_{-\infty}^{\infty} x^n \, d\sigma(x), \quad n = 0, 1, 2, \ldots . \quad (**)$$

Nevanlinna (1922) gave the parametrization

$$I_{\sigma_f}(z) = \int \frac{1}{t-z} \, d\sigma_f(t) = -\frac{A(z)f(z) - C(z)}{B(z)f(z) - D(z)}, \quad z \in \mathbb{C} \setminus \mathbb{R}$$

of all the solutions σ_f to $(**)$, where $f \in \mathcal{N} \cup \{\infty\}$. Here A, B, C, D are certain entire functions defined in terms of the orthogonal polynomials associated with (s_n).

The class $\mathcal{N}_A$ for a closed set $A \subseteq \mathbb{R}$

As we have seen, $f \in \mathcal{N}$ can be extended to a holomorphic function in the lower half-plane, and it is natural to ask, if there is an analytic continuation of f across some part of the real axis. This is formalized in the following:

Definition

For a closed set $A \subseteq \mathbb{R}$ we denote by $\mathcal{N}_A$ the set of $f \in \mathcal{N}$ for which there exists $F \in \mathcal{H}(\mathbb{C} \setminus A)$ such that

$$F(z) = \begin{cases} f(z), & \operatorname{Im} z > 0 \\ \overline{f(\overline{z})}, & \operatorname{Im} z < 0. \end{cases}$$

If F exists it is clearly determined on $\mathbb{R} \setminus A$ by the real values $F(x) = \lim_{y \to 0^+} f(x + iy)$.

Characterization of $\mathcal{N}_A$

Theorem

A Pick function f with representation $(*)$ belongs to $\mathcal{N}_A$ if and only if $\mathrm{supp}(\sigma) \subseteq A$, and in the affirmative case the right-hand side of $(*)$ defines the holomorphic extension to $\mathbb{C} \setminus A$.

Note that $\mathrm{Log} \in \mathcal{N}_{]-\infty,0]}$.

Given an open interval $I =]a, b[$ a function $f : I \to \mathbb{R}$ is called operator monotone if $f(A) \leq f(B)$ for all self-adjoint operators A, B in a Hilbert space satisfying $A \leq B$ and having spectrum contained in I. Loewner proved that for a function to be operator monotone it is enough to consider $n \times n$-matrices A, B of arbitrary size n. In the matrix case $f(A)$ is defined in an elementary way using diagonalization. In the general case $f(A)$ is defined via the functional calculus. Loewner further proved, that the set of operator monotone functions is exactly $\mathcal{N}_{\mathbb{R} \setminus I}$.

Completely monotonic functions

A function $f :]0, \infty[\to \mathbb{R}$ is called completely monotonic if it is C^∞ and

$$(-1)^n f^{(n)}(x) \geq 0, \quad n \geq 0,\ x > 0.$$

The set of completely monotonic functions is denoted $\mathcal{C}$. It is a convex cone and stable under multiplication as is seen directly from the definition. It is less obvious that $\mathcal{C}$ is closed under pointwise convergence, but follows from the following result:

Theorem (Bernstein (1928))

A function $f :]0, \infty[\to \mathbb{R}$ is completely monotonic if and only if it is the Laplace transform of a positive measure μ on $[0, \infty[$, i.e.

$$f(x) = \mathbb{L}\mu(x) = \int_0^\infty e^{-xs}\, d\mu(s), \quad x > 0. \tag{1}$$

The measure μ in the theorem is not necessarily finite. Since $f \in \mathcal{C}$ is decreasing, $\lim_{x\to 0^+} f(x) = f(0+)$ exists and equals $\mu([0, \infty[)$.

How to prove complete monotonicity? Stieltjes transforms

The integral representation of $f \in \mathcal{C}$ shows that f can be extended to a holomorphic function in the right half-plane $\{z \mid \operatorname{Re} z > 0\}$. If the calculation of the high derivatives of f are too complicated, one may try to find the measure $\exp(-xs)d\mu(s)$ by Fourier inversion of $y \to f(x+iy)$ for fixed $x > 0$, but that can be very difficult too.
A function $f :]0,\infty[\to [0,\infty[$ is called a Stieltjes function if it has the representation

$$f(x) = a + \int_0^\infty \frac{d\mu(s)}{x+s},$$

where $a \geq 0$ and μ is a positive measure on $[0,\infty[$ such that $\int 1/(1+s)d\mu(s) < \infty$.
Note that

$$f(x) = \mathbb{L}[a\delta_0 + \mathbb{L}\mu(s)1_{]0,\infty[}(s)\, ds :](x),$$

So the set $\mathcal{S}$ of Stieltjes functions is a convex subcone of $\mathcal{C}$.

