Experimental Approaches to Kuttner's Problem

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CONTENTS

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For $\lambda \in (0, 2)$, let $k(\lambda)$ denote the smallest positive value of κ so that the truncated power function $\varphi_{\lambda,\kappa}(t) = (1-|t|^{\lambda})_+^{\kappa}$ is positive definite. We give lower and upper estimates of Kuttner's function $k(\lambda)$ through detailed numerical and symbolic computations, and we show analytically that $k\left(\frac{4n+1}{2n+1}\right) \leq 2n+1$ for $n \in \mathbb{N}$.

1. INTRODUCTION

A complex-valued function φ is said to be *positive definite* if the matrix

$$\big(\varphi(t_i - t_j)\big)_{i,j=1}^{k}$$

is nonnegative definite for all finite systems of real numbers $t_1, \ldots, t_k$. Positive definite functions have significant applications in probability theory, statistics, and approximation theory, where they occur as characteristic functions, covariance functions, and radial basis functions, respectively. The celebrated theorem of Bochner [1933] characterizes continuous, positive definite functions as the Fourier transforms of nonnegative finite measures.

Wintner [1942] raised the question for which values of $\lambda > 0$ and $\kappa > 0$ the truncated power function

$$\varphi_{\lambda,\kappa}(t) = \big(1 - |t|^{\lambda}\big)_+^{\kappa} = \begin{cases} (1-|t|^{\lambda})^{\kappa} & \text{if } |t| \leq 1, \\ 0 & \text{if } |t| \geq 1, \end{cases}$$

is positive definite (see [Gneiting 2000] for an extensive discussion of, and corrections to, Wintner's results). The question is an appealing special case of a recent problem of Bisgaard and Sasvári [1997]. By Bochner's theorem and Fourier inversion, $\varphi_{\lambda,\kappa}$ is positive definite if and only if

$$\int_0^1 (1-t^{\lambda})^{\kappa} \cos(\omega t)\, dt \geq 0 \quad \text{for } \omega \geq 0. \qquad (1\text{–}1)$$

Rephrased this way, the problem superficially looks simple, but it is not. Kuttner [1944] showed that $\varphi_{\lambda,\kappa}$ is not positive definite if $\lambda \geq 2$, regardless of

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the value of κ. For each $\lambda \in (0,2)$, there exists a positive number $k(\lambda)$ such that $\varphi_{\lambda,\kappa}$ is positive definite if and only if $\kappa \geq k(\lambda)$. The function $k(\lambda)$, for $\lambda \in (0,2)$, is known as *Kuttner's function.* It is continuous and strictly increasing, and satisfies

$$\begin{aligned} \lim_{\lambda \to 0} k(\lambda) &> 0, \\ k(1) &= 1, \\ \lim_{\lambda \to 2} k(\lambda) &= \infty, \\ k(\lambda) &> \lambda \quad \text{if } \lambda \neq 1. \end{aligned}$$

Almost 60 years after Wintner's and Kuttner's contributions, exact values of $k(\lambda)$, for $\lambda \neq 1$, are still out of reach. Here we provide estimates of Kuttner's function based on extensive experimentation. In Section 2 we find upper bounds through an application of a criterion of Pólya type. Specifically, we prove that

$$k\left(\frac{4n+1}{2n+1}\right) \leq 2n+1 \quad \text{for } n = 0, 1, \ldots; \tag{1–2}$$

this provides upper bounds for all $\lambda \in (0,2)$ and settles a problem of Zastavnyi [2000, p. 79]. The estimate implies similar inequalities and Pólya-type criteria for norm-dependent positive definite functions in $\mathbb{R}^d$. In Section 3 we apply a numerical approach to find lower bounds on Kuttner's function; in particular, we show that

$$\lim_{\lambda \to 0} k(\lambda) > 0.4279. \tag{1–3}$$

Our findings are illustrated in Figure 1. The estimates divide the (λ, κ) plane into three regions; for parameter values on or above the upper estimate, $\varphi_{\lambda,\kappa}$ is positive definite; for parameter values on or beneath the lower estimate, it is not. Between the two bounds, rigorous results are not available, but we expect the lower estimates in Table 2 to be sharp within an accuracy of 10^{-4}.

