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DIFFERENTIAL CRITERIA FOR POSITIVE DEFINITENESS

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Abstract. We show how the Mellin transform can be used to derive differential criteria for integral representations of functions as scale mixtures, and apply this idea to derive differential criteria for positive definiteness of functions in a manner similar to that of Gneiting (1999,2001). We also give a simple derivation of Williamson's result on multiply monotone functions (Williamson, 1956), with a limiting process giving the Bernstein-Widder theorem.

1. Introduction

Recently, Gneiting (1999,2000) has derived differential criteria for positive definiteness based on finding necessary and sufficient conditions that a function be representable as a scale mixture of a certain function known to be positive definite. The use of differential criteria for integral representations is also seen in the Bernstein-Widder theorem on completely monotone functions, and in Schoenberg (1942) and Williamson's (1956) theorem on multiply monotone functions. In this paper we show how the Mellin transform can be used to facilitate the analysis of scale mixture representations and the derivation differential criteria for such representations.

1.1. Scale mixtures.

Let f and g be real-valued functions, continuous on $[0,\infty]$. We say that f is a *scale mixture* of g if there is a non-decreasing function μ, bounded on $[0,\infty]$ such that,

$$f(x) \;=\; \int_0^\infty \frac{1}{\xi}\, g\!\left(\frac{x}{\xi}\right) d\mu(\xi) \quad \forall\, x \in [0,\infty] \tag{1}$$

where the integral will generally be the Riemann-Stieltjes integral. [1]

If μ is also continuous, then $d\mu(\xi) = h(\xi)\, d\xi$, with h non-negative and integrable on $(0,\infty)$, and $f(x) = \int_0^\infty \xi^{-1} g(x/\xi) h(\xi)\, d\xi$. We refer to the latter as the *scale convolution* of g and h. It is related to ordinary convolution through the change of variables, $x = e^z$ and $\xi = e^t$, which yields,

$$f \circ \exp = \big(g \circ \exp\big) * \big(h \circ \exp\big) \tag{2}$$

where $*$ denotes convolution and $\circ$ denotes composition. [2]

[1]We generally use the Riemann-Stieltjes integral rather than the Lebesgue integral since the latter requires absolute integrability. We will however use Lebesgue integrals when they exist, and write $f \in L(0,\infty)$ when f is Lebesgue integrable on $(0,\infty)$.

[2]The two types of convolution arise together in the consideration of the distribution function of sums and products of measurable functions. It is well known that the distribution function of a finite sum is the (ordinary) convolution of the respective distribution functions. Similarly, if $X(\omega)$ and $Y(\omega)$ are non-negative μ-measurable functions with continuously differentiable distribution

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1.1.1. *Examples.* (i) The class of functions that are completely monotonic on $(0,\infty)$ is equivalent to the class of scale mixtures of e^{-x} by the Bernstein-Widder theorem. (ii) The class of functions $f(r)$ such that $f(\|x\|)$ is positive definite on $\mathbb{R}^n$, is equivalent to the class of scale mixtures of $r^{-\nu}J_\nu(r)$ where $\nu = (n-1)/2$ [2, Thm. 1].

In this paper we shall be interested primarily in the fact that scale mixtures preserve positive definiteness. Thus, a test determining whether a function f is a scale mixture of a given positive definite function, is also a test determining whether f is positive definite.