Sergei Bernstein (1880-1968), Ukrainian

The formula for Stieltjes functions show that they have a holomorphic extension to the cut plane $\mathbb{C}\setminus]-\infty,0]$, and they can be characterized via complex analysis. The result is attributed to M. G. Krein in Akhiezer's book about the moment problem.

Theorem (Krein)

A function $f:]0,\infty[\to\mathbb{R}$ is a Stieltjes function if and only if $f(x)\geq 0$ for $x>0$ and it has a holomorphic extension (also denoted f) to the cut plane $\mathbb{C}\setminus]-\infty,0]$ satisfying $\operatorname{Im} f(x+iy)\leq 0$ for $y>0$.

Properties of Stieltjes functions. Examples

(i) $f \in \mathcal{S} \setminus \{0\} \Rightarrow \frac{1}{f(1/x)} \in \mathcal{S}$

(ii) $f \in \mathcal{S} \setminus \{0\} \Rightarrow \frac{1}{xf(x)} \in \mathcal{S}$

(iii) $f \in \mathcal{S} \setminus \{0\} \Rightarrow 1/f, -f \in \mathcal{N}$

(iv) $f, g \in \mathcal{S},\ 0 < \alpha < 1 \Rightarrow f^\alpha g^{1-\alpha} \in \mathcal{S}$.

Property (ii) was established by Reuter (1956) in work about integral equations and independently by Masayuki Itô (1974) in potential theory, but already Stieltjes noticed it in a letter to Hermite from 1894. The property (iv) shows that the cone $\mathcal{S}$ is logarithmically convex.

Examples: For $\alpha > 0$: $x^{-\alpha} \in \mathcal{C}$. $\quad x^{-\alpha} \in \mathcal{S} \iff 0 < \alpha \leq 1$.

$$e^\alpha - (1+1/x)^{\alpha x} = \frac{1}{\pi}\int_0^1 \frac{(t/(1-t))^{\alpha t}\sin(\alpha\pi t)}{x+t}dt \in \mathcal{S}, 0 < \alpha < 1.$$

This is a formula obtained by Berg and Alzer in 2002. (More later)

Positive operator monotone functions on $]0,\infty[$

Theorem

For a function $f :]0,\infty[\to [0,\infty[$ the following conditions are equivalent:

(i) *f can be extended to a function in $\mathcal{N}_{]-\infty,0]}$.*

(ii) *f has the representation*

$$f(x) = \alpha x + x \int_0^\infty \frac{d\sigma(t)}{x+t},$$

where $\alpha \geq 0$ and σ is a positive measure on $[0,\infty[$ satisfying $\int (1+t)^{-1}\, d\sigma(t) < \infty$.

(iii) *$f(x)/x \in \mathcal{S}$.*

These functions are called complete Bernstein functions by René Schilling (1994) in connection with Lévy processes.

Introduction to a paper by Berg, Massa and Peron

For $\alpha > 0, x > 0$ it is classical that $h_\alpha(x) := (1 + 1/x)^{\alpha x}$ increases from 1 to e^α as $x \to \infty$. It is a small exercise to prove that the function is concave iff $\alpha \leq 3.69127...$, where the number is the minimum value of a certain function. In other words h'_α is positive and decreasing for $0 < \alpha \leq 3.69127...$.

In 2003 I posed the question: For which $\alpha \geq 0$ is h'_α completely monotonic?.

Graphs suggested that the answer is an interval $[0, \alpha^*]$ with $2 < \alpha^* < 3$. Several people worked on this during more than 15 years and came up with various approximations to α^*.

In joint work with Massa and Peron in 2019 we obtained the approximation

$$\alpha^* \approx 2.29965\,64432\,53461\,30332$$

together with some explanation of what α^* is, based on complex and harmonic analysis.

The corresponding holomorphic function

For $\alpha \in \mathbb{C}$ we consider the holomorphic function

$$h_\alpha(z) = (1+1/z)^{\alpha z} := \exp(\alpha z \,\mathrm{Log}(1+1/z)), \quad z \in \mathcal{A} = \mathbb{C} \setminus]-\infty, 0]$$

where $\mathrm{Log} : \mathcal{A} \to \mathbb{C}$ is the principal logarithm, holomorphic in $\mathcal{A}$ and real on the positive half-axis.

We have $\lim_{|z|\to\infty} h_\alpha(z) = \exp(\alpha)$ and define

$$f_\alpha(z) = \exp(\alpha) - h_\alpha(z), \quad z \in \mathcal{A}.$$

An equivalent formulation of the original problem is

For which $\alpha \geq 0$ is f_α a completely monotonic function?
Berg-Alzer proved in 2002 that $f_\alpha \in \mathcal{S}$ (hence completely monotonic) for $0 < \alpha \leq 1$.