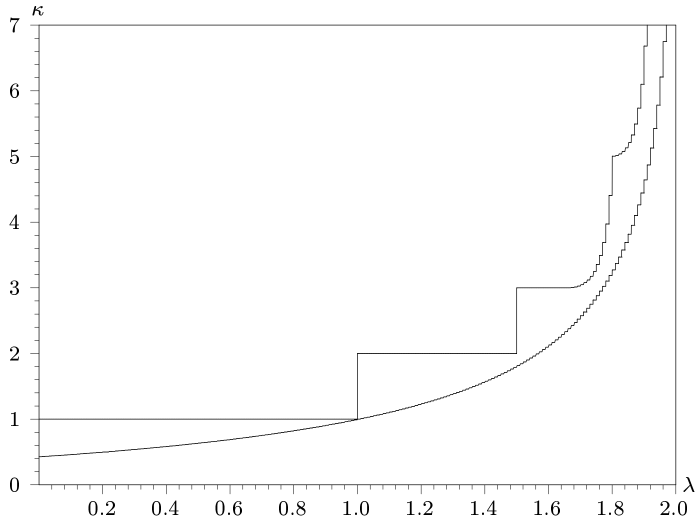

FIGURE 1. Lower and upper bounds of Kuttner's function.

2. UPPER ESTIMATES OF KUTTNER'S FUNCTION

As mentioned, Zastavnyi [2000, p. 79] called for explicit upper bounds on Kuttner's function. We address the problem through criteria of Pólya type, an approach suggested by [Gneiting 2000; 2001]. In particular, we prove the crucial estimate (1–2).

Whenever convenient, we identify a symmetric function $\varphi(|t|)$, $t \in \mathbb{R}$, with its restriction $\varphi(t)$, $t \geq 0$. We can then formulate a classical criterion ([Pólya 1949]; see also [Sasvári 1998]):

Criterion 1 (Pólya). *If $\varphi : [0,\infty) \to \mathbb{R}$ is a continuous and convex function that satisfies $\varphi(0) = 1$ and $\lim_{t\to\infty} \varphi(t) = 0$, then $\varphi(|t|)$, where $t \in \mathbb{R}$, is positive definite.*

This criterion applies to the truncated power function $\varphi_{\lambda,\kappa}$ if and only if $\lambda \leq 1$ and $\kappa \geq 1$. This does not go beyond the results of [Kuttner 1944]; Kuttner knew that $k(\lambda)$ is an increasing function with $k(1) = 1$. To proceed, we rely on an analogue of the criterion of [Gneiting 2001].

Criterion 2 (Gneiting). *Let $\varphi : [0,\infty) \to \mathbb{R}$ be a continuous function with $\varphi(0) = 1$ and $\lim_{t\to\infty} \varphi(t) = 0$. Let n be a positive integer, and suppose that $\varphi(t)$ posesses derivatives of all orders up to $2n$ for $t > 0$. Put*

$$\begin{aligned} \eta_1(t) &= \left(\frac{d}{du}\right)^n \varphi(u^{1/2}) \Big|_{u=t^2}, \\ \eta_2(t) &= \left(\frac{d}{dt}\right)^{n-1} \eta_1'(t^{1/2}). \end{aligned} \tag{2–1}$$

If $\eta_2(t)$ is convex for $t > 0$, then $\varphi(|t|)$, $t \in \mathbb{R}$, is positive definite.

Definition 3. Let n be a positive integer. If a function $\varphi : [0,\infty) \to \mathbb{R}$ satisfies the conditions of Criterion 2, we call it a function of type $\mathcal{P}_n$.

According to [Gneiting 2001, Proposition 2.1], φ is of type $\mathcal{P}_n$ if and only if it is a scale mixture of a certain basis function φ_n, that is, the representation

$$\varphi(t) = \int_{(0,\infty)} \varphi_n(rt)\, dF(r) \quad \text{for } t \geq 0 \qquad (2\text{–}2)$$

holds, where F is a probability measure on $(0, \infty)$. Furthermore, the even continuation $\varphi_n(|t|)$, $t \in \mathbb{R}$, of the basis function is precisely $2n$-times differentiable at $t = 0$. We return to these observations when we subsequently check whether the truncated power function $\varphi_{\lambda,\kappa}$ is of type $\mathcal{P}_n$, for $n = 1, 2, \ldots$ A positive answer will evidently provide an upper estimate of Kuttner's function. Figure 2 summarizes the results of extensive calculations with Maple. For $n = 1, 2, 3$, and 4, the graph of the function $k_n(\lambda)$ divides the (λ, κ) plane into two regions; for parameter values above the graph, $\varphi_{\lambda,\kappa}$ is of type $\mathcal{P}_n$; for parameter values below the graph, it is not.

