CONSTRUCTIVE THEORY OF FUNCTIONS, Varna 2002
(B. Bojanov, Ed.), DARBA, Sofia, 2003, pp. 267-274.

Localization of the Spherical Gauss-Weierstrass Kernel

Noemí Laín Fernández* and Jürgen Prestin

In [2], Narcowich and Ward introduced a new uncertainty product U for functions on the sphere. In this paper we show that the spherical Gauss-Weierstrass kernel is asymptotically best localized with respect to the product U. The method of proof is based on series expansions of the corresponding inner products.

1. An Uncertainty Relation

In many occasions one is interested in working with functions that are somehow concentrated in both space and momentum domain. As is known, it is not possible to confine a function arbitrarily and simultaneously to space and momentum. Nevertheless, it is possible to derive a so-called *uncertainty relation* which measures a trade-off between space localization and angular momentum. In [2], Narcowich and Ward introduced an uncertainty principle for the unit sphere $\Omega \subset \mathbb{R}^3$ using the operator $O : F \mapsto OF$, which maps any real-valued function $F \in L^2(\Omega)$ into the normal field $OF : \Omega \to \mathbb{R}^3$, $\xi \mapsto \xi F(\xi)$, as position operator and the surface curl operator $L^* : F \mapsto L^*F$, which associates to any real-valued function F the tangential vector field $L^*F : \Omega \to \mathbb{R}^3$, $\xi \mapsto L^*F(\xi) = \xi \times \nabla^* F(\xi)$, as momentum operator. Here, ∇^* denotes the surface gradient. Before establishing the uncertainty principle, let us introduce the following notation, cf. also [1, 2].

(I) Localization in space domain: We define the "center of gravity of the spherical window" in space domain ξ_F^O as the expectation value of the position operator O, i.e.,

$$\xi_F^O := \langle OF, F\rangle = \int_\Omega OF(\eta)F(\eta)\, dw(\eta) = \int_\Omega \eta F(\eta)^2\, dw(\eta) \in \mathbb{R}^3.$$

*Supported by the DFG Graduiertenkolleg 357 *Effiziente Algorithmen und Mehrskalenmethoden.*

In a similar way, we can define the *variance in space domain* as the variance of the operator O, i.e.,

$$\sigma_F^O := \int_\Omega \|OF(\eta) - \xi_F^O F\|_2^2 \, dw(\eta) = 1 - \|\xi_F^O\|_2^2.$$

(II) LOCALIZATION IN MOMENTUM DOMAIN: As mentioned at the beginning, we make now use of the surface curl operator $L^* : F \mapsto L^*F$, where L^*F is the tangential vector field which associates to each point $\xi \in \Omega$ the vector $L^*F(\xi) = \xi \times \nabla^* F(\xi)$. In a similar way, we can introduce the center in momentum domain as the expectation value of the operator L^*:

$$\xi_F^{L^*} := \langle L^*F, F\rangle = \int_\Omega (L^*F(\eta))\, F(\eta)\, dw(\eta) \in \mathbb{R}^3.$$

It can be shown that if F is a twice-continuously differentiable function then the expectation value $\xi_F^{L^*}$ is equal to $\mathbf{0}$. Defining the *variance in momentum domain* as the variance of the operator L^*, one obtains

$$\begin{aligned}\sigma_F^{L^*} &:= \int_\Omega \|L^*F(\eta) - \xi_F^{L^*} F(\eta)\|_2^2 \, dw(\eta) = \int_\Omega L^*F(\eta) \cdot L^*F(\eta)\, dw(\eta) \\ &= -\int_\Omega F(\eta)\Delta^* F(\eta)\, dw(\eta) = \xi_F^{-\Delta^*},\end{aligned}$$

where in the penultimate step we have applied Stokes' Theorem to the function FL^*F and used the fact that Ω is closed. Now that we have introduced the fundamental concepts concerning localization in space and in momentum domain we are in a position to state the uncertainty principle. For the proof we refer to [1, Chapter 5] and [2].

Theorem 1. *Let F be a twice-continuously differentiable real-valued function on Ω with $\|F\|=1$. Then*

$$\sigma_F^O\, \sigma_F^{L^*} \geq \|\xi_F^O\|_2^2.$$

If ξ_F^O is non-vanishing, then

$$\operatorname{var}_O(F) \cdot \operatorname{var}_{L^*}(F) \geq 1,$$

where $\operatorname{var}_O(F) := \dfrac{\left(\sigma_F^O\right)^{1/2}}{\|\xi_F^O\|_2}$ *and* $\operatorname{var}_{L^*}(F) := \left(\sigma_F^{L^*}\right)^{1/2}$.

