ANZIAM J. 61(2019), 416–430
doi:10.1017/S1446181120000012

APPROXIMATION OF AND BY COMPLETELY MONOTONE FUNCTIONS

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(Received 14 October, 2019; accepted 9 January, 2020; first published online 6 March 2020)

Abstract

We investigate convergence in the cone of completely monotone functions. Particular attention is paid to the approximation of and by exponentials and stretched exponentials. The need for such an analysis is a consequence of the fact that although stretched exponentials can be approximated by sums of exponentials, exponentials cannot in general be approximated by sums of stretched exponentials.

2010 *Mathematics subject classification*: primary 41A30; secondary 41A10, 44A10, 76A10.

Keywords and phrases: complete and absolute monotonicity, stretched exponential, approximation, completely monotone and Kohlrausch functions, uniform and pointwise convergence.

1. Introduction

In the Boltzmann model of linear viscoelasticity [11], the stress σ and strain rate $\dot{\gamma}$ at points on the line are related via the convolution equation

$$\sigma(t) = \int_{-\infty}^{t} G(t-s)\dot{\gamma}(s)\,ds \quad (t > -\infty).$$

Here $G : [0, \infty) \to (0, \infty)$ is the relaxation modulus, a function characterizing the behaviour of the material under consideration. Fading memory and conservation of energy arguments lead to G being completely monotone (CM). Taking the case where $\gamma(s) = 0$ for $s < 0$ gives a convolution equation on the half-line, for which one of the standard approaches is the use of the Laplace transform [12, Ch. 2], which leads inexorably to consideration of the Laplace transform of G. Even though many CM functions, such as the Kohlrausch, have simple formulae, their Laplace transform may

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not be known in amenable form. It is therefore expedient to consider how they may be approximated by other CM functions whose transforms are easy to calculate. It is a common practice to use sums of negative exponentials in this role, with direct justification coming from the Maxwell spring and dashpot model [11, Ch. 1 Section D].

The popularity and importance of the Kohlrausch (Williams–Watts, stretched exponential) functions [2, 3] for parameters $\alpha > 0$ and $0 < \beta < 1$,

$$t \mapsto \exp(-\alpha t^{\beta}) \quad (t \geq 0),$$

relates not only to it being a two-parameter family of functions that yields excellent fits to decay data, not possible on occasions by even a large sum of negative exponentials when β is not near 1 [28], but also to it representing a practical example of the challenges that arise in the approximation of and by CM functions. In fact, for a wide range of applications, including polymer dynamics, bone and muscle rheology, and modelling of glassy states [8–10, 18, 23, 24], a Kohlrausch function is often the choice to fit and interpret the associated experimental decay data. On the other hand, there are of course some restrictions to their applicability (see the discussion in [7]).

In addition, as shown in Section 4, when considering the approximation of the exponential $\exp(-t)$ by Kohlrausch functions, it cannot be assumed that good approximations of a given CM function can be generated by a sum from some other family of CM functions.

In outline, Section 2 defines and gives some basic results about CM functions, and Section 3 discusses pointwise convergence of CM functions, in particular, which implies much stronger convergence results. Section 4 shows that convex combinations of Kohlrausch functions fail to approximate negative exponentials except in a trivial manner; Section 5 discusses approximation by polynomials in $(1 + x)^{-1}$. Section 6 gives a further brief discussion and concludes. Finally, Appendix A shows that pointwise convergence in suitable spaces of monotonic functions is in fact given by a metric, leading to simplifications of convergence arguments.

2. Background

We begin with the basic definition.

Definition 2.1. A function $f : (0, \infty) \to [0, \infty)$ is completely monotone if it is C^{∞} and satisfies

$$(-1)^n f^{(n)}(t) \geqslant 0 \quad (t > 0, n = 0, 1, \ldots). \tag{2.1}$$

In addition, following Widder [27, Chapter IV], we will say that a function $f : [0, \infty) \to [0, \infty)$ is CM if it is continuous at 0 and satisfies (2.1). We will also have occasions to refer to functions being absolutely monotone, where the $(-1)^n$ factor in (2.1) is omitted.

The class of CM functions on $(0, \infty)$ will be denoted by CM. This is the class $\mathcal{CM}$ of Schilling et al. [26]. When dealing with functions on $[0, \infty)$, the notation $CM(\mathbb{R}^+)$ will be used. As is implicit here, we will use the notation $\mathbb{R}^+$ for the closed half-line

$[0, \infty)$. It will be seen that the inclusion, or otherwise, of the origin plays an important role. For a general discussion of properties of CM we refer to Schilling et al. [26], although the focus of matters considered here is rather different to theirs [26].

The fundamental fact concerning the class CM is the following consequence of Bernstein [4] (see, for example, [27, Theorem IV.12b], [12, Theorem 5.2.5] or [26, Theorem 1.4]). The original is from Bernstein's work [4, page 56], where it is couched in terms of absolutely monotone functions.