Search for functions φ_α by Fourier inversion of f_α

Since the derivatives of h_α become very complicated we search for functions φ_α such that

$$f_\alpha(x) = \int_0^\infty e^{-xs}\varphi_\alpha(s)\,ds, \quad \alpha \in \mathbb{C}, x > 0,$$

because by Bernstein's Theorem the problem is reduced to

For which α is φ_α non-negative on $[0,\infty[$?

It turns out by Fourier inversion that

$$\varphi_\alpha(s) = \frac{1}{2\pi i}\int_{C(r,c)} f_\alpha(z)e^{sz}\,dz, \quad \alpha, s \in \mathbb{C}$$

is an entire function, which is independent of $c > 1, r > 0$. Here $C(r,c)$ denotes the rectangle with corners $-c \pm ir, \pm ir$ considered as a closed contour with positive orientation.

First step in the Fourier inversion

Notice that f_α extends to a holomorphic function in $\mathbb{C} \setminus [-1, 0]$. In fact, for $z \neq 0, |z| < 1$

$$g_\alpha(z) := e^\alpha - \exp(\alpha z^{-1} \operatorname{Log}(1+z)) = e^\alpha - \exp((\alpha(1 - z/2 + z^2/3 - \ldots)),$$

so defining $g_\alpha(0) = 0$ we have that g_α is holomorphic in the unit disc and

$$f_\alpha(z) := g_\alpha(1/z), \quad |z| > 1$$

yields a holomorphic extension of f_α to $\mathbb{C} \setminus [-1, 0]$.
The power series of g_α can be written

$$g_\alpha(z) = e^\alpha \sum_{n=1}^{\infty} (-1)^{n-1} p_n(\alpha) z^n, \quad |z| < 1,$$

where $p_n(\alpha)$ is a sequence of polynomials in α given next.

The polynomials $p_n(\alpha)$

Let $(p_n)_{n\geq 0}$ denote the sequence of polynomials defined by

$$p_0(\alpha)=1, \quad p_1(\alpha)=\frac{\alpha}{2}, \quad p_2(\alpha)=\frac{\alpha}{3}+\frac{\alpha^2}{8},\ldots, \tag{2}$$

and in general

$$p_{n+1}(\alpha)=\frac{\alpha}{n+1}\sum_{k=0}^{n}\frac{k+1}{k+2}p_{n-k}(\alpha), \quad n\geq 0. \tag{3}$$

$$p_n(\alpha)=\sum_{k=1}^{n}c_{n,k}\alpha^k, \quad n\geq 1, c_{n,k}>0$$

$$c_{n,1}=\frac{1}{n+1}, \quad c_{n,n}=\frac{1}{2^n n!}.$$

There is a complicated formula for $c_{n,k}$ in terms of Stirling numbers.

Bell partition polynomials

To get the polynomials $p_n(\alpha)$ we use a classical formula from combinatorics

$$\exp\left(\sum_{k=1}^{\infty}\frac{a_k}{k!}z^k\right)=\sum_{n=0}^{\infty}\frac{B_n(a_1,\ldots,a_n)}{n!}z^n,$$

where B_n are the exponential Bell partition polynomials. It is known that

$$B_0=1,\quad B_1(a_1)=a_1,\quad B_2(a_1,a_2)=a_1^2+a_2,$$

and in general we have the recursion formula

$$B_{n+1}(a_1,\ldots,a_{n+1})=\sum_{k=0}^{n}\binom{n}{k}B_{n-k}(a_1,\ldots,a_{n-k})a_{k+1}.$$

Application of the Bell partition polynomials

We know that for $z \in \mathbb{D}, z \neq 0$, then
$h_\alpha(1/z) = \exp(\alpha z^{-1} \operatorname{Log}(1+z))$ is holomorphic in $\mathbb{D}$.
Defining $a_k = (-1)^k \alpha k!/(k+1),\ k \geq 1$, this gives

$$\begin{aligned} f_\alpha(1/z) &= e^\alpha - e^\alpha \exp\left(\sum_{k=1}^\infty (-1)^k \alpha \frac{z^k}{k+1}\right) \\ &= -e^\alpha \sum_{n=1}^\infty \frac{B_n(a_1,\ldots,a_n)}{n!} z^n = e^\alpha \sum_{n=1}^\infty (-1)^{n-1} p_n(\alpha) z^n, \end{aligned}$$

where we have defined

$$p_n(\alpha) := (-1)^n \frac{B_n(a_1,\ldots,a_n)}{n!}.$$

This gives the recursion for p_n.