The figure and similar experiments for higher values of n suggest a clear pattern, and Theorem 4 summarizes the results that we have been able to show.

Theorem 4. *Let n be a positive integer.*

(a) *There exists a function $k_n(\lambda)$, $\lambda \in (0, 2)$, such that $\varphi_{\lambda,\kappa}$ is of type $\mathcal{P}_n$ if and only if $\kappa \geq k_n(\lambda)$.*

(b) *If $k_n(\lambda) \leq \kappa$ and κ is an integer, then $k_n(\lambda') \leq \kappa$ for all $\lambda' \leq \lambda$.*

(c) $k_n(\lambda) = 2n{+}1$ *if* $\lambda \leq \lambda_{(n)} = (4n{+}1)/(2n{+}1)$.

(d) *There exists a number $\lambda^{(n)}$ satisfying $\lambda_{(n)} \leq \lambda^{(n)}$ and*

$$\lambda^{(n)} \leq \sup\left\{\lambda \in (0,2) : \exp(-t^\lambda) \textit{ is of type } \mathcal{P}_n\right\} < 2. \qquad (2\text{–}3)$$

Furthermore, $k_n(\lambda) < \infty$ if $\lambda < \lambda^{(n)}$, and $k_n(\lambda) = \infty$ if $\lambda > \lambda^{(n)}$.

We conjecture, but do not know how to prove, that $\lambda_{(n)} < \lambda^{(n)}$, that $k_n(\lambda)$ is continuous and strictly increasing for $\lambda \in (\lambda_{(n)}, \lambda^{(n)})$, and that

$$\lim_{\lambda \to \lambda^{(n)}} k_n(\lambda) = \infty.$$

We believe furthermore that the first relation in (2–3) is an equality, and that $\lambda^{(n)}$ increases with n.

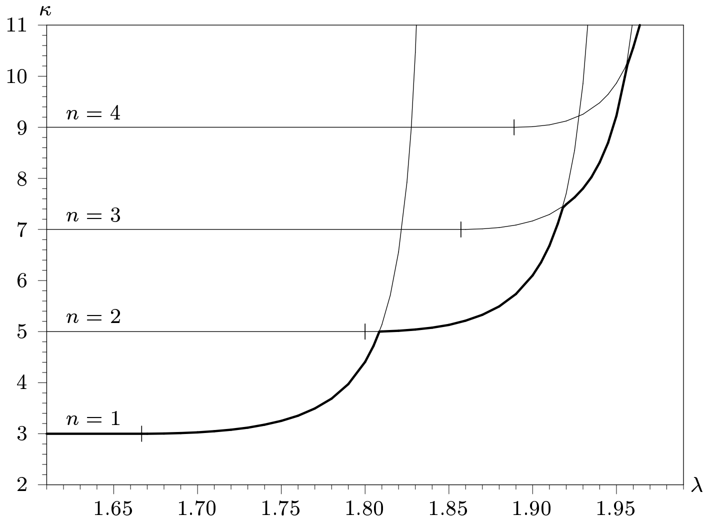

FIGURE 2. The graphs of the function $k_n(\lambda)$ for $n = 1, 2, 3$, and 4 indicate whether $\varphi_{\lambda,\kappa}$ is of type $\mathcal{P}_n$ (above the graph) or not (below it). The vertical tick marks correspond to $\lambda_{(n)} = (4n{+}1)/(2n{+}1)$, and the thick line illustrates the upper estimate (2–7) for Kuttner's function.