THEOREM 2.2 (Bernstein [4]). *A function* $f : (0, \infty) \to \mathbb{R}^+$ *is* CM *if and only if there is a positive locally finite Borel measure* μ *on* $\mathbb{R}^+$ *such that*

$$f(t) = \int_0^\infty e^{-st}\, d\mu(s) \quad (t > 0). \tag{2.2}$$

The measure μ *is finite if and only if* f *extends continuously to a function in* $CM(\mathbb{R}^+)$.

Note that μ is necessarily unique, and is such that the integrals (2.2) are finite for each $t > 0$. We will refer to μ as the Bernstein measure for f.

REMARK 2.3. The measure μ in Theorem 2.2 need not be finite, but its local finiteness is automatic. For taking $M > 0$, for $t > 0$ we have

$$\int_0^M d\mu \le e^{tM} \int_0^M e^{-st}\, d\mu(s) \le e^{tM} \int_0^\infty e^{-st}\, d\mu(s) = e^{tM} f(t) < \infty.$$

The Bernstein measure of a simple CM function may be quite complicated: for the Kohlrausch function $\exp(-t^\beta)$ with $0 < \beta < 1$, (2.2) becomes [21]

$$\exp(-t^\beta) = \int_0^\infty \phi(\beta, t) \exp(-pt)\, dp \quad (0 < \beta < 1, t \ge 0),$$

where

$$\phi(\beta, t) = \frac{1}{\pi} \int_0^\infty \exp(-tu) \exp(-u^\beta \cos(\beta\pi)) \sin(u^\beta \sin(\beta\pi))\, du.$$

Further discussion on this is given in Section 4; from an application perspective, see [16, 28].

We will need the following elementary fact.

PROPOSITION 2.4. *Take* $0 < \beta \le 1$, *and* μ *a positive measure on* $\mathbb{R}^+$ *such that*

$$f(t) = \int_0^\infty \exp(-st^\beta)\, d\mu(s) < \infty \quad (t > 0). \tag{2.3}$$

Then for $t > 0$, *we may differentiate through the integral sign in (2.3) to get*

$$\frac{df}{dt}(t) = -\beta t^{\beta-1} \int_0^\infty s \exp(-st^\beta)\, d\mu(s) \quad (t > 0). \tag{2.4}$$

Further, in the case $\beta = 1$, *for* $n = 1, 2, \ldots,$

$$\frac{d^n f}{dt^n}(t) = \int_0^\infty (-s)^n e^{-st}\, d\mu(s) \quad (0 < t < \infty).$$

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3. Pointwise approximations by completely monotone functions

It is convenient to set up some notation. For a set S of nonnegative functions or measures on $[0,\infty)$, define

$$\mathrm{sp}^+(S) = \Big\{ \sum_{k=0}^{n} \alpha_k f_k, \alpha_k \ge 0, f_k \in S, n = 1, 2, \ldots \Big\}.$$

This is just the cone of nonnegative linear combinations of elements of S.

Since equation (2.2) can be viewed as a limiting sum of negative exponentials, it follows from Theorem 2.2 that $\{\exp(-\lambda s), \lambda \ge 0\}$ 'generates' $CM(\mathbb{R}^+)$. In fact, $CM(\mathbb{R}^+)$ is the uniform closure of $\mathrm{sp}^+\{\exp(-\lambda s), \lambda \ge 0\}$ [15, Theorem 4]. This result was essentially known much earlier – the analogous result for absolutely monotone functions is the work of Bernstein [4, Théorème E]. As noted by Schilling et al. [26, Remark 1.9], Theorem 2.2 can also be viewed as a Choquet representation of elements of the convex cone $CM(\mathbb{R}^+)$ in terms of extremal elements, reinforcing that the natural 'basic' elements are the negative exponentials, together with δ_0, the point mass at 0. Finally, we remark that Liu [15, Theorem 5] and Loy and Anderssen [17] together show that for $1 \le p < \infty$,

$$\overline{\mathrm{sp}^+\{\exp(-\lambda s), \lambda \ge 0\}}^{\|\cdot\|_p} = CM(\mathbb{R}^+) \cap L^p(\mathbb{R}^+).$$

We present another consequence of (2.2). A different proof was given by Schlling et al. [26, Corollary 1.6] and Berg and Frost [6, Proposition 9.5] of essentially the same result. The argument here is based on classical convergence results from complex analysis, using the fact that any $\phi \in CM$ extends to a function holomorphic on $\Re z > 0$ by setting

$$\widetilde{\phi}(z) = \int_0^\infty e^{-zs}\, d\mu(s) \quad (\Re z > 0),$$

where μ is the Bernstein measure for ϕ. Here $\Re$ denotes the real part. Further, for any $\eta > 0$,

$$|\widetilde{\phi}(z)| \le |\phi(\Re z)| \le |\phi(\eta)| \quad (\Re z \ge \eta), \tag{3.1}$$

since ϕ is decreasing on $(0,\infty)$.

Recall that a function f being in the pointwise closure of a set X of functions on $(0,\infty)$, or, equivalently, being the pointwise limit of functions from X, means that, given $\varepsilon > 0$ and finitely many points $x_1, \ldots, x_k$ in $(0,\infty)$, there is $g \in X$ such that $|g(x_j) - f(x_j)| < \varepsilon$, $j = 1, \ldots, k$ (see the formal discussion in Appendix A).