1.2. **The Mellin transform.** It is well known that the Fourier and Laplace transforms can be used to solve integral equations of the convolution type. Given (2), these transforms can also be used to solve equations of the scale convolution type. The latter however can be solved without changing variables using the Mellin transform [5, 4, 1], which is defined by,

$$\mathcal{M}\left[f(x)\,;s\right] \;\equiv\; \tilde{f}(s) \;\equiv\; \int_0^\infty x^{s-1} f(x)\,dx \tag{3}$$

for $s \in \mathbb{C}$ such that the integral is convergent. If $x^k g(x)$ and $x^k h(x) \in L(0,\infty)$ for some $k \in \mathbb{R}$ then [5, Thm. 44],

$$f(x) = \int_0^\infty \frac{1}{\xi}\, g\!\left(\frac{x}{\xi}\right) h(\xi)\,d\xi \quad\Rightarrow\quad \tilde{f}(s) = \tilde{g}(s)\tilde{h}(s) \tag{4}$$

and $x^k f(x) \in L(0,\infty)$. Then we can solve for $h(x)$ by inverting the transform. If $x^k f(x) \in L(0,\infty)$, then (3) can be inverted almost everywhere using the formula [5, Thm. 28],

$$\mathcal{M}^{-1}[\tilde{f}(s)\,;x] \;\equiv\; \frac{1}{2\pi i}\int_{k-i\infty}^{k+i\infty} x^{-s}\tilde{f}(s)\,ds \;=\; \frac{f(x+)+f(x-)}{2} \tag{5}$$

where $f(x+)$ and $f(x-)$ denote the right and left hand limits of f at x. Thus, for example, when h in (4) is continuous on $(0,\infty)$, we have,

$$h(x) = \mathcal{M}^{-1}\Big[\frac{\tilde{f}(s)}{\tilde{g}(s)}\,;x\Big], \quad x \in (0,\infty)$$

We can similarly solve integral equations of the form $f(x) = \int_0^\infty g(\xi x)h(\xi)\,d\xi$. First note the following two properties, which follow readily from the definition (3):

$$\mathcal{M}\left[x^a f(x)\,;s\right] = \frac{1}{a}\tilde{f}\left(\frac{s}{a}\right), \quad \mathcal{M}\left[f(x^a)\,;s\right] = \tilde{f}(s+a) \tag{6}$$

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functions $G(x)$ and $H(x)$, then for the distribution function F of $X(\omega)Y(\omega)$ we have,

$$F(x) = \int_0^\infty G\!\left(\frac{x}{\xi}\right) dH(\xi) \;=\; \int_0^\infty H\!\left(\frac{x}{\xi}\right) dG(\xi)$$

and for the derivative $f(x) \equiv F'(x)$, we have,

$$f(x) = \int_0^\infty \frac{1}{\xi}\, g\!\left(\frac{x}{\xi}\right) h(\xi)\,d\xi \;=\; \int_0^\infty \frac{1}{\xi}\, h\!\left(\frac{x}{\xi}\right) g(\xi)\,d\xi$$

We thus have $\mathcal{M}\left[t^{-1}h(t^{-1})\,;s\right] = \tilde{h}(1-s)$, and it follows that,

$$f(x) = \int_0^\infty g(\xi x)h(\xi)\,d\xi \quad \Rightarrow \quad \tilde{f}(s) = \tilde{g}(s)\tilde{h}(1-s) \tag{7}$$

The integral in (7) is also referred to as a scale mixture.

Another basic property we shall use is the "scaling property":

$$\mathcal{M}\left[f(ax)\,;s\right] = a^{-s}\tilde{f}(s) \tag{8}$$

Thus far, we have only considered functions for which $x^{k-1}f(x) \in L(0,\infty)$ for some $k \in \mathbb{R}$. In order to justify the use of transforms of functions like $\cos(x)$, for which $x^{k-1}f(x)$ is not absolutely integrable for any $k \in \mathbb{R}$, we require the following theorem [5, Thm. 32], which applies to functions for which there exists a $k \in \mathbb{R}$ such that $x^{k-1+it}f(x)$ is uniformly integrable with respect to t.

Theorem. *Let the integral $\int_0^\infty x^{s-1}f(x)\,dx \equiv \tilde{f}(s)$ be uniformly convergent (as the limits are approached independently) for $s = k+it$, t in any finite interval. Then,*

$$\frac{1}{2\pi i}\lim_{\lambda\to\infty}\int_{k-i\lambda}^{k+i\lambda}\left(1-\frac{|t|}{\lambda}\right)x^{-s}\tilde{f}(s)\,ds \;=\; \frac{f(x+)+f(x-)}{2} \tag{9}$$

for all $x > 0$ such that $f(x+)$ and $f(x-)$ exist.

