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LETTER TO THE EDITOR

On the completeness of certain sets of functions in $L^2(0, \infty)$

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Abstract. The set of $L^2(0, \infty)$ functions $\{\exp(-\frac{1}{2}\xi r^\beta) r^{\gamma(n+\alpha)}; n = 0, 1, \ldots\}$, which is known to be complete for $\beta = 1$, $\gamma = 2$, is shown to be incomplete for all $0 < 2\beta < \gamma$ and complete for all $0 < \gamma \leq 2\beta$.

The properties of infinite sets of linearly independent square integrable functions are of enormous importance in the context of obtaining approximations to functions such as the bound state wavefunctions in quantum mechanics. That an arbitrary set of functions of this type does not necessarily form a complete set is well known. On the other hand, necessary and sufficient conditions for completeness which can be applied to arbitrary situations do not exist. A completeness discussion of the existing body of knowledge in this area, with a special emphasis on quantum mechanical applications, is presented in a series of articles by Klahn and Bingel (1977a, b, c) and Klahn (1981). Two sets of functions for which concrete results are available are the set of powers $\{x^{\lambda_i}; i = 1, 2, \ldots\}$, which form a complete set in $0 \leq x < 1$ if and only if λ_i is a monotonically increasing set, $\lambda_1 > -\frac{1}{2}$ and $\Sigma_i \lambda_i^{-1} = \infty$ (Müntz's theorem, cf Kaczmarz and Steinhaus (1935)) and the non-harmonic Fourier series, consisting of $\{\exp(i\lambda_n t); n = 0, 1, 2, \ldots\}$ which form complete sets on $-\pi < t < \pi$ if and only if $|\lambda_n - n| < \frac{1}{4}$ for all n (Kadec's $\frac{1}{4}$ theorem (Young 1980)). For the set of integers, $\lambda_n = n$, the completeness of $\{x^n; n = 0, 1, \ldots\}$ is the Weierstrass approximation theorem and the completeness of $\{\exp(int); n = 0, 1, \ldots\}$ is the Fourier expansion theorem. Thus the Müntz and Kadec theorems are statements about the stability of the Weierstrass and Fourier sets with respect to 'sufficiently small' perturbations of the integers. Stability is used in the present context to indicate the property that sets sufficiently close to a given complete set are complete as well (Young 1980, p 37).

We note in passing that not all sets of powers which are complete under Müntz's theorem are equally efficient from the point of view of their rate of convergence. This is treated by the Jackson theorem, which, in the extended form discussed by Newman (1973), states that if $\lambda_{i+1} - \lambda_i \leq 2$ for (almost) all i, the rate of convergence of the power series approximation to a function defined in $[0, 1]$ is $1/n$, becoming slower when the powers are more thinly spread.

Our purpose in the present letter is to discuss the completeness of certain commonly employed sets of square integrable functions in $L^2(0, \infty)$. Although most of the results are available in the mathematical literature, their relevance to computational quantum mechanics has been largely ignored.

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Stieltjes, in a memoir discussed by Borel (1928), investigated the extent to which an essentially positive function $f(u)$ $(0 \leq u < \infty)$ is determined by its moments

$$C_n = \int_0^\infty f(u) u^n \, du \qquad n = 0, 1, 2, \ldots.$$

He pointed out that there exist functions $\varphi(u)$ for which

$$\int_0^\infty \varphi(u) u^n \, du = 0 \qquad n = 0, 1, 2, \ldots$$

which means that $f(u)$ and $f(u) + \varphi(u)$ have the same set of moments. One such function, given by Stieltjes, is

$$\varphi(u) = \exp(-u^\alpha) \sin(u^\alpha) \qquad \text{with } \alpha = \tfrac{1}{4}.$$

Hamburger (cf Freud 1971) pointed out that the above result holds for any $0 < \alpha < \frac{1}{2}$.

Let us consider the set $\{\varphi_n = \exp(-\frac{1}{2}\xi r^\beta) r^{\gamma(n+\alpha)}; \, n = 0, 1, 2, \ldots\}$. Certain special cases, such as $\beta = 1$, $\gamma = 1$, $\alpha > -1$ (Szegö 1939) and $\beta = 1$, $\gamma = 2$, $\alpha \geq 0$ (Klahn and Bingel 1977b) are well known to be complete in $L^2(0, \infty)$. Let us also consider the set $\{\Psi_p = \exp(-\frac{1}{2}\xi r^\beta) r^{\gamma p} \sin(\xi k r^\beta)/r; \, k > 0\}$. Note that both φ_n and Ψ_p are square integrable.

Now

$$I_{np} = \int_0^\infty \varphi_n \Psi_p \, dr = -\mathrm{Im} \int_0^\infty \exp[-\xi r^\beta (1 + ik)] r^{\gamma(n+p+\alpha)-1} \, dr. \qquad (1)$$

Defining $x = \xi r^\beta$ we obtain

$$\begin{aligned} I_{np} &= -\frac{1}{\beta} \xi^{-(\gamma/\beta)(n+p+\alpha)} \, \mathrm{Im} \int_0^\infty \exp[-x(1+ik)] x^{(\gamma/\beta)(n+p+\alpha)-1} \, dx \\ &= -\frac{1}{\beta} \xi^{-(\gamma/\beta)(n+p+\alpha)} \, \mathrm{Im} \frac{\Gamma((\gamma/\beta)(n+p+\alpha))}{(1+ik)^{(\gamma/\beta)(n+p+\alpha)}} \end{aligned} \qquad (2)$$

(see also equation 5, in § 3.944 of Gradshteyn and Ryzhik (1980)). Clearly, if $(1+ik)^{\gamma/\beta}$ is real, then $I_{np} = 0$ for all values of n and p. In that case each member of $\{\varphi_n\}$ is orthogonal to each member of $\{\psi_p\}$, which means that neither set is complete in $L^2(0, \infty)$.