Theorem 3.1. *CM is closed under pointwise limits on* $(0,\infty)$.

Proof. Suppose that f is the pointwise limit of CM functions on $(0,\infty)$. Fix $1 > \eta > 0$. Then as in Theorem A.1, there is a sequence $(f_n) \subset CM$ with $f_n \to f$ locally uniformly on $(0,\infty)$. Furthermore, the sequence is bounded on $[\eta,\infty)$ by $f(\eta) + 1$, thanks to monotonicity.

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But then from (3.1), $(\widetilde{f_n})$ is a bounded sequence of functions analytic on $\Re z > \eta$ and pointwise convergent on the set $\{1 + 1/j \mid j \in \mathbb{N}\}$. The Vitali–Porter theorem [25, § 2.4] now applies to $(\widetilde{f_n})$ to give locally uniform convergence on $\Re z > \eta$ to an analytic function F. It follows that for each $k \in \mathbb{N}$, $\widetilde{f_n}^{(k)} \to F^{(k)}$ locally uniformly on (η, ∞). But $\widetilde{f_n} = f_n$ on $(0, \infty)$, so that $F = f$ on (η, ∞), and $f_n^{(k)} \to f^{(k)}$ locally uniformly on (η, ∞) for each $k \in \mathbb{N}$.

This can be done for $\eta = 2^{-1}, 3^{-1}, \ldots$, giving a doubly indexed sequence (f_n^k), such that for each k, $f_n^k \to f$ locally uniformly on (k^{-1}, ∞). Then the diagonal sequence (f_n^n) converges to f locally uniformly on $(0, \infty)$. The derivatives of (f_n^n) being locally uniformly convergent means that f is C^∞, and consequently CM. □

Corollary 3.2 [26, Corollary 1.7]. *Suppose that $(f_n) \subset CM$ converges pointwise to f. Then $f \in CM$, and $f_n^{(k)} \to f^{(k)}$ locally uniformly on $(0, \infty)$.*

Corollary 3.3. *Suppose that f lies in the pointwise closure of $CM(\mathbb{R}^+)$. Then $f \in CM$, and $f \in CM(\mathbb{R}^+)$ if and only if, in addition, f is continuous at 0.*

Proof. Theorem 3.1 gives $f \in CM$ and the result is immediate. □

Note that an immediate consequence of Corollary 3.3 is that the stress function derived from the Prandtl–Eyring model [9, equation (24)] for positive constants A, B, C and τ,

$$\varphi(t) = A \tanh^{-1}\left[\tanh(B)\exp\left(-\frac{t}{\tau}\right)\right] + C,$$

lies in $CM \setminus CM(\mathbb{R}^+)$. Just recall the power series expansion of $\tanh^{-1}$. Of course the same expansion gives the (discrete) Bernstein measure of φ directly.

Remark 3.4. In the topology of pointwise convergence on $(0, \infty)$, $CM(\mathbb{R}^+)$ is dense in CM. For given $f \in CM$ with Bernstein measure μ, set $\mu_n = \mu|_{[0,n]}$. Set f_n to be the Laplace transform of μ_n. Then $f_n \in CM(\mathbb{R}^+)$, and $f_n \to f$ pointwise on $(0, \infty)$.

By its very formulation, Theorem 3.1 gives no information about convergence or otherwise at 0. The role of behaviour at 0 has arisen in Corollary 3.3. Adding a condition at 0 also gives the following convergence result for $CM(\mathbb{R}^+)$.

Theorem 3.5. *Suppose that f lies in the pointwise closure of $CM(\mathbb{R}^+)$ and is continuous at 0. Then there is a sequence (f_n) in $CM(\mathbb{R}^+)$ which converges locally uniformly to f on $\mathbb{R}^+$.*

Proof. As in Remark A.2, we have a sequence (f_n) with $f_n \to f$ pointwise on $\mathbb{R}^+$, locally uniformly on $(0, \infty)$. Let the Bernstein measures for (f_n) and f be (μ_n) and μ, respectively.

Since $\|\mu_n\| = f_n(0) \to f(0) = \|\mu\|$, by going to a subsequence, and scaling as necessary, we may suppose without loss of generality that these are equal for all n.

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It suffices to show uniform convergence on $[0, 1]$. Take $\varepsilon > 0$. Choose $1 > \eta > 0$ such that for $0 \le t \le \eta$,

$$\|\mu\| \ge \int_0^\infty e^{-st}\, d\mu(s) \ge \|\mu\| - \varepsilon$$

and, using continuity of f at 0, a crucial condition,

$$f(t) \ge f(0) - \varepsilon.$$

Then for such t,

$$\begin{aligned} |f_n(t) - f(t)| &< \left|\int_0^\infty e^{-st}\, d\mu_n(s) - \|\mu_n\|\right| + \varepsilon \\ &= \int_0^\infty (1 - e^{-st})\, d\mu_n(s) + \varepsilon \\ &\le \int_0^\infty (1 - e^{-s\eta})\, d\mu_n(s) + \varepsilon \\ &= f(0) - f_n(\eta) + \varepsilon \\ &\le |f(0) - f_n(0)| + |f_n(0) - f_n(\eta)| + \varepsilon \\ &< 3\varepsilon \end{aligned} \tag{3.2}$$

for sufficiently large n. But we know that $f_n \to f$ uniformly on $[\eta, 1]$ from Theorem 3.1, so for sufficiently large n,

$$|f_n(t) - f(t)| \le \varepsilon \quad (\eta \le t \le 1). \tag{3.3}$$

Equations (3.2) and (3.3) together show uniform convergence on $[0, 1]$. □

REMARK 3.6. Clearly local uniform convergence on $\mathbb{R}^+$ necessitates continuity at 0. As noted in Remark A.2, this does not follow from the other hypothesis on f.