We can take (9) as the most general definition of the Mellin inverse since the $C(1)$ summation in (9) is equivalent to the ordinary summation in (5) when the latter exists.

Like the Laplace transform, the Mellin transform can be used to convert integro-differential equations into algebraic equations. We use in particular the following relation. Let D denote the differential operator. The transform of the operator D^n is given by,

$$\mathcal{M}\left[D^n f(x)\,;s\right] = (-1)^n\frac{\Gamma(s)}{\Gamma(s-n)}\tilde{f}(s-n) \tag{10}$$

and from (6), we have,

$$\mathcal{M}\left[(-x)^n D^n f(x)\,;s\right] = \frac{\Gamma(s+n)}{\Gamma(s)}\tilde{f}(s) \tag{11}$$

These formulae are valid for negative n, where $D^{-n} \equiv I^n$ denotes the nth iterated integral, where $I \equiv \int_0^x$. For example, if f is integrable on $(0,x)$, we have,

$$\mathcal{M}\left[\int_0^x f(t)\,dt\,;s\right] = -\frac{1}{s}\tilde{f}(s+1) \tag{12}$$

For f integrable on (x,∞), $t>0$, we have,

$$\mathcal{M}\left[\int_x^\infty f(t)\,dt\,;s\right] = \frac{1}{s}\tilde{f}(s+1) \tag{13}$$

We will also use the following result on differentiation in the transform domain,

$$\mathcal{M}\left[(\log x)^n f(x)\,;s\right] \;=\; \frac{d^n}{ds^n}\tilde{f}(s) \tag{14}$$

Regarding the Mellin transform of Stieltjes integrals, we note that if μ is non-decreasing and bounded on $(0,\infty)$, and $\mu(x)$ is $O(x^\epsilon)$, $\epsilon > 0$, as $x \to 0$, then $\tilde{\mu}(s)$ exists for $0 < \mathrm{Re}(s) < \epsilon$, and,

$$\int_0^\infty x^{s-1} d\mu(x) = (s-1)\tilde{\mu}(s-1) \tag{15}$$

in this region.

We define the class of functions $\mathcal{M}_k$, $k \in \mathbb{R}$, to consist of all real-valued functions on $(0,\infty)$ such that either (i) $x^{k-1}f(x)$ is absolutely integrable on $(0,\infty)$, or (ii) f is bounded on $[0,\infty)$, and $\int_0^\infty x^{k-1+it} f(x)\,dx$ is uniformly convergent for t in any finite interval. If $f \in \mathcal{M}_k$, then $\mathcal{M}^{-1}[\mathcal{M}[f(x)\,;s]\,;x] = f(x)$ at all points of continuity of f, where the contour integral is taken on the line $\mathrm{Re}(s) = k$. Based on the preceding, we formulate the following theorem for the type of scale mixture considered in the sequel.

Lemma 1. *If $f, g \in \mathcal{M}_k$ for some $k \in \mathbb{R}$, then there exists a function μ non-decreasing and bounded on $(0,\infty)$ such that,*

$$f(x) = \int_0^\infty g(x\xi)\, d\mu(\xi) \tag{16}$$

if and only if,

$$\mathcal{M}^{-1}\Big[\frac{1}{s}\,\frac{\tilde{f}(-s)}{\tilde{g}(-s)}\,;x\Big] \tag{17}$$

is non-decreasing and bounded on $(0,\infty)$.