Second step in the Fourier inversion

We next look at f_α on the imaginary axis when $\alpha \in \mathbb{C} \setminus \{0\}$.
As a function of $y \in \mathbb{R}$

$$F_\alpha(y) := \begin{cases} f_\alpha(iy) = e^\alpha - \left(1 + y^{-2}\right)^{i\alpha y/2} \exp(\alpha y \operatorname{Arctan}(1/y)), & y \neq 0, \\ e^\alpha - 1, & y = 0, \end{cases}$$

is continuous and tends to 0 for $|y| \to \infty$. It belongs to $L^2(\mathbb{R}) \setminus L^1(\mathbb{R})$.

Proof.

We have for $y \neq 0$

$$\exp(i\alpha y \operatorname{Log}(1 - i/y)) = \exp(i\alpha y[\log \sqrt{1 + y^{-2}} - i \operatorname{Arctan}(1/y)]),$$

where $\operatorname{Arctan} : \mathbb{R} \to] - \pi/2, \pi/2[$ is the inverse of tan. The continuity of F_α for $y = 0$ follows, and the behavior at $\pm\infty$ including the integrability properties follows because $f_\alpha(iy) \sim (\alpha \exp(\alpha))/iy$ for $|y| \to \infty$. □

Use of Plancherel's Theorem

There exists an L^2-function G_α on $\mathbb{R}$ such that

$$f_\alpha(iy) = \lim_{R\to\infty} \int_{-R}^{R} G_\alpha(s)\exp(-iys)\,ds, \quad y \in \mathbb{R}$$

and

$$G_\alpha(s) = \lim_{R\to\infty} \frac{1}{2\pi} \int_{-R}^{R} f_\alpha(iy)\exp(iys)\,dy, \quad s \in \mathbb{R}.$$

In both cases the limits are in the norm of $L^2(\mathbb{R})$.
If we let R tend to infinity through a suitable sequence $R_n \to \infty$, we can also obtain pointwise convergence almost everywhere.

Use of holomorphy of $f_\alpha(z)\exp(sz)$ in the right half-plane

This gives by Cauchy's integral theorem

$$\int_{-R}^{R} f_\alpha(iy)e^{isy}\,i\,dy = \int_{-\pi/2}^{\pi/2} f_\alpha(Re^{it})e^{sRe^{it}}Re^{it}\,i\,dt.$$

The absolute value of the integrand to the right is bounded by

$$\frac{C}{R}e^{sR\cos(t)}R$$

for a suitable $C > 0$ depending on α. If we assume $s < 0$, then $sR\cos t \to -\infty$ for $R \to \infty$ when $-\pi/2 < t < \pi/2$, so the integral to the right tends to 0 by dominated convergence.

Conclusion: $G_\alpha(s) = 0$ for $s < 0$

Use of holomorphy of f_α outside $[-1, 0]$

Theorem (1)

For $\alpha \in \mathbb{C}$, the function

$$\varphi_\alpha(s) = \frac{1}{2\pi i} \int_{C(r,c)} f_\alpha(z) e^{sz}\, dz, \quad s \in \mathbb{C}$$

is an entire function, which is independent of $c > 1, r > 0$.

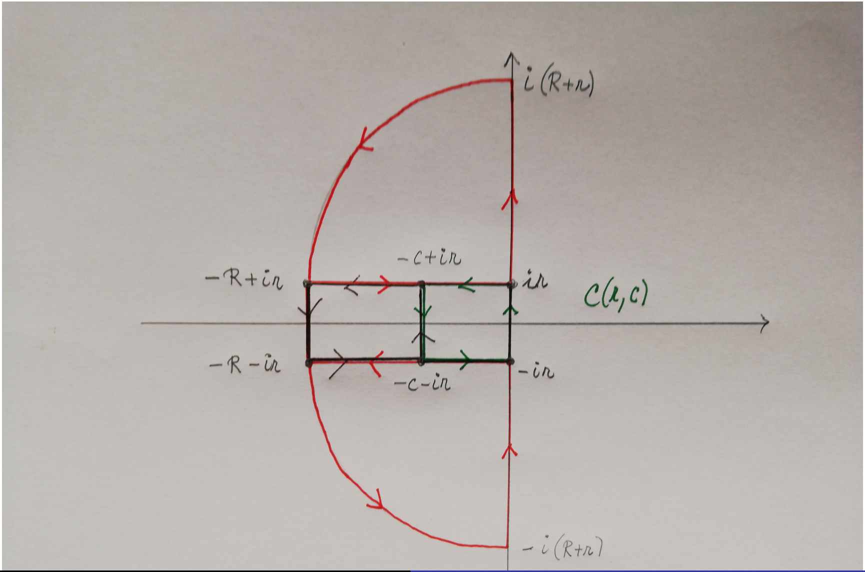
$$\varphi_\alpha(s) = e^\alpha \sum_{n=0}^{\infty} (-1)^n p_{n+1}(\alpha) \frac{s^n}{n!}, \quad s \in \mathbb{C}.$$