For simplicity of notation we will denote by $U(F)$ the uncertainty product,

$$U(F) = \operatorname{var}_O(F) \cdot \operatorname{var}_{L^*}(F).$$

In the next corollary we establish an explicit formula for the computation of the uncertainty product of zonal functions of the form

$$F(\xi) = \sum_{k=0}^{\infty} c_k \,\frac{2k+1}{4\pi}\, P_k(\xi \cdot e_3), \tag{1}$$

where P_k denotes the Legendre polynomial of degree k normalized according to the condition $P_k(1) = 1$ and $\{\sqrt{2k+1}\, c_k\} \in \ell^2(\mathbb{N}_0)$.

Corollary 1. *Let $F \in C^2(\Omega)$ be of the form (1) and $F \neq const.$ The uncertainty product $U(F)$ of the function F is then evaluated as*

$$U(F) = \left(\left(\frac{\sum\limits_{k=0}^{\infty} (2k+1)\, c_k^2}{2 \sum\limits_{k=1}^{\infty} k\, c_k\, c_{k-1}} \right)^2 - 1 \right)^{1/2} \left(\frac{\sum\limits_{k=1}^{\infty} k(k+1)(2k+1)\, c_k^2}{\sum\limits_{k=0}^{\infty} (2k+1)\, c_k^2} \right)^{1/2} . \qquad (2)$$

For the proof and further localization results we refer to [3].

2. The Gauss-Weierstrass Kernel

By using the integral formulation of the uncertainty principle for zonal functions and making use of the so-called *Gaussian kernel*

$$G(t) := e^{-\frac{\lambda}{2}(1-t)}, \qquad t \in [-1,1],\ \lambda > 0,$$

it is shown in [1, Chapter 5] that the best lower bound of the uncertainty product U is one. Additionally, numerical experiments have given evidence of the fact that the *Gauss-Weierstrass kernel* W_ρ, defined by

$$W_\rho(t) := \sum_{n=0}^{\infty} e^{-n(n+1)\rho}\, \frac{2n+1}{4\pi}\, P_n(t), \qquad t \in [-1,1],$$

also yields the best value of the uncertainty product when ρ tends to zero. In this section we prove that indeed $U(W_\rho) \to 1$ as $\rho \to 0$ by studying the behavior of the uncertainty product in its series representation (2).

Theorem 2. *Let W_ρ be the* Gauss-Weierstrass kernel*. Then*

$$\begin{aligned}
&\lim_{\rho\to 0} U(W_\rho)^2 \\
&\quad = \lim_{\rho\to 0}\ \operatorname{var}_O(W_\rho)^2 \cdot \operatorname{var}_{L^*}(W_\rho)^2 \\
&\quad = \lim_{\rho\to 0} \left(\left(\frac{\sum\limits_{k=0}^{\infty} (2k+1) e^{-2k(k+1)\rho}}{2 \sum\limits_{k=1}^{\infty} k\, e^{-2k^2\rho}} \right)^2 - 1 \right) \cdot \frac{\sum\limits_{k=1}^{\infty} k\,(k+1)(2k+1)\, e^{-2k(k+1)\rho}}{\sum\limits_{k=0}^{\infty} (2k+1)\, e^{-2k(k+1)\rho}} \\
&\quad = 1.
\end{aligned}$$