Proof. Suppose that (16) holds with μ non-decreasing and bounded on $(0,\infty)$, and let $\mu(0+) = 0$. Note that $\int_0^\infty x^{s-1} d\mu(x) = (s-1)\tilde{\mu}(s-1)$. We have,

$$\int_0^\infty x^{s-1}\bigg[\int_0^\infty g(x\xi)\,d\mu(\xi)\bigg]dx \;=\; \int_0^\infty\bigg[\int_0^\infty x^{s-1} g(x\xi)\,dx\bigg]d\mu(\xi) \;=\; -s\,\tilde{g}(s)\tilde{\mu}(-s)$$

where $s = k + it$, and the interchange in the order of integration is justified since $g \in \mathcal{M}_k$ and thus either g is bounded, in which case the bracketed integral on the left is absolutely convergent, or $x^{k-1}g(x)$ is absolutely integrable, in which case the bracketed integral on the right is absolutely convergent. Thus,

$$\frac{1}{s}\,\frac{\tilde{f}(-s)}{\tilde{g}(-s)} \;=\; \tilde{\mu}(s)$$

and the Mellin inverse of the left side is equal to $\mu(x)$ at all points of continuity of μ, and to $(\mu(x+) + \mu(x-))/2$ at points of discontinuity, and is thus non-decreasing and bounded.

Conversely, suppose that (17) is non-decreasing and bounded on $[0,\infty)$. Then □

We assume in the sequel that any non-decreasing bounded function μ used in an integral satisfies $\mu(0) = 0$ and is thus uniquely determined at points of continuity.

2. Differential criteria for scale-mixture representations

The derivation of differential criteria for the representation of functions as scale-mixtures is based on the

2.1. **Multiply monotone functions.** A function is defined to be n-times monotone, $n \geq 2$, if $(-1)^n f^{(n-2)}(x)$ is non-negative, non-increasing, and convex for $x > 0$. It is shown in [3] that an n-times monotone function f can be represented in the form,

$$f(t) = \int_0^\infty (1-ut)_+^{n-1} d\gamma(u) \tag{18}$$

where $\gamma(t)$ is non-decreasing, and $(a)_+ \equiv \max(a,0)$. The argument in [3] is based on the integration by parts development of the Taylor series expansion of f.

Alternatively, using Lemma 1 to invert (18), we have

$$\gamma(t) \ = \ \mathcal{M}^{-1}[\frac{1}{s}\tilde{f}(-s)\left(\mathcal{M}\left[(1-t)_+^{n-1}\,;-s\right]\right)^{-1};t] \tag{19}$$

at all points of continuity. For the Mellin transform of $(1-t)_+^{n-1}$, we have,

$$\mathcal{M}\left[(1-t)_+^{n-1}\,;s\right] \ = \ \int_0^1 t^{s-1}(1-t)^{n-1}dt \ = \ \frac{\Gamma(s)\Gamma(n)}{\Gamma(s+n)}$$

where we identify the integral as the Beta function. Noting that $\mathcal{M}^{-1}[\tilde{\gamma}(-s)\,;t] = -\gamma(t^{-1})$, we have for (19),

$$-\gamma\left(\frac{1}{t}\right) = \frac{1}{\Gamma(n)}\,\mathcal{M}^{-1}[-\frac{1}{s}\frac{\Gamma(s+n)}{\Gamma(s)}\tilde{f}(s)\,;t] \tag{20}$$

Using (13), (15), and (10) we have,

$$\begin{aligned}\mathcal{M}\left[\int_t^\infty (-u)^{n-1}df^{(n-1)}(u)\,;s\right] \ &= \ \frac{1}{s}(-1)^{n-1}\int_0^\infty u^{s+n-1}df^{(n-1)}(u)\\ &= \ \frac{1}{s}\,(-1)(s+n-1)\frac{\Gamma(s+n-1)}{\Gamma(s)}\tilde{f}(s) \ = \ -\frac{1}{s}\frac{\Gamma(s+n)}{\Gamma(s)}\tilde{f}(s)\end{aligned}$$