Moreover, the function

$$s \mapsto \begin{cases} \varphi_\alpha(s), & \text{when } 0 \le s < \infty, \\ 0, & \text{when } -\infty < s < 0, \end{cases}$$

is equal to $G_\alpha(s)$ for almost all $s \in \mathbb{R}$.

Change of contour $C(r, c)$



Finishing the proof of Theorem 1

This gives

$$\varphi_\alpha(s) = \frac{1}{2\pi i}\int_{-i(r+R)}^{i(r+R)} f_\alpha(z)e^{sz}\,dz + \frac{1}{2\pi i}\int_{L(R)} f_\alpha(z)e^{sz}\,dz,$$

where $L(R)$ is the path in the left half-plane from $i(r+R)$ to $-i(r+R)$. For $s>0$ the first integral converges to $G_\alpha(s)$ a.e. and the last integral converges to 0 for a suitable sequence $R = R_n \to \infty$.

The power series of φ_α

From the compactness of the contour $C(r,c)$ we get

$$\varphi_\alpha(s) = \sum_{n=0}^{\infty} \frac{s^n}{n!} \frac{1}{2\pi i} \int_{C(r,c)} f_\alpha(z) z^n \, dz.$$

Using that $f_\alpha(z)z^n$ is holomorphic outside $[-1,0]$, we can replace the contour $C(r,c)$ by the circle $|z| = R_0$, where $R_0 > \sqrt{c^2+r^2} > 1$. We next use the Laurent expansion

$$f_\alpha(z) = g_\alpha(1/z) = e^\alpha \sum_{k=1}^{\infty} (-1)^{k-1} p_k(\alpha) z^{-k}, \quad |z| > 1,$$

and get

$$\begin{aligned} \frac{1}{2\pi i} \int_{C(r,c)} f_\alpha(z) z^n \, dz &= \sum_{k=1}^{\infty} e^\alpha (-1)^{k-1} p_k(\alpha) \frac{1}{2\pi i} \int_{|z|=R_0} z^{n-k} \, dz \\ &= e^\alpha (-1)^n p_{n+1}(\alpha). \end{aligned}$$

φ_α is completely monotonic iff $0 \le \alpha \le 1$

If $(p_{n+1}(\alpha))_{n\ge 0}$ is a Stieltjes moment sequence, i.e.,

$$p_{n+1}(\alpha) = \int_0^\infty x^n \, d\sigma_\alpha(x), \quad n \ge 0, \quad \sigma_\alpha \ge 0, \tag{4}$$

then it is easy to see that

$$\varphi_\alpha(s) = e^\alpha \int_0^\infty e^{-sx} \, d\sigma_\alpha(x), \quad s \in \mathbb{C}, \tag{5}$$

and in particular $\varphi_\alpha(s) \ge 0$ for $s \ge 0$ and hence $0 \le \alpha \le \alpha^*$.

Theorem (2)

The following conditions are equivalent:

(i) $(p_{n+1}(\alpha))_{n\ge 0}$ *is a Stieltjes moment sequence.*

(ii) φ_α *is completely monotonic.*

(iii) $0 \le \alpha \le 1$.

If the equivalent conditions hold, then σ_α *from* (4) *is supported by* $[0,1]$*, and* $(p_{n+1}(\alpha))_{n\ge 0}$ *is a Hausdorff moment sequence.*

Integral representation of φ_α for $0 < \alpha \leq 1$

In the formula

$$\varphi_\alpha(s) = \frac{1}{2\pi i} \int_{C(r,c)} f_\alpha(z) e^{sz}\, dz, \quad \alpha, s \in \mathbb{C}$$

we let $r \to 0$ and for $0 < \alpha < 1$ we get after some work

$$\varphi_\alpha(s) = \frac{1}{\pi} \int_0^1 (x/(1-x))^{\alpha x} \sin(\alpha \pi x) e^{-sx}\, dx, \quad s \geq 0.$$

We next let $\alpha \to 1^-$ and again after some work an extra term comes out: Furthermore,

$$\varphi_1(s) = e^{-s} + \frac{1}{\pi} \int_0^1 (x/(1-x))^{x} \sin(\pi x) e^{-sx}\, dx, \quad s \geq 0.$$

NB. The middle formula has no sense for $\alpha > 1$.