As noted in Remark A.3, convergence will generally not be uniform on $\mathbb{R}^+$. However, the condition for uniform convergence is easily given.

THEOREM 3.7. *Suppose that $f_n \to f$ pointwise in $CM(\mathbb{R}^+)$. Then the convergence is uniform on $\mathbb{R}^+$ if and only if* $\lim_n \lim_{t\to\infty} |f_n(t) - f(t)| = 0$.

PROOF. Let the Bernstein measures for (f_n) and f be (μ_n) and μ, respectively. Then $\lim_{t\to\infty} f_n(t) = \mu_n(\{0\})$, $\lim_{t\to\infty} f(t) = \mu(\{0\})$. Set $\mu_n' = \mu_n - \mu_n(\{0\})$, $\mu' = \mu - \mu(\{0\})$. Take $\varepsilon > 0$, and choose $M > 0$ such that

$$\int_0^\infty e^{-sM}\, d\mu'(s) < \varepsilon.$$

Since $f(M) = \int_0^\infty e^{-sM}\, d\mu'(s) + \mu(\{0\})$ and $f_n(M) = \int_0^\infty e^{-sM}\, d\mu_n'(s) + \mu_n(\{0\})$, we have for $t \ge M$,

$$\begin{aligned} |f_n(t) - f(t)| &\le \left|\int_0^\infty e^{-st}\, d\mu_n'(s) - \int_0^\infty e^{-st}\, d\mu'(s)\right| + |\mu_n(\{0\}) - \mu(\{0\})| \\ &\le \int_0^\infty e^{-sM}\, d\mu_n'(s) + \int_0^\infty e^{-sM}\, d\mu'(s) + |\mu_n(\{0\}) - \mu(\{0\})| \\ &\le 2\varepsilon + |\mu_n(\{0\}) - \mu(\{0\})| \end{aligned}$$

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provided n is sufficiently large, because of pointwise convergence at M. But we already have uniform convergence on $[0, M]$, and so on $\mathbb{R}^+$ provided $|\mu_n(\{0\}) - \mu(\{0\})| \to 0$.

Conversely, if convergence is uniform, take $\varepsilon > 0$ and then N such that $\|f_n - f\|_\infty < \varepsilon$ for $n > N$. Then, for such n,

$$|\mu_n(\{0\}) - \mu(\{0\})| = \lim_{t\to\infty} |f_n(t) - f(t)| \le \varepsilon.$$

Thus $|\mu_n(\{0\}) - \mu(\{0\})| \to 0$. □

For $f_n(t) = \exp(-t/n)$, we have $\mu_n = \delta_{1/n}$ and $\mu = \delta_0$, so that $\mu_n(\{0\}) - \mu(\{0\}) = -1$ for each n.

Finally, we have a weak* version of part of [6, Proposition 9.5].

Theorem 3.8. *Suppose that $f_n \to f$ pointwise in $CM(\mathbb{R}^+)$. Take the (finite) Bernstein measures μ_n for f_n, and μ for f. Then $\mu_n \overset{\text{weak}^*}{\to} \mu$. However, in general, $\|\mu_n - \mu\| \not\to 0$.*

Proof. Since $f_n(0) = \|\mu_n\| \to f(0) = \|\mu\| < \infty$, $(f_n(0))$ is bounded, and so (μ_n) is bounded, and so has a weak* limit point σ. By Theorem A.4, take a subsequence (n_k) such that $\mu_{n_k} \overset{\text{weak}^*}{\to} \sigma$.

Fixing $s \ge 0$, we have

$$\int_0^\infty e^{-st}\, d\mu(t) = f(s) = \lim_k f_{n_k}(s) = \lim_k \int_0^\infty e^{-st}\, d\mu_{n_k}(t) = \int_0^\infty e^{-st}\, d\sigma(t).$$

It follows that

$$\int_0^\infty e^{-st}\, d\mu(t) = \int_0^\infty e^{-st}\, d\sigma(t),$$

and this holding for each $s \ge 0$ shows that $\mu = \sigma$. Thus (μ_n) has a weak* unique limit point, namely μ.