Using this in (20), we have,

$$\gamma(t) \ = \ -\frac{1}{\Gamma(n)}\int_{1/t}^\infty (-u)^{n-1}df^{(n-1)}(u) \ = \ \frac{1}{\Gamma(n)}\int_{0^+}^t (-u)^{1-n}\,df^{(n-1)}\left(\frac{1}{u}\right) \tag{21}$$

which is equivalent to equation 1.2 of [3]. Thus f is n-times monotone if and only if $\gamma(t)$ defined by (21) is non-decreasing, i.e. $-f^{(n-1)}(t)$ is non decreasing on $(0,\infty)$.

2.2. **Complete monotonicity.** A function is defined to be completely monotonic if it satisfies the inequalities $f^{(n)}(x) \geq 0$ for $x > 0$, $n = 1, \ldots, \infty$. The Bernstein-Widder theorem states that a function f is completely monotonic if and only if it can be represented in the form,

$$f(x) = \int_0^\infty e^{-tx}d\mu(t) \tag{22}$$

with μ non-decreasing on $(0,\infty)$.gh

Lemma 2. *f is completely monotonic on $(0,\infty)$ if and only if*

$$\mathcal{M}^{-1}[\Gamma(s)\tilde{f}(s)\,;t] \tag{23}$$

is non-decreasing and bounded on $(0,\infty)$.

Proof. □

3. Positive definiteness on $\mathbb{R}^n$

Let $\mathcal{P}_n$ denote the class of functions positive definite on $\mathbb{R}^n$. Schoenberg [2] used the polar representation of radial symmetric functions (functions of $\|x\|_2$) and Bochner's theorem to show that a real valued radially symmetric function f on $\mathbb{R}^n$ is positive definite if and only if $f(x) = g(\|x\|)$ with

$$g(r) = \int_0^\infty r^{-\nu} J_\nu(ru)\, d\alpha(u)$$

where $\alpha(u)$ is non-decreasing and bounded for $u \geq 0$, and $\nu = (n-2)/2$. Using the fact that [4, p. 263],

$$\mathcal{M}\left[r^{-\nu} J_\nu(r)\,;s\right] = 2^{s-n/2} \frac{\Gamma\left(\dfrac{s}{2}\right)}{\Gamma\left(\dfrac{n-s}{2}\right)} \tag{24}$$

with Lemma 1 and the scaling property (8), we have,

$$\alpha(2^{-n/2}u) = \mathcal{M}^{-1}[s \frac{\Gamma\left(\frac{n+s}{2}\right)}{\Gamma\left(\frac{-s}{2}\right)}\, \tilde{g}(-s)\,; u]$$

at all points of continuity.

Lemma 3. *$f \in \mathcal{P}_n$ if and only if,*

$$\mathcal{M}^{-1}[\Gamma(s) \cos\left(\frac{\pi s}{2}\right) \tilde{f}(s)\,; t] > 0 \qquad \forall\, t \geq 0 \tag{25}$$

Proof. □

Theorem 1. *$f \in \mathcal{P}_n$ if and only if $XXX \in \mathcal{P}_1$.*

Proof. □

Theorem 2. *f is positive definite on $\mathbb{R}$ if and only if,*

$$\frac{1}{\sqrt{x}} \int_0^\infty \exp\left(-\frac{t^2}{x}\right) f(t)\, dt$$

is completely monotonic.

Proof. □

4. Functions with compact support

Substituting $x = e^{-z}$ in (3), we see that the Mellin transform is equivalent to the bilateral Laplace transform of $f(e^{-x})$. Now let $f(x)$ be concentrated on $[0, 1]$, with $f(0) = 1$ and $f(1) = 0$. Then the support of $f(e^{-x})$ is $[0, \infty)$, and the Mellin transform of f is equivalent to the one-sided Laplace transform of $f(e^{-x})$.

Theorem 3.

Proof. □

Theorem 4.

Proof. □

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