Study of φ_α when α is small

From

$$\varphi_\alpha(s) = e^\alpha \sum_{n=0}^{\infty} p_{n+1}(\alpha) \frac{(-s)^n}{n!}, \quad p_n(\alpha) = \frac{\alpha}{n+1} + \cdots + \frac{\alpha^n}{2^n n!}, \; n \geq 1$$

we get

$$\lim_{\alpha \to 0} \frac{\varphi_\alpha(s)}{\alpha e^\alpha} = \sum_{n=0}^{\infty} \frac{(-s)^n}{(n+2)n!}, = \begin{cases} \dfrac{1-(1+s)e^{-s}}{s^2}, & \text{when } s \neq 0, \\ \dfrac{1}{2}, & \text{when } s = 0, \end{cases}$$

uniformly for s in compact subsets of the complex plane.
The limit function is completely monotonic and in particular positive for $s \geq 0$.
The zeros of the limit function are given by $1 + s = e^s$, which has no real solutions except $s = 0$. The complex zeros can be expressed by the Lambert W function.

The Bessel function J_1

It is the entire function given by

$$J_1(z) = \sum_{n=0}^{\infty} (-1)^n \frac{(z/2)^{2n+1}}{n!(n+1)!}.$$

The zeros of J_1 are $0, \pm j_1, \pm j_2, \ldots$, where

$$j_1 \approx 3.83170,\ j_2 \approx 7.01558,\ j_3 \approx 10.17346$$

Study of φ_α when α is large

For $|\alpha| \to \infty$ we get

$$\frac{\varphi_\alpha(s/\alpha)}{\alpha\, e^\alpha} = \sum_{n=0}^{\infty} \frac{p_{n+1}(\alpha)}{\alpha^{n+1}} \frac{(-s)^n}{n!} \to \sum_{n=0}^{\infty} \frac{(-s)^n}{2^{n+1}(n+1)!n!} = \frac{J_1(\sqrt{2s})}{\sqrt{2s}}$$

uniformly for s in compact subsets of the complex plane, where J_1 is the Bessel function of order 1.

Given $n \in \mathbb{N}$, φ_α has at least n simple zeros $s_1(\alpha), s_2(\alpha), \ldots, s_n(\alpha)$ such that $0 < |s_1(\alpha)| < |s_2(\alpha)| < \ldots < |s_n(\alpha)|$ for $|\alpha|$ sufficiently large, and they satisfy

$$\lim_{|\alpha|\to\infty} \alpha s_k(\alpha) = \frac{j_k^2}{2} \qquad \text{for all } k \le n. \tag{6}$$

If in addition $\alpha > 0$, then $s_j(\alpha) > 0$, $j = 1, \ldots, n$. This shows that φ_α stops being positive when α is sufficiently large and it oscillates with more and more positive zeros real as α increases to infinity.

The power series for φ_a is eventually alternating when $\alpha > 0$

Theorem (3)

For $\alpha > 0$, $n \geq 0$, we know that $p_n(\alpha) > 0$ and

$$\frac{p_{n+1}(\alpha)}{p_n(\alpha)} \leq \widehat{\alpha} := \begin{cases} 1, \textit{ when } 0 \leq \alpha \leq 1, \\ 2\alpha, \textit{ when } 1 < \alpha < 2, \\ \alpha, \textit{ when } 2 \leq \alpha. \end{cases} \qquad (7)$$

Then the power series for φ_α satisfies the Alternating Series Test for $n \geq \widehat{\alpha}s$, which allows to obtain an error bound for the truncated series.

In fact,

$$p_{n+1}(\alpha)\frac{s^n}{n!} \leq p_n(\alpha)\frac{s^{n-1}}{(n-1)!} \iff \frac{p_{n+1}(\alpha)}{np_n(\alpha)} \leq \frac{1}{s}$$

so the power series satisfies the alternating series test for $n \geq \widehat{\alpha}s$.

Summary of numerical calculations

Theorem (4)