For example, demonstrating the final statement, let μ be the Lebesgue measure on $[0, 1]$, and set

$$\mu_n = 2^{-n} \sum_{i=0}^{2^n-1} \delta_{2^{-n}i}.$$

Then $\mu_n \overset{\text{weak}^*}{\to} \mu$, since for any $f \in C_0(\mathbb{R}^+)$, $\int f(s)\, d\mu_n(s)$ is just a Riemann sum for $\int_0^1 f(s)\, d\mu(s)$, and $\mu_n \not\to \mu$ in norm. □

4. Approximations by Kohlrausch functions

The popularity of the parametric Kohlrausch (stretched exponential) functions is based on the ansatz that, in terms of the two parameters, they will always yield a good approximation to any smooth relaxation curve. The justification is based on graphical comparisons [20]. However, what is required is a mathematical examination of the validity of the ansatz. Since the Kohlrausch function is both a CM function and a

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relaxation function, and the latter are often assumed to be CM [1], an examination of the validity of the ansatz can be viewed as a special case of the approximation of and by CM functions. To test the validity of the ansatz in this context, we here assume that the relaxation function is $\exp(-t)$, and examine the question of approximating it by a sum of Kohlrausch functions.

The Bernstein measures of the Kohlrausch functions $\exp(-\alpha t^\beta)$ are β-stable densities. They are unimodal, and for $0 < \beta < 1$ they have "heavy tails" and decay like $x^{-\beta-1}$ for large x. In particular, they have infinite means (see [13, § 4.3.2] for details). On the other hand, $\varphi(t) = \exp(-t)$ has Bernstein measure the point mass δ_1. Suppose that φ could be approximated pointwise by positive linear combinations $\{\varphi_n\}$ of Kohlrausch functions with index $\beta < 1$, with corresponding Bernstein measures $\{\mu_n\}$. Then, by Theorem 3.8,

$$\mu_n \overset{\text{weak}^*}{\to} \delta_1, \quad \text{that is,} \int_0^\infty \psi(t)\, d\mu_n \to \psi(1)$$

for each $\psi \in C_0[0, \infty)$. In particular, for each $0 < h < 1 < R$,

$$\mu_n([0, 1-h] \cup [1+h, R]) \to 0 \quad \text{and} \quad \mu_n([1-h, 1+h]) \to 1. \tag{4.1}$$

This would seem to be very unlikely because of the "heavy tails".

Indeed, taking $\beta = 1/2$ (the only value in $(0, 1)$ where the Bernstein measure is known in terms of elementary functions), we have [13, § 4.3.2],

$$\exp(-\alpha t^{1/2}) = \int_0^\infty \exp\Big(-\frac{\alpha^2}{4p}\Big)\Big(\frac{\alpha^2}{4\pi p^3}\Big)^{1/2} \exp(-pt)\, dp \quad (\alpha > 0, t \geq 0). \tag{4.2}$$

The densities in (4.2) peak at $p = \alpha^2/6$, with the maximum value $A\alpha^{-2}$, where $A = 3\exp(-3/2)\sqrt{6/\pi} < 0.9251$. So the total mass from 0 to the maxima is bounded by $A/6 < 0.1542$. It follows that if $\varphi_n(t) = \sum_{k=1}^{k_n} a_{k_n} \exp(-\alpha_{k_n} t^{1/2})$, values of k_n with $\alpha_{k_n} \neq \sqrt{6}$ will not contribute to the "peaking" at 1 required by (4.1). Clustering of α_{k_n} near 1 will result in a broad peak there, again inconsistent with (4.1).

In fact, we give a more direct and precise argument as follows. For $0 < \beta < 1$, suppose that μ is a positive measure on $\mathbb{R}^+$, and that for all $t > 0$,

$$\exp(-t) = \int_0^\infty \exp(-st^\beta)\, d\mu(s). \tag{4.3}$$

Taking the derivative, (2.4) gives

$$\exp(-t) = \beta t^{\beta-1} \int_0^\infty s \exp(-st^\beta)\, d\mu(s) \quad (t > 0).$$

As $t \downarrow 0$, we have the left-hand side converging to 1 and $t^{\beta-1} \uparrow \infty$, but

$$\int_0^\infty s\exp(-st^\beta)\, d\mu(s) \to \int_0^\infty s\exp(-s)\, d\mu(s) > 0,$$

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which is a contradiction. (Note that the right-hand-side integral here may be ∞.) Thus (4.3) fails to hold.

Indeed, since $\mathrm{sp}^+\{\delta_x \mid x \geq 0\}$ is weak* dense in the positive finite measures on $\mathbb{R}^+$, it would follow from (4.3) that, with $\overline{(\cdots)}^{pw}$ denoting closure in the topology of pointwise convergence on $\mathbb{R}^+$,

$$\exp(-t) \in \overline{\mathrm{sp}^+\{\exp(-\alpha t^\beta) \mid \alpha \geq 0\}}^{pw}. \tag{4.4}$$

Taking (4.4) itself as an assumption, and putting $s = t^\beta$ and $\gamma = \beta^{-1} > 1$,

$$g(s) = \exp(-s^\gamma) \in \overline{\mathrm{sp}^+\{\exp(-\alpha s) \mid \alpha \geq 0\}}^{pw}.$$

So by Theorem 3.1, the function g is CM. But

$$g''(s) = \{-\gamma(\gamma - 1) + \gamma^2 s^\gamma\} s^{\gamma-2} \exp(-s^\gamma),$$

which is negative for $s > 0$ sufficiently small, a contradiction.