The crucial estimate (1–2) is immediate from part (c). The first inequality in (2–3) allows us to compute upper bounds on $\lambda^{(n)}$; for example,

$$\lambda^{(1)} < 1.8418, \qquad \lambda^{(2)} < 1.9489,$$
$$\lambda^{(3)} < 1.9789, \qquad \lambda^{(4)} < 1.9902.$$

Proof of Theorem 4. (a) For $\lambda \in (0, 2)$, let $k_n(\lambda) = \inf\{\kappa > 0 : \varphi_{\lambda,\kappa} \text{ is of type } \mathcal{P}_n\}$ if the infimum exists; if not, let $k_n(\lambda) = \infty$. Then $\varphi_{\lambda,\kappa}$ is not of type $\mathcal{P}_n$ if $\kappa < k_n(\lambda)$, and it is of type $\mathcal{P}_n$ if $\kappa = k_n(\lambda)$, by a continuity argument. A corollary of [Williamson 1956, p. 198] shows that $\varphi_{\lambda,\kappa'}$ is a scale mixture of $\varphi_{\lambda,\kappa}$ whenever $\kappa' \geq \kappa$. In other words, the representation

$$\varphi_{\lambda,\kappa'}(t) = \int_{(0,\infty)} \varphi_{\lambda,\kappa}(st)\, dG(s) \quad \text{for } t \geq 0 \qquad (2\text{–}4)$$

holds, where G is a probability measure on $(0, \infty)$. We know from the representation (2–2) that a function φ is of type $\mathcal{P}_n$ if and only if it is a scale mixture of the basis function φ_n. If we insert (2–4) into (2–2) we see that $\varphi_{\lambda,\kappa'}$ is of type $\mathcal{P}_n$, because it is a scale mixture of φ_n.

(b) Suppose that $k_n(\lambda) \leq \kappa$ where κ is an integer. By [Gneiting 1999, Proposition 4.5], $\varphi_{\lambda',\kappa}$ is a scale mixture of $\varphi_{\lambda,\kappa}$ whenever $\lambda' \leq \lambda$. An argument in analogy to that in part (a) shows that $k_n(\lambda') \leq \kappa$.

(c) For $t \in (0,1)$, expand

$$\begin{aligned}\varphi_{(4n+1)/(2n+1),\,2n+1}(t) &= \left(1 - t^{(4n+1)/(2n+1)}\right)^{2n+1} \\ &= \sum_{j=0}^{2n+1} (-1)^j \binom{2n+1}{j} t^{j(4n+1)/(2n+1)}, \quad (2\text{–}5)\end{aligned}$$

and differentiate termwise to find $\eta_2(t)$. The chain rule for higher derivatives of composite functions [Gradshteyn and Ryzhik 1994, Eq. 0.430.2] shows that $\eta_2(t)$ is continuous but not differentiable at $t = 1$. Nevertheless, $\eta_2(t)$ will be convex if we can prove that $\eta''(t)$ exists and is positive for $t \in (0,1)$. Direct calculation based on (2–1) and (2–5) yields

$$\eta_2''(t) = 2\sum_{j=1}^{2n}\left((-1)^j\binom{2n+1}{j}\Big(\frac{4n+1}{4n+2}\,j\Big)^{(n)} \times \Big(\frac{4n+1}{4n+2}\,j - n - \frac{1}{2}\Big)^{(n)} t^{j(4n+1)/(4n+2)-2n-3/2}\right), \quad (2\text{–}6)$$

where $m^{(k)} = m(m-1)\cdots(m-k)$. Notice that we can write

$$\eta_2''(t) = t^{-2n-3/2}p\big(t^{(4n+1)/(4n+2)}\big),$$

where p is a polynomial of degree $2n$. The first $n+1$ coefficients of p are nonnegative and its final n coefficients are negative. By Descartes' rule of signs (see [Albert 1943], for example), p has at most one positive root. Furthermore, we show in the appendix that the expression on the right-hand side of (2–6) has a root at $t = 1$. Thus, the unique positive root of the polynomial $p(t)$ is at $t = 1$ and $p(t)$ is positive for $t \in (0,1)$. We conclude that $\eta_2''(t)$ is positive for $t \in (0,1)$, too, and that $\eta_2(t)$ is convex for $t \in (0,\infty)$. In view of part (b), we have shown that $k_n(\lambda) \le 2n+1$ if $\lambda \le (4n+1)/(2n+1)$.