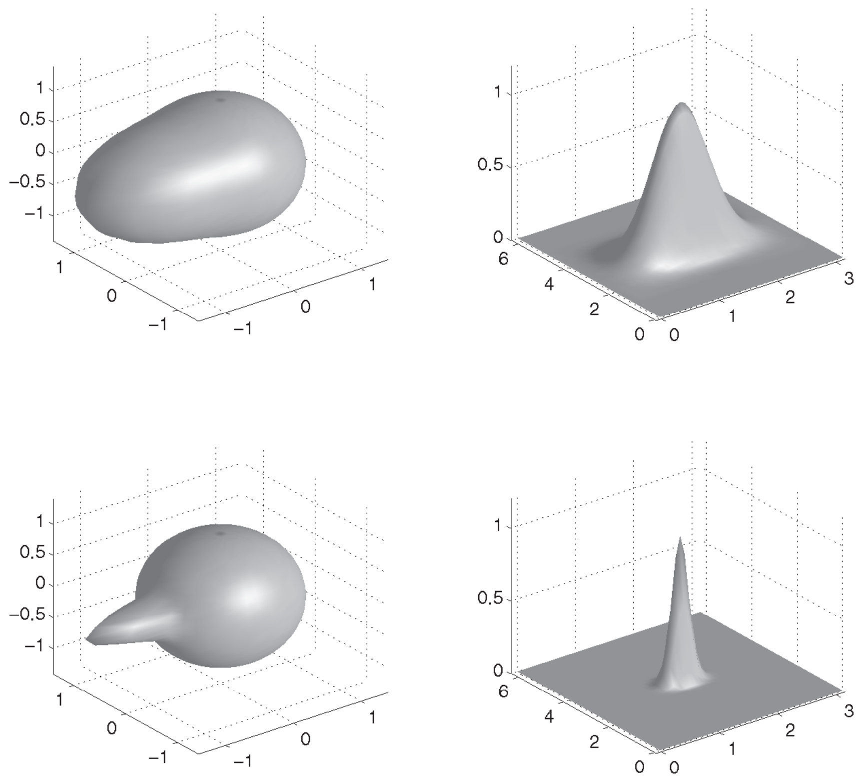

Figure 1: Plots of the Gauss-Weierstrass kernel: on the left as spherical function, on the right as function in spherical coordinates for values of $\rho = 0.1$ and $\rho = 0.01$.

For the proof of the theorem we need the following two lemmas.

Lemma 1. *Let* $0 < \rho < 1$. *It holds*

$$(i) \quad 1 + \tfrac{1}{2\rho} - \tfrac{e^{(\rho-1)/2}}{\sqrt{\rho}} < \sum_{k=0}^{\infty} (2k+1) e^{-2k(k+1)\rho} < 1 + \tfrac{1}{2\rho} + \tfrac{e^{(\rho-1)/2}}{\sqrt{\rho}},$$

$$(ii) \quad \tfrac{1}{4\rho} - \tfrac{1}{2e\sqrt{\rho}} < \sum_{k=1}^{\infty} k\, e^{-2k^2\rho} < \tfrac{1}{4\rho} + \tfrac{1}{2e\sqrt{\rho}} + \tfrac{e^{-2\rho}-1}{4\rho},$$

$$(iii) \quad \tfrac{1}{4\rho^2} - \tfrac{3}{2\sqrt{2}\,\rho^{3/2}} < \sum_{k=1}^{\infty} k(k+1)(2k+1) e^{-2k(k+1)\rho} < \tfrac{1}{4\rho^2} + \tfrac{3}{2\sqrt{2}\,\rho^{3/2}}.$$

Moreover,

$$\sum_{k=1}^{\infty} k^{\alpha} e^{-2k^2\rho} < \rho^{-(\alpha+1)/2}(1 + \delta_{\alpha,0}) \qquad (\alpha = 0, \ldots, 4). \tag{3}$$

Proof. The proof follows directly from applying the trapezoidal quadrature rule

$$\int_0^\infty f(x)\,dx - \max_{x\in\mathbb{R}_+} f(x) < \sum_{k=1}^{\infty} f(k) < \int_0^\infty f(x)\,dx + \max_{x\in\mathbb{R}_+} f(x) - \int_0^1 f(x)\,dx$$

to the functions

(i) $f(x) = (2x+1)\,e^{-2x(x+1)\rho}$,

(ii) $f(x) = x\,e^{-2x^2\rho}$,

(iii) $f(x) = x\,(x+1)\,(2x+1)\,e^{-2x(x+1)\rho}$, and finally

$f(x) = x^\alpha e^{-2x^2\rho}$, $(\alpha = 0, \dots, 4)$.

Lemma 2. *Let* $0 < \rho < 1$. *Then it holds*

$$\lim_{\rho\to 0}\left(\sum_{k=0}^{\infty}(2k+1)\,e^{-2k(k+1)\rho} - 2\sum_{k=1}^{\infty} k\,e^{-2k^2\rho}\right) = \frac{1}{2}.$$