So positive linear combinations of Kohlrausch functions with a fixed β, $0 < \beta < 1$, cannot be used to approximate negative exponentials. Clearly, if varying β is allowed, then approximation is possible, since $\exp(-t) = \lim_{\beta \to 1-} \exp(-t^\beta)$ uniformly on $\mathbb{R}^+$.

The same argument shows that

$$\exp(-t^\gamma) \notin \overline{\mathrm{sp}^+\{\exp(-\alpha t^\beta) \mid \alpha \geq 0\}}^{pw}$$

for any (fixed) $\beta < \gamma$.

However, what about the possibility that for some $0 \leq \eta < 1$,

$$\exp(-t) \in \overline{\mathrm{sp}^+\{\exp(-\alpha t^\beta) \mid \alpha \geq 0, 0 \leq \beta \leq \eta < 1\}}^{pw}?$$

Suppose that for $t \geq 0$,

$$\exp(-t) = \lim_n \sum_i a_i^{(n)} \exp(-\alpha_i^{(n)} t^{\beta_i^{(n)}}),$$

where $\alpha_i^{(n)}, a_i^{(n)} \geq 0, 0 \leq \beta_i^{(n)} \leq \eta < 1$, each sum being finite. Theorem 3.7 shows that convergence is uniform on $\mathbb{R}^+$. Evaluation at $t = 0$ shows that $\lim_n \sum_i a_i^{(n)} = 1$, so without loss of generality we may suppose that $\sum_i a_i^{(n)} = 1$ for each n.

Theorem 3.1 shows that for $t > 0$ we can differentiate to get

$$\exp(-t) = \lim_n \sum_i \alpha_i^{(n)} \beta_i^{(n)} a_i^{(n)} \exp(-\alpha_i^{(n)} t^{\beta_i^{(n)}}) t^{\beta_i^{(n)}-1}. \tag{4.5}$$

Now for $t \geq 0$, $t\exp(-t) \leq e^{-1}$, and by assumption, $0 \leq \beta_i^{(n)} \leq \eta < 1$. Putting $t = 1$ in (4.5), we thus have

$$\frac{1}{e} = \lim_n \sum_i \alpha_i^{(n)} \beta_i^{(n)} a_i^{(n)} \exp(-\alpha_i^{(n)}) \leq \frac{\eta}{e} \sum_i a_i^{(n)} < \frac{1}{e},$$

a contradiction.

Thus $\exp(-t)$ cannot be approximated pointwise by positive linear combinations of Kohlrausch functions with exponent β bounded away from 1.

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5. Approximation by polynomials

By Corollary 3.3,

$$\overline{\mathrm{sp}^+\{(1+x)^{-n} \mid n=0,1,\ldots\}}^{pw} \subset CM(\mathbb{R}^+).$$

Suppose that $f_1 : [0,1] \to (0,\infty)$ is absolutely monotone. Then f_1 is the uniform limit of a sequence (P_n) of polynomials with nonnegative coefficients [27, Theorem 9b]. Set $f_2 : x \mapsto (1+x)^{-1} : [0,\infty) \to (0,1]$. Then $f_2 \in CM(\mathbb{R}^+)$, whence $f_1 \circ f_2 \in CM(\mathbb{R}^+)$ [27, Theorem 2b]. (Widder [27] gives no explicit argument, but the result is immediate from the formula of Faà di Bruno [14].) It follows that $P_n((1+x)^{-1})$ is a sequence of $CM(\mathbb{R}^+)$ functions converging to $f_1 \circ f_2$, which thus lies in $CM(\mathbb{R}^+)$.

Conversely, if $f \in CM(\mathbb{R}^+)$ were approximable by a sequence (P_n) of polynomials in $(1+x)^{-1}$ with nonnegative coefficients, then, since the inverse of $x \mapsto (1+x)^{-1}$ is $t \mapsto t^{-1} - 1$, we would have $f(t^{-1}-1)$ so approximable by $P_n(t)$ on $(0,1]$. That is, $f(t^{-1}-1)$ would be absolutely monotone on $(0,1]$. This is false for $f(x) = \exp(-x)$, since then $f(t^{-1}-1) = e \cdot \exp(-t^{-1})$, and for $0.5 < t \le 1$,

$$\frac{d^2}{dt^2}(\exp(-t^{-1})) = \exp(-t^{-1})t^{-4}(1-2t) < 0.$$

Looking at Kohlrausch functions for $0 < t < 1$,

$$\frac{d^2}{dt^2}(\exp(-(t^{-1}-1)^{\beta})) = \frac{\beta\exp(-(t^{-1}-1)^{\beta})(t^{-1}-1)^{\beta}[\beta\{(t^{-1}-1)^{\beta}-1\}+2t-1]}{(t-1)^2t^2}.$$

The final factor in the numerator on the right-hand side vanishes at $t = 1/2$. It follows that $\exp(-(t^{-1}-1)^{\beta})^{(2)}$ is not absolutely monotone [27, Corollary IV.3a], and hence neither is $\exp(-(t^{-1}-1)^{\beta})$. But then $\exp(-t^{\beta})$ is not approximable by the polynomials in $(1+x)^{-1}$ with nonnegative coefficients.