It remains to prove that $k_n(\lambda) \ge 2n+1$. If $\kappa \le 2n$, $\varphi_{\lambda,\kappa}$ is not sufficiently smooth at $t = 1$ and therefore not of type $\mathcal{P}_n$. For $\kappa \in (2n, 2n+1)$, we apply the chain rule for higher derivatives of composite functions to find $\eta_2'(t)$. The argument is analogous to the reasoning in the appendix, and we merely note that $\eta_2'(t)$ involves derivatives $(d^j/dt^j)\left((1-t)^\kappa\right)$ of order $j = 1,\ldots,2n+1$. The first $2n$ derivatives and the associated terms are bounded at $t = 1$, but the derivative of order $2n+1$ and the associated term in the sum for $\eta_2'(t)$ have a singularity at $t = 1$. Thus, $\eta_2(t)$ is not convex and $\varphi_{\lambda,\kappa}$ is not of type $\mathcal{P}_n$.

(d) Let $\lambda^{(n)} = \sup\{\lambda \in (0,2) : k_n(\lambda) < \infty\}$; then $\lambda_{(n)} \le \lambda^{(n)}$, $k_n(\lambda) = \infty$ if $\lambda > \lambda^{(n)}$, and $k_n(\lambda) < \infty$ if $\lambda < \lambda^{(n)}$, by part (b). To prove the first inequality in (2–3), recall from the results of Williamson [1956] that $\exp(-t^\lambda)$ is a scale mixture of $(1-t^\lambda)_+^\kappa$ for all $\kappa > 0$. Similarly to the argument in part (a), we see that $\exp(-t^\lambda)$ is of type $\mathcal{P}_n$ whenever $k_n(\lambda)$ is finite. To prove the third inequality, assume that $\exp(-t^{\lambda_j})$ is of type $\mathcal{P}_n$ for a sequence λ_j, $j = 1,2,\ldots$, which tends to 2 as $j \to \infty$. A continuity argument implies that $\exp(-t^2)$ is of type $\mathcal{P}_n$, too. This contradicts the representation (2–2) for functions of type $\mathcal{P}_n$, because $\exp(-t^2)$ is analytic and does not admit a scale mixture representation in terms of a basis function $\varphi_n(|t|)$ whose derivative of order $2n+1$ does not exist. □

We now apply Criterion 3 and Theorem 4 to find upper bounds on Kuttner's function $k(\lambda)$, $\lambda \in (0,2)$. If $\lambda \le 1$, $k(\lambda) \le 1$ by Pólya's criterion; if $\lambda \le \frac{3}{2}$, $k(\lambda) \le 2$ by [Gneiting 2001, Proposition 3.1]; and if $\lambda \le \frac{5}{3}$, $k(\lambda) \le 3$ by the estimate (1–2). Part (c) of Theorem 4 shows that these estimates are best possible with the present tools. For $\lambda > \frac{5}{3}$, let l_λ be the smallest positive integer n such that $\lambda \le \lambda^{(n)}$; and let $u_\lambda \ge l_\lambda$ be the smallest positive integer n such that $\lambda \le \lambda_{(n)}$. The upper estimates of Kuttner's function $k(\lambda)$, for $\lambda = 1.71, 1.72, \ldots, 1.99$, in Table 1 have been found as

$$k(\lambda) \le \min_{l_\lambda \le n \le u_\lambda} k_n(\lambda) \quad (2\text{–}7)$$

and complement the results in [Gneiting 2000; 2001]. Theorem 4 shows that they are best possible with the given tools.

Finally, we note that the estimates in Table 1 and Eq. (1–2) lead to similar inequalities and criteria of Pólya type for norm-dependent positive definite

λ	u.b.	λ	u.b.	λ	u.b.	λ	u.b.
1	1	1.76	3.3534	1.84	5.0763	1.92	7.4897
3/2	2	1.77	3.4930	1.85	5.1317	1.93	7.8008
5/3	3	1.78	3.6884	1.86	5.2123	1.94	8.3116
1.71	3.0481	1.79	3.9718	1.87	5.3277	1.95	9.2243
1.72	3.0784	1.80	4.4063	1.88	5.4936	1.96	10.5621
1.73	3.1199	1.81	5.0038	1.89	5.7357	1.97	12.0171
1.74	3.1760	1.82	5.0161	1.90	6.1004	1.98	14.5770
1.75	3.2514	1.83	5.0392	1.91	6.6814	1.99	19.7466