(i) $\alpha^* \approx 2.29965\,64432\,53461\,30332.$

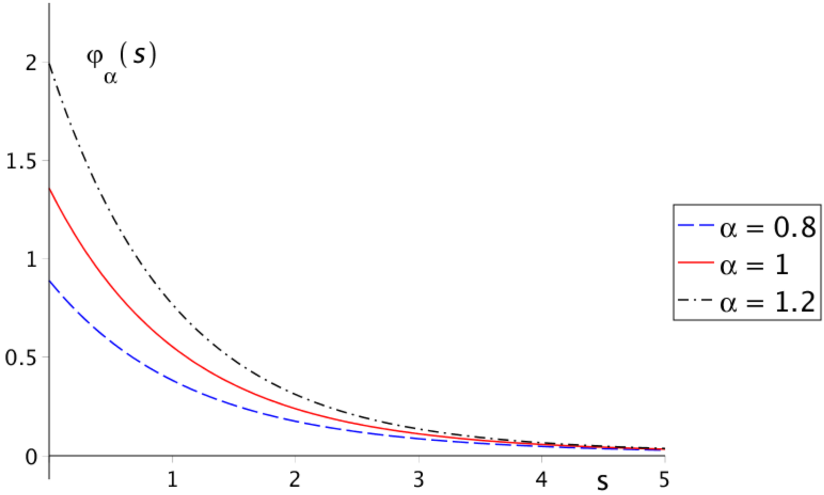
(ii) *For* $0 < \alpha < \alpha^*$ *we have* $\varphi_\alpha(s) > 0$ *for* $s \geq 0$.

(iii) $\varphi_{\alpha^*}(s) \geq 0$ *for* $s \geq 0$ *and it has a unique zero of multiplicity two at* $s^* \approx 5.27004\,87522\,76132\,37103.$

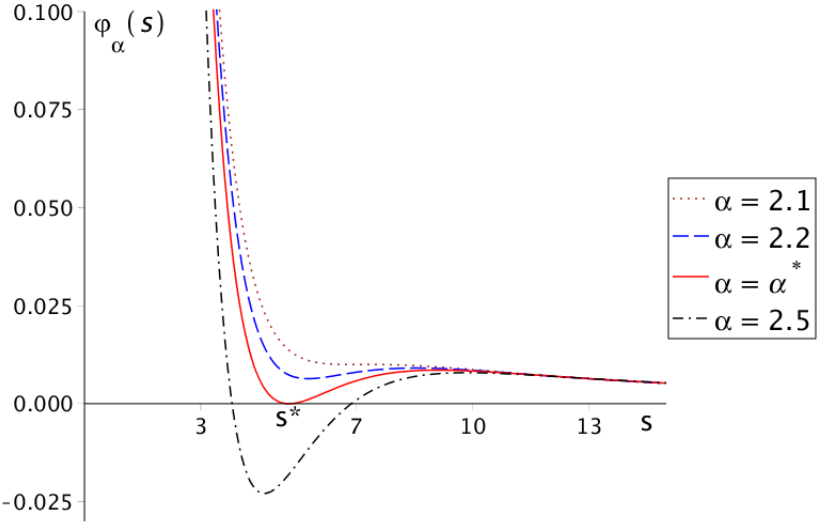
(iv) *For* $\alpha^* < \alpha$, φ_α *has a finite number of positive zeros* $0 < s_1(\alpha) < s_2(\alpha) < \ldots < s_n(\alpha)$ *which are all simple with the exception that the last can be double.*

(v) $s_1(\alpha)$ *is a simple zero with* $\varphi'_\alpha(s_1(\alpha)) < 0$, *moreover* $s_1(\alpha)$ *is a decreasing function on* $]\alpha^*, \infty[$.

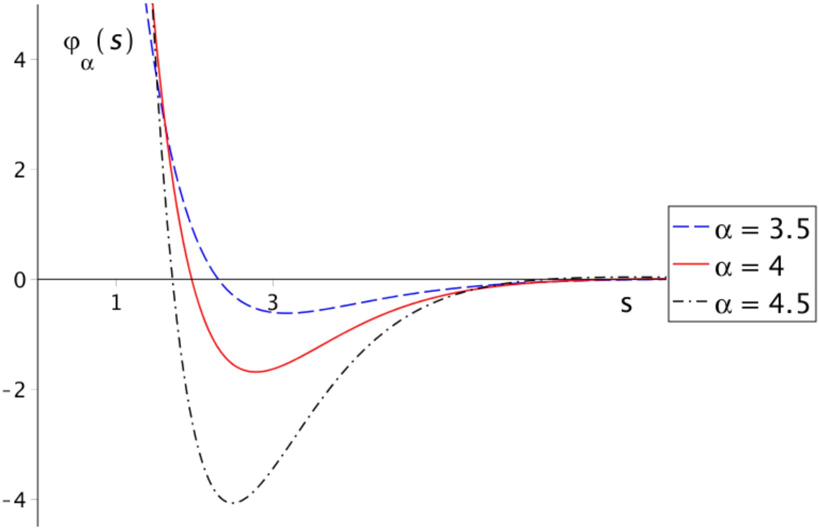
For some of these results we have no rigorous proofs.