We can also show this, and much more, using Bernstein measures. Recall that $(1+x)^{-n}$ has Bernstein measure $\exp(-t)t^{n-1}/(n-1)!$, so for any polynomial $p(x) = \sum_{k=1}^{n} a_k x^k$ with nonnegative coefficients, $p((1+x)^{-1})$ has Bernstein measure

$$\exp(-t)\Big(\sum_{k=1}^{n} a_k \frac{t^{k-1}}{(k-1)!}\Big).$$

Suppose that $p_n((1+x)^{-1}) \overset{pw}{\to} f(x)$, where f has Bernstein measure μ of compact support S. Set $p_n(x) = \sum_{k=1}^{k_n} a_k^{(n)} x^k$ with $a_k^{(n)} \ge 0$. Then by Theorem 3.8 we would have

$$\exp(-t)\Big(\sum_{k=1}^{k_n} a_k^{(n)} \frac{t^{k-1}}{(k-1)!}\Big) \overset{\text{weak}^*}{\to} \mu. \tag{5.1}$$

Take $s > \sup S$ and $\varphi \in C_0(\mathbb{R}^+)$ which is 0 on the support of μ, and $\varphi(t) = 1$ on a neighbourhood of s. Then

$$\int_0^s \exp(-t)\Big(\sum_{k=1}^{k_n} a_k^{(n)} \frac{t^{k-1}}{(k-1)!}\Big)\varphi(t)\,dt \to 0.$$

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The integrand being nonnegative, this gives, for some $r < s$ with $[0, r] \supset S$,

$$\int_r^s \exp(-t)\Big(\sum_{k=1}^{k_n} a_k^{(n)} \frac{t^{k-1}}{(k-1)!}\Big)\,dt \to 0. \tag{5.2}$$

But on $[r, s]$,

$$\exp(-t)\Big(\sum_{k=1}^{k_n} a_k^{(n)} \frac{t^{k-1}}{(k-1)!}\Big) > \exp(-s)\Big(\sum_{k=1}^{k_n} a_k^{(n)} \frac{r^{k-1}}{(k-1)!}\Big),$$

whence, from (5.2),

$$\sum_{k=1}^{k_n} a_k^{(n)} \frac{r^{k-1}}{(k-1)!} \to 0.$$

This means that

$$\sum_{k=1}^{k_n} a_k^{(n)} \frac{t^{k-1}}{(k-1)!} \to 0$$

uniformly on $[0, r] \supset S$. But then by (5.1), $\mu = 0$. Thus a nonzero $CM(\mathbb{R}^+)$ function f which is pointwise approximable by nonnegative polynomials in $(1 + x)^{-1}$ has Bernstein measure of noncompact support; *a fortiori*, f is not a finite nonnegative linear combination of negative exponentials.

In fact, this works provided the support S does not contain a neighbourhood of ∞. For suppose that $s_n \to \infty$, and for all n, $s_n \notin S$. Apply the argument above to some s_{n_0} to see that $\mu[0, s_{n_0}] = 0$. Hence $\mu = 0$, as before.

6. Discussion and conclusion

The two most widely used families of functions in $CM(\mathbb{R}^+)$ are the negative exponentials $\exp(-\alpha t)$ and the Kohlrausch functions $\exp(-\alpha t^\beta)$ for $0 < \beta < 1$, $\alpha > 0$. It is well known that positive linear combinations of the former can be used to approximate the latter (or, indeed, any function in $CM(\mathbb{R}^+)$) in a variety of ways – pointwise, locally uniformly and in $\|\cdot\|_p$ for $1 \le p < \infty$. This is another reason, in a sense complementary to that mentioned in Section 1, for the use of finite positive linear combinations of negative exponentials to be commonly used when modelling relaxation processes. In this paper, we have considered various notions of convergence in $CM(\mathbb{R}^+)$, showing in particular that pointwise convergence necessitates both local uniform convergence of the functions and weak* convergence of the associated Bernstein measures. These results have then been used to show that Kohlrausch functions with indices constrained away from 1 cannot be used to approximate negative exponentials, and neither can polynomials in $(1 + x)^{-1}$ with nonnegative coefficients. An indirect consequence is that care must be taken when using Kohlrausch functions to model relaxation phenomena; an accurate value of the index is very important.

Appendix A

Many of our results concern the topology of pointwise convergence on spaces X of real-valued functions on $(0, \infty)$ or $\mathbb{R}^+$. Here, we explain this topology and show that it simplifies in the situation we are considering.

We denote this topology by *pw*; it is given by the (uncountably many) seminorms

$$p_F(f) = \max\{|f(x_i)| \mid x_i \in F\} \quad (f \in X),$$

where F runs over all finite subsets $\{x_1, x_2, \ldots, x_k\}$ of $(0, \infty)$ or $\mathbb{R}^+$. This topology is not given by a metric, and to speak of convergence one needs to use nets, rather than just sequences. Here, we have arranged matters so as to avoid explicit use of this terminology. We have also made no use of the vague topology, in distinction to [5, 26]. It turns out, however, that in many of the circumstances under consideration in this paper, sequences do in fact suffice to describe convergence. One might possibly expect this to be due to Theorem A.4. However, the following elementary result gets closer to the reason – the functions of interest are monotonic, decreasing and continuous.