TABLE 1. Upper bounds for Kuttner's function.

functions in $\mathbb{R}^d$. Let $\|x\|_\alpha = (|x_1|^\alpha + \cdots + |x_d|^\alpha)^{1/\alpha}$ denote the l_α (quasi)norm of $x \in \mathbb{R}^d$, and let $n = 0, 1, 2, \ldots$ Then we may combine results of Zastavnyi [2000] with the estimate (1–2) to show that the norm-dependent function

$$\varphi(x) = \left(1 - \|x\|_\alpha^\lambda\right)_+^\kappa \quad \text{for } x \in \mathbb{R}^d$$

is positive definite whenever

$$0 < \lambda \le \alpha \le \frac{4n+1}{2n+1} \quad \text{and} \quad \kappa \ge 2d\,(n+1) - 1.$$

This settles a problem of Richards [1986], gives explicit upper bounds on the Richards–Askey function [Gneiting 1998, Section 3], and provides criteria of Pólya type for $\|\cdot\|_\alpha$-dependent function. We refer to [Gneiting 2001, Section 4] and leave details to the reader.

3. LOWER ESTIMATES OF KUTTNER'S FUNCTION

Our approach in this section is based on the following criterion of Kuttner [1944]. We note the connection to nonnegative trigonometric sums [Askey 1975, Lecture 9], to the Fourier integral (1–1), and to nonnegative integrals of Bessel functions [Misiewicz and Richards 1994].

Criterion 5 (Kuttner). *The truncated power function $\varphi_{\lambda,\kappa}$ is positive definite if and only if*

$$\psi_{\lambda,\kappa;\,n}(\omega) = \frac{1}{2} + \sum_{j=1}^{n} \left(1 - \left(\frac{j}{n}\right)^\lambda\right)^\kappa \cos(\omega j) \ge 0$$

for $\omega \in [0, \pi]$, $n = 1, 2, \ldots$

The criterion suggests numerical tests for positive definiteness. If, for a given $\lambda \in (0, 2)$, we can find values of κ, n, and ω such that $\psi_{\lambda,\kappa;\,n}(\omega) < 0$, then we have shown that $k(\lambda) > \kappa$. We developed and implemented the following algorithm, which uses a number $\lambda \in (0, 2)$, $\lambda \ne 1$, and a positive integer n as input.

1. Put $\kappa = \lambda$ and $\delta = \max\left(\lambda, \frac{1}{4}\right)$.
2. Minimize $\psi_{\lambda,\kappa+\delta;\,n}(\omega)$ over $\omega \in [0, \pi]$. This is done in a golden section search, and facilitated by the empirical observation that the first local minimum of the trigonometric sum is also the global minimum. If the minimum is negative, then $\kappa+\delta$ is a lower bound for $k(\lambda)$; put $\kappa = \kappa+\delta$. Otherwise, put $\delta = \delta/2$.
3. Repeat until $\delta < 10^{-10}$.

For given λ and n, the algorithm returns the lower bound κ and the location of the minimum of the associated trigonometric sum. We repeat this for increasing values of n, and use the asymptotic relationship

$$\frac{1}{n}\,\psi_{\lambda,\kappa;\,n}\!\left(\frac{\omega}{n}\right) \longrightarrow \int_0^1 (1 - t^\lambda)^\kappa \cos(\omega t)\, dt$$

for $\omega \ge 0$, $n \to \infty$, to locate the minimum efficiently as n increases. Table 2 and the lower graph in Figure 1 summarize our results. We used values of n between 10^4 and 10^7, with smaller values of λ calling for larger values of n. Extensive experimentation suggests that the lower estimates for $\lambda = 0.01$, 0.02, …, 1.99 cannot be improved within the numerical precision of Table 2. In other words, we conjecture that the difference between the true value of $k(\lambda)$ and our lower estimate is less than 10^{-4}.