Proof. As a first step we apply the Euler-Maclaurin summation formula to the function

$$f(x) = (2x+1)\,e^{-2x(x+1)\rho} - 2\,x\,e^{-2x^2\rho}$$

and obtain

$$\begin{aligned}\sum_{k=0}^{m} f(k) &= \int_0^m f(x)\,dx + \frac{f(0)}{2} - \frac{f(m)}{2} + \int_0^m f'(x)\left(x - \lfloor x\rfloor - \frac{1}{2}\right)dx \\ &= \int_0^m f(x)\,dx + \frac{f(0)}{2} - \frac{f(m)}{2} + \sum_{q=0}^{m-1}\int_q^{q+1} f'(x)\left(x - q - \frac{1}{2}\right)dx.\end{aligned}$$

Observe that, by taking the limit $m \to \infty$,

$$\lim_{m\to\infty}\int_0^m f(x)d\,x = \int_0^\infty \left((2x+1)\,e^{-2x(x+1)\rho} - 2\,x\,e^{-2x^2\rho}\right)dx = 0$$

and $\lim_{m\to\infty} f(b) = 0$. Since $f(0) = 1$, our problem reduces to showing that

$$\lim_{\rho\to 0}\sum_{q=0}^{\infty}\int_q^{q+1} f'(x)\left(x - q - \frac{1}{2}\right)dx = 0.$$

Some calculations with *Mathematica* yield that

$$g_q(\rho) := \int_q^{q+1} f'(x)\left(x - q - \frac{1}{2}\right)dx = \frac{1}{2\rho}\,e^{-2\rho(q^2+3q+2)}\,G_q(\rho),$$

with

$$\begin{aligned}G_q(\rho) := \rho\big(&-2\,e^{6q\rho+4\rho}\,q + e^{4\rho(q+1)}\,(2q+1) - 2\,e^{2\rho(q+1)}\,(q+1) + 2q + 3\big) \\ &+ e^{6q\rho+4\rho} - e^{4\rho(q+1)} - e^{2\rho(q+1)} + 1.\end{aligned}$$

Expanding now $G_q(\rho)$ in Taylor series around the origin gives

$$G_q(\rho) = -2\rho^2 + \frac{\rho^3}{6}\, G_q^{(3)}(\xi)$$

where $0 < \xi < \rho$. After some straightforward calculations, using also the mean value theorem, one can estimate

$$\begin{aligned}\left|G_q^{(3)}(\xi)\right| &\le 16\, e^{6\rho q + 4\rho} \\ &\quad \times \max\{27\rho q^2\,(q+1)^2 + q\,(3q+2),\ 12\,(q+1)^2 + 4\rho q^3\,(1+3q)\}.\end{aligned}$$

Consequently, for

$$27\rho q^2\,(q+1)^2 + q\,(3q+2) \ge 12\,(q+1)^2 + 4\rho q^3\,(1+3q),$$

one obtains that

$$\begin{aligned}|g_q(\rho)| &= \left|\frac{1}{2\rho}\, e^{-2\rho(q^2+3q+2)}\left(-2\rho^2 + \frac{\rho^3}{6}\, G_q^{(3)}(\xi)\right)\right| \\ &\le e^{-2\rho q^2}\left(\rho + \frac{8}{3}\,\rho^2 q + \left(4\rho^2 + 36\rho^3\right) q^2 + 72\rho^3 q^3 + 36\rho^3 q^4\right).\end{aligned}$$

Hence,

$$\begin{aligned}\sum_{k=0}^{\infty}(2k+1)\, e^{-2k(k+1)\rho} - 2\sum_{k=1}^{\infty} k\, e^{-2k^2\rho} &\le \frac{1}{2} + |g_0(\rho)| + \sum_{q=1}^{\infty}|g_q(\rho)| \\ &\le \frac{1}{2} + |g_0(\rho)| + 42\sqrt{\rho} + \frac{224}{3}\,\rho + 36\rho^{3/2} \\ &\le \frac{1}{2} + |g_0(\rho)| + 42\sqrt{\rho} + 111\rho,\end{aligned}$$

where in the last two steps we have applied the estimate (3) to each of the terms $q^\alpha e^{-2\rho q^2}$ $(\alpha = 0, \ldots, 4)$ and made use of the fact that $\rho < 1$. Since

$$\lim_{\rho\to 0}|g_0(\rho)| = \lim_{\rho\to 0}\left|\int_0^1 f'(x)\,\left(x - \frac{1}{2}\right)\, dx\right| = 0,$$

the result follows now from taking the limit $\rho \to 0$.