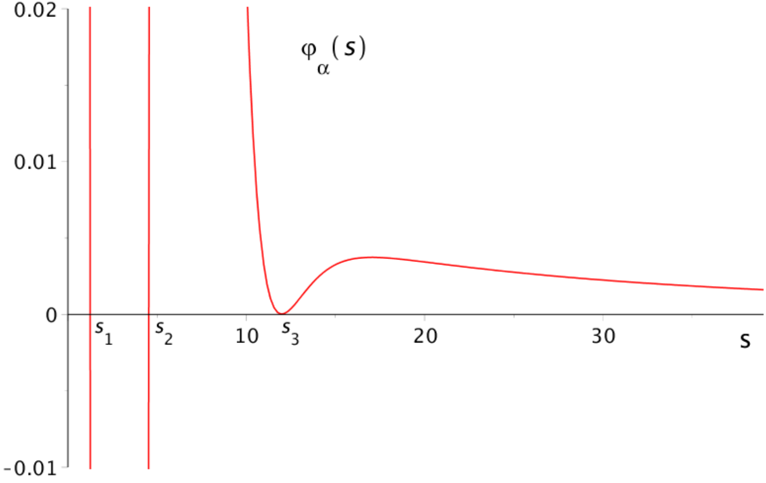
φ_α is > 0 for the shown values of α, completely monotonic when $0 < \alpha \leq 1$.



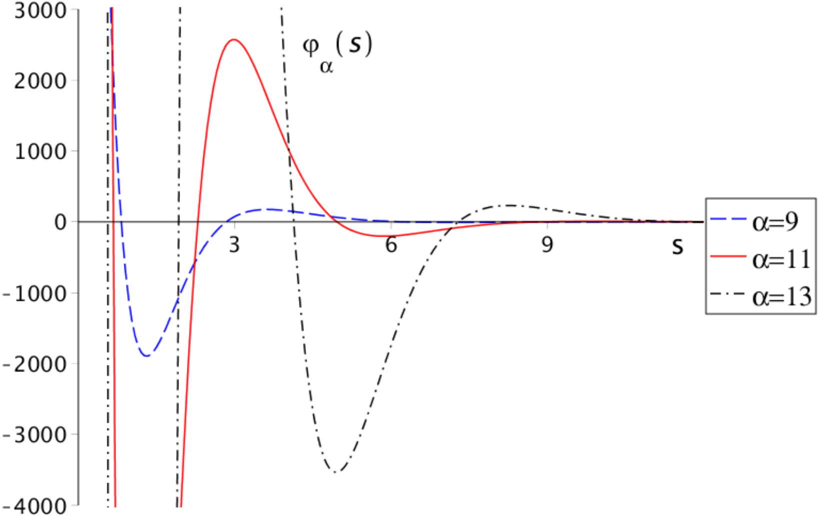
0.100
0.075
0.050
0.025
0.000
-0.025
φ α (s)
3
s*
7
10
13
s
α = 2.1
α = 2.2
α = α*
α = 2.5



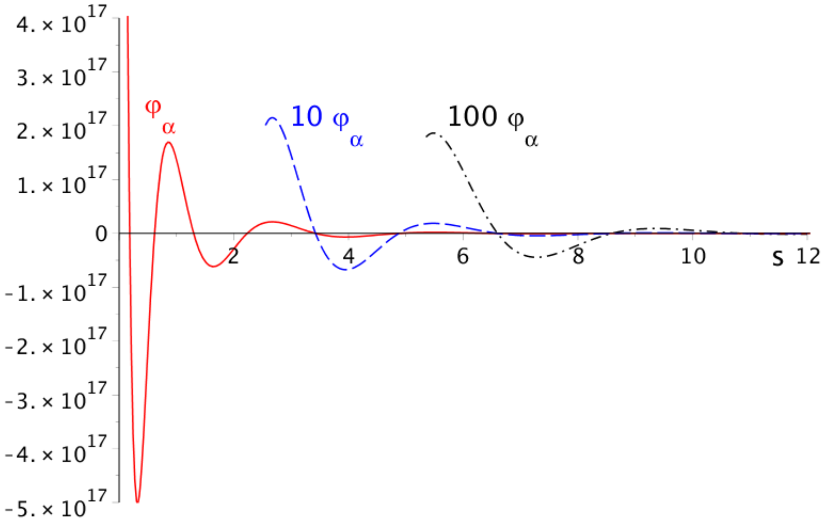
The first zero $s_1(\alpha)$ is decreasing for $\alpha > \alpha^*$.



For $\alpha \approx 5.988$ a new double zero appears on the right of s_1 and s_2.



For bigger α more oscillations appear.



For $\alpha = 40$ we see the oscillations in different scales.

Some references

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Thank you for your attention