λ	l.b.	λ	l.b.	λ	l.b.	λ	l.b.
0.01	0.4312	0.40	0.5853	1.00	1.0000	1.60	2.1313
0.02	0.4344	0.45	0.6098	1.05	1.0519	1.65	2.3324
0.03	0.4377	0.50	0.6357	1.10	1.1081	1.70	2.5759
0.04	0.4410	0.55	0.6630	1.15	1.1691	1.75	2.8794
0.05	0.4444	0.60	0.6918	1.20	1.1235	1.80	3.2733
…	…	0.65	0.7224	1.25	1.3086	1.85	3.8162
0.10	0.4617	0.70	0.7548	1.30	1.3889	1.90	4.6443
0.15	0.4798	0.75	0.7893	1.35	1.4779	1.95	6.2097
0.20	0.4989	0.80	0.8260	1.40	1.5772	…	…
0.25	0.5189	0.85	0.8651	1.45	1.6889	1.97	7.4633
0.30	0.5399	0.90	0.9069	1.50	1.8158	1.98	8.5063
0.35	0.5620	0.95	0.9518	1.55	1.9615	1.99	10.3650

TABLE 2. Lower bounds for Kuttner's function. (The dots indicate a transition in the λ increment.)

More accurate estimates for small values of λ suggest that $\lim_{\lambda\to 0} k(\lambda) = 0.4279\ldots$ Kuttner [1944, p. 84] shows that

$$\int_0^1 (-\log t)^\kappa \cos(\omega t)\, dt \ge 0 \quad \text{for } \omega \ge 0$$

if $\kappa \ge \lim_{\lambda\to 0} k(\lambda)$. The integral becomes numerically tractable if we change coordinates to $u = -\log t$ and approximate the tail integral by the incomplete gamma function. The inequality is violated if $\kappa = 0.4279$ and $\omega = 5.40324$, which proves the estimate (1–3), $\lim_{\lambda\to 0} k(\lambda) > 0.4279$.

APPENDIX

In this appendix we provide a technical detail in the proof of Theorem 4(c). We denote the right-hand side of (2–6) by $\eta_2''(t)$, which we consider as a function of $t \in (0,\infty)$. Our goal is to show that this function has a root at $t = 1$. Toward this end, we recall the construction of $\eta_2''(t)$ through Eq. (2–1), where $\varphi(t)$ is given by (2–5), so that

$$\varphi(u^{1/2}) = \bigl(1 - u^{(4n+1)/(4n+2)}\bigr)^{2n+1}.$$

The chain rule for higher derivatives of composite functions [Gradshteyn and Ryzhik 1994, Eq. 0.430.2] shows that

$$\begin{aligned}\Bigl(\frac{d}{du}\Bigr)^n \varphi(u^{1/2}) &= \sum (-1)^{j_1+\cdots+j_n} \frac{n!}{j_1!\cdots j_n!}\,(2n{+}1)^{(j_1+\cdots+j_n-1)}\bigl(1-u^{(4n+1)/(4n+2)}\bigr)^{2n+1-(j_1+\cdots+j_n)}\\ &\quad\times\Bigl(\frac{4n{+}1}{4n{+}2}\,u^{\frac{4n+1}{4n+2}-1}\Bigr)^{j_1}\Bigl(\frac{1}{2!}\Bigl(\frac{4n{+}1}{4n{+}2}\Bigr)^{(1)}u^{\frac{4n+1}{2n+1}-2}\Bigr)^{j_2}\cdots\Bigl(\frac{1}{n!}\Bigl(\frac{4n{+}1}{4n{+}2}\Bigr)^{(n-1)}u^{\frac{4n+1}{2n+1}-n}\Bigr)^{j_n}\\ &= \sum c_{j_1,\dots,j_n}\,u^{(j_1+\cdots+j_n)(4n+1)/(4n+2)-(j_1+2j_2+\cdots+nj_n)}\bigl(1-u^{(4n+1)/(4n+2)}\bigr)^{2n+1-(j_1+\cdots+j_n)},\end{aligned}$$

where $m^{(k)} = m(m-1)\cdots(m-k)$, and where the sum extends over all n-tuples $(j_1, j_2, \dots, j_n)$ of nonnegative integers for which $j_1 + 2j_2 + \cdots + nj_n = n$. Thus, we can write

$$\eta_1(t) = \Bigl(\frac{d}{du}\Bigr)^n \varphi(u^{1/2})\Big|_{u=t^2} = \sum_{k=1}^n c_k\, t^{k(4n+1)/(2n+1)-2n}\bigl(1-t^{(4n+1)/(2n+1)}\bigr)^{2n+1-k},$$

where $c_k = \sum_{j_1+\cdots+j_n=k} c_{j_1,\dots,j_n}$ for $k = 1,\dots,n$; in particular,

$$c_n = (-1)^n\frac{(2n{+}1)!}{(n{+}1)!}\Bigl(\frac{4n{+}1}{4n{+}2}\Bigr)^n, \qquad c_{n-1} = (-1)^n\frac{n(n-1)(2n)!}{4(n{+}2)!}\Bigl(\frac{4n{+}1}{4n{+}2}\Bigr)^{n-1}. \tag{A–1}$$