In a similar way, if

$$27\rho q^2\,(q+1)^2 + q\,(3q+2) < 12\,(q+1)^2 + 4\rho q^3\,(1+3q),$$

then

$$|g_q(\rho)| \le e^{-2\rho q^2}\left(\rho + 16\rho^2 + 32\rho^2 q + 16\rho^2 q^2 + \frac{16}{3}\,\rho^3 q^3 + 16\rho^3 q^4\right)$$

and consequently,

$$\begin{aligned}\sum_{k=0}^{\infty}(2k+1)\,e^{-2k(k+1)\rho} - 2\sum_{k=1}^{\infty} k\,e^{-2k^2\rho} &\le \frac{1}{2} + |g_0(\rho)| + \sum_{q=1}^{\infty} |g_q(\rho)| \\ &\le \frac{1}{2} + |g_0(\rho)| + 34\sqrt{\rho} + \frac{112}{3}\rho + 32\rho^{3/2} \\ &\le \frac{1}{2} + |g_0(\rho)| + 34\sqrt{\rho} + 70\rho.\end{aligned}$$

Accordingly, the result follows from considering $\rho \to 0$.

Now, after we have collected the necessary ingredients, we are in a position to prove our main result.

Proof of Theorem 2. In order to show the theorem it is sufficient to find an upper bound of $U(W_\rho)$ which tends to one when ρ approximates zero. Since

$$\begin{aligned}U(W_\rho) = &\frac{\sum_{k=0}^{\infty}\left((2k+1)\,e^{-2k(k+1)\rho} + 2k\,e^{-2k^2\rho}\right)}{\left(2\sum_{k=1}^{\infty} k\,e^{-2k^2\rho}\right)^2} \\ &\times \sum_{k=0}^{\infty}\left((2k+1)\,e^{-2k(k+1)\rho} - 2k\,e^{-2k^2\rho}\right)\cdot\frac{\sum_{k=1}^{\infty} k\,(k+1)\,(2k+1)\,e^{-2k(k+1)\rho}}{\sum_{k=0}^{\infty}(2k+1)\,e^{-2k(k+1)\rho}},\end{aligned}$$

we can now use the asymptotics established in Lemma 1 and Lemma 2. Simply note that for $\rho < 1$

$$\begin{aligned}&\frac{\sum_{k=0}^{\infty}\left((2k+1)\,e^{-2k(k+1)\rho} + 2k\,e^{-2k^2\rho}\right)}{\left(2\sum_{k=1}^{\infty} k\,e^{-2k^2\rho}\right)^2}\cdot\frac{\sum_{k=1}^{\infty} k\,(k+1)\,(2k+1)\,e^{-2k(k+1)\rho}}{\sum_{k=0}^{\infty}(2k+1)\,e^{-2k(k+1)\rho}} \\ &\quad\le \frac{1+\frac{1}{2\rho}+\frac{1}{\sqrt{\rho}}+2\left(\frac{1}{4\rho}+\frac{1}{2\,e\,\sqrt{\rho}}\right)}{\left(\frac{1}{2\rho}-\frac{1}{e\,\sqrt{\rho}}\right)^2}\cdot\frac{\frac{1}{4\rho^2}+\frac{3}{2\sqrt{2}\,\rho^{3/2}}}{1+\frac{1}{2\rho}-\frac{1}{\sqrt{\rho}}} \\ &\quad= \frac{2\,(3\sqrt{2\rho}+1)\,e\,\left(e\rho+(1+e)\sqrt{\rho}+e\right)}{\left(2\rho-2\sqrt{\rho}+1\right)(e-2\sqrt{\rho})^2} \\ &\quad< 2+504\sqrt{\rho}.\end{aligned}$$

Consequently, by Lemma 2,

$$U(W_\rho) \le \left(\frac{1}{2} + 42\sqrt{\rho} + 111\rho\right)\cdot(2+504\sqrt{\rho}) \le (1+336\sqrt{\rho}+77334\rho) \to 1,$$

which completes the proof.

Note that the order of convergence of $U(W_\rho) - 1$ is indeed $\sqrt{\rho}$. However, the constants given here are in no way best possible.

References

[1] W. Freeden, T. Gervens, and M. Schreiner, "Constructive Approximation on the Sphere", Clarendon Press, Oxford, 1998.

[2] F. J. Narcowich and J. D. Ward, Nonstationary wavelets on the m-sphere for scattered data, *Appl. Comput. Harmon. Anal.* **3**, 4 (1996), 324–336.

[3] N. Laín Fernández, Optimal space-localized polynomials on the sphere, in preparation.

Noemí Laín Fernández

Institute