Now, $1 + ik = (1 + k^2)^{1/2} e^{i\phi}$ where $\phi = \tan^{-1}(k)$. Since $0 < k < \infty$, $0 < \phi < \pi/2$. Therefore, I_{np} will vanish if $\exp(i\phi\gamma/\beta)$ is real, i.e. $\phi\gamma/\beta = \pi m$ where m is a positive integer.

For $m = 1$ it follows that a value of ϕ in the range $0 < \phi < \pi/2$ exists provided that $0 < \beta/\gamma < \frac{1}{2}$ which means that for $0 < 2\beta < \gamma$ the set $\{\varphi_n\}$ is incomplete. Higher values of m give no additional information.

To determine the properties of $\{\varphi_n\}$ for $0 < \gamma \leq 2\beta$ we note that $\{\exp(-\frac{1}{2}\xi r) r^{2(n+\alpha)}; \, n = 0, 1, 2 \ldots\}$ is known to be complete (Klahn and Bingel 1977b). This set corresponds to $\beta = 1$ and $\gamma = 2$. Note that, by the transformation used in the evaluation of the integral, equation (2), it follows that all sets of the form $\{\exp(-\frac{1}{2}\xi r^{1/2}) r^{n+\alpha}; \, n = 0, 1, 2 \ldots\}$ are complete.

Consider a set of the form $\{\exp(-\frac{1}{2}\xi r^{\beta_0}) r^{n+\alpha}; \, n = 0, 1, \ldots\}$. For $\beta_0 < \frac{1}{2}$ this set was shown to be incomplete, whereas for $\beta_0 = \frac{1}{2}$ it is complete. Assume that for some $\beta_0 > \frac{1}{2}$

the set is incomplete. This means that a square integrable function, $g(r)$, exists, such that

$$\int_0^\infty g(r)\exp(-\tfrac{1}{2}\xi r^{\beta_0})r^{n+\alpha}\,\mathrm{d}r=0 \tag{3}$$

for all n.

Let $\tilde{g}(r)=g(r)\exp[\tfrac{1}{2}\xi(r^{1/2}-r^{\beta_0})]$, $(\beta_0>\tfrac{1}{2})$. Since for $r\to\infty$ $(r^{1/2}-r^{\beta_0})\to-\infty$, $\tilde{g}(r)$ is square integrable if $g(r)$ is also. Furthermore, from equation (3) it follows that

$$\int_0^\infty \tilde{g}(r)\exp(-\tfrac{1}{2}\xi r^{1/2})r^{n+\alpha}\,\mathrm{d}r=0$$

for all n. This is in contradiction to the fact that $\{\exp(-\tfrac{1}{2}\xi r^{1/2})r^{n+\alpha}\}$ is complete. Thus, $\{\exp(-\tfrac{1}{2}\xi r^{\beta})r^{n+\alpha};\ n=0,1\ldots\}$ is complete for all $\beta\geqslant\tfrac{1}{2}$. By the transformation mentioned above it follows that $\{\exp(-\tfrac{1}{2}\xi r^{\beta})r^{\gamma(n+\alpha)}\}$ is complete whenever $2\beta\geqslant\gamma>0$.

Consider the set $\{\omega^{1/2}(r)r^i;\ i=0,1\ldots\}$ and assume that a function $g(r)$ exists, for which $\int_0^\infty\omega^{1/2}(r)r^i g(t)\,\mathrm{d}r=0$ for all i. Any $\tilde{g}(r)=\omega^{1/2}\tilde{\omega}^{-1/2}g(r)$ which is square integrable corresponds to an incomplete set $\{\tilde{\omega}^{1/2}r^i\}$. $\tilde{g}(r)$ is square integrable if $\omega/\tilde{\omega}$ is bounded from above (for all r). Thus for $\omega^{1/2}=\exp(-\tfrac{1}{2}r^{\beta})(\beta<\tfrac{1}{2})$ $\tilde{\omega}^{1/2}$ can be of the form $\tilde{\omega}^{1/2}=\exp(-f(r))$ where $f(r)<r^{\beta}$. Thus any weight of the form $\tilde{\omega}^{1/2}=\exp(-f(r))$ with $f(r)<r^{1/2}$ corresponds to an incomplete set $\{\exp(-f(r))r^n\}$ over $0\leqslant r<\infty$. Closely related ideas were discussed by Stieltjes, as presented by Borel (1978), in the context of the moment problem referred to above.

These results are in interesting contrast with Müntz's theorem since, according to the latter $\{x^{\gamma n};\ n=0,1,2\ldots\}$ is complete (in $0<x<1$) for any $\gamma>0$. The not so intuitively obvious nature of this contrast is a sobering example of where the naive commonsense we usually feel confortable with can go astray.

Yet another contrast between a finite interval and an infinite one involves the fact that over a finite interval any set $\{\omega(x)^{1/2}x^n\}$ is complete in L^2, where $\omega(x)$ is a weight function which is only assumed to be positive (almost everywhere) and integrable (Erdélyi 1953).

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