It is then immediate that

$$\begin{aligned}\eta_1'(t) = \sum_{k=1}^n c_k\Bigl(\frac{4n{+}1}{2n{+}1}k - 2n\Bigr)\, t^{k(4n+1)/(2n+1)-2n-1}\bigl(1-t^{(4n+1)/(2n+1)}\bigr)^{2n+1-k}&\\ -\sum_{k=1}^n c_k\,(2n{+}1-k)\,\frac{4n{+}1}{2n{+}1}\,t^{(k+1)(4n+1)/(2n+1)-2n-1}\bigl(1-t^{(4n+1)/(2n+1)}\bigr)^{2n-k}&\end{aligned}$$

and

$$\eta_1'(t^{1/2}) = \sum_{k=1}^n c_k\, f_k(t)\bigl(1-t^{(4n+1)/(4n+2)}\bigr)^{2n+1-k} - \sum_{k=1}^n c_k\, g_k(t)\bigl(1-t^{(4n+1)/(4n+2)}\bigr)^{2n-k}, \tag{A–2}$$

where

$$f_k(t) = \Bigl(\frac{4n{+}1}{2n{+}1}k - 2n\Bigr)\, t^{k(4n+1)/(4n+2)-n-1/2}, \qquad g_k(t) = (2n{+}1-k)\,\frac{4n{+}1}{2n{+}1}\, t^{(k+1)(4n+1)/(4n+2)-n-1/2}, \tag{A–3}$$

for $k = 1,\dots,n$. Finally, we recall that

$$\eta_2''(t) = \Bigl(\frac{d}{dt}\Bigr)^{n+1}\bigl(\eta_1'(t^{1/2})\bigr).$$

To show that $\eta_2''(1) = 0$, we apply Leibniz's rule to each term in the representation (A–2) for $\eta_1'(t^{1/2})$. There are $2n$ terms in the representation, and taking the derivative of order $n{+}1$ splits each into $n{+}1$ terms.

Notice that all but four of the resulting $2n(n+1)$ terms in the sum for $\eta_2''(t)$ vanish at $t = 1$. We combine the exceptional terms in a remainder

$$\begin{aligned}\rho(t) = c_n\, f_n(t)\Big(\frac{d}{dt}\Big)^{n+1}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n+1} - c_{n-1}\, g_{n-1}(t)\Big(\frac{d}{dt}\Big)^{n+1}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n+1} \\ - c_n\, g_n(t)\Big(\frac{d}{dt}\Big)^{n+1}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n} - c_n\,(n+1)\,\frac{d}{dt}\big(g_n(t)\big)\Big(\frac{d}{dt}\Big)^{n}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n}\end{aligned} \quad \text{(A–4)}$$

and proceed to show that $\rho(t)$ vanishes at $t = 1$, too. Expanding the higher order derivatives by the chain rule yields

$$\begin{aligned}\Big(\frac{d}{dt}\Big)^{n+1}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n}\Big|_{t=1} &= (-1)^{n+1}\,\frac{n(n+1)!}{4(2n+1)}\Big(\frac{4n+1}{4n+2}\Big)^{n}, \\ \Big(\frac{d}{dt}\Big)^{n+j}\big(1 - t^{(4n+1)/(4n+2)}\big)^{n+j}\Big|_{t=1} &= (-1)^{n+j}\,(n+j)!\,\Big(\frac{4n+1}{4n+2}\Big)^{n+j} \quad \text{for } j = 0, 1.\end{aligned} \quad \text{(A–5)}$$

If we insert (A–1), (A–3), and (A–5) in (A–4), we find that $\rho(1) = 0$. We have shown that $\eta_2''(t)$ has a root at $t = 1$.

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