This result was given by Berg and Forst [6, 9.7] as "easily seen". In view of the subtleties involved and its importance in reducing to sequential arguments, we think it is appropriate to give a proof. The following argument was prompted in part by Pólya and Szegö [22, Part 2, Problem 127].

Theorem A.1. *Let X be the set of monotonic and decreasing convex functions on $(0, \infty)$. The topology pw on X is the same as the topology ρ of local uniform convergence, which makes X into a complete metric space.*

Proof. First note that being monotonic, decreasing and convex is a property determined by triplets of points in X, so that X is a closed subset of the set of all real-valued functions on $(0, \infty)$ under the topology *pw*. Furthermore, convexity ensures that the functions in X are continuous.

Suppose then that f lies in the pointwise closure of $S \subset X$. Fix $[a, b] \subset (0, \infty)$ and $\varepsilon > 0$. For $n \in \mathbb{N}$ so large that $f(a) - f(b) < n\varepsilon$, partition $[f(b), f(a)]$ into n equal intervals $f(a) = y_0 > y_1 > \cdots > y_n = f(b)$. Take points $a = x_0 < \cdots < x_n = b$ such that $f(x_i) = y_i$, $i = 0, 1, \ldots, n$. This is possible, since f is continuous and so has connected range.

Since f lies in the pointwise closure of S, there is $g \in S$ such that $|g(x_i) - f(x_i)| < \varepsilon$ for $i = 0, 1, \ldots n$.

Given $x \in [a, b]$, take j such that $f(x) \in [y_{j+1}, y_j]$, so that $x \in [x_j, x_{j+1}]$. Then

$$f(x_j) + \varepsilon > g(x_j) \geq g(x) \geq g(x_{j+1}) > f(x_{j+1}) - \varepsilon,$$

so that for any $x \in [a, b]$,

$$\begin{aligned} |g(x) - f(x)| &\leq |g(x) - g(x_j)| + |g(x_j) - f(x_j)| + |f(x_j) - f(x)| \\ &< 5\varepsilon. \end{aligned}$$

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It follows that for each $n \in \mathbb{N}$, we can find $g_n \in S$ such that

$$\max\{|g_n(x) - f(x)| \mid 2^{-n} \le x \le 2^n\} < n^{-1}.$$

In particular, $g_n \to f$ locally uniformly on $(0, \infty)$.

Define semi-metrics ρ_n on X by

$$\rho_n(f, g) = \max\{|g(x) - f(x)| \mid 2^{-n} \le x \le 2^n\} \quad (f, g \in X, n \in \mathbb{N}),$$

and then a metric by

$$\rho(f, g) = \sum_{n=1}^{\infty} 2^{-n} \frac{\rho_n(f, g)}{1 + \rho_n(f, g)}.$$

Then convergence under ρ is exactly local uniform convergence.

The above shows that if $f \in \overline{S}^{pw}$ then $f \in \overline{S}^{\rho}$. The converse is obvious, and so the topology pw and the metric topology given by ρ are the same on X. Completeness is immediate from the first line of the proof. □

Remark A.2. Taking $\mathbb{R}^+$ in place of $(0, \infty)$, the same argument, amended to require that the $g \in S$ also satisfies $|g(0) - f(0)| < \varepsilon$, shows that there is $(g_n) \subset S$ such that $g_n \to f$ pointwise on $\mathbb{R}^+$, and locally uniformly on $(0, \infty)$. Local uniform convergence on $\mathbb{R}^+$ will not hold in general. Take $f_n(t) = \exp(-nt)$, $n \ge 1, t \ge 0$. Then $f_n(t) \to 0$, $t > 0$, but $f_n(0) = 1$ for all n. Thus, convergence cannot be uniform on any interval $[0, \delta]$ $\delta > 0$.

Remark A.3. Given a sequence (f_n) in X with $f_n \to f$ on $\mathbb{R}^+$, it does *not* follow that the convergence is uniform. Take $f_n(t) = \exp(-t/n)$. Clearly $f_n \to 1$ on $\mathbb{R}^+$, but certainly not uniformly (see Theorem 3.7).

Recall that the Riesz representation theorem identifies the space of finite Borel measures $M(\mathbb{R}^+)$, under the total variation norm, as the dual space of $C_0(\mathbb{R}^+)$, the space of continuous functions vanishing at ∞, under the supremum norm. The proof of Theorem 3.8 uses the following standard metrizability result (see [19, Theorem 2.6.23] for a proof).

Theorem A.4. *The weak* topology in $M(\mathbb{R}^+)$ is metrizable on bounded sets.*

The weak* topology on $M(\mathbb{R}^+)$ itself is not metrizable [19, Proposition 2.6.12].

Acknowledgements

The authors wish to thank the reviewers for their helpful suggestions.

https://doi.org/10.1017/S1446181120000012 Published online by Cambridge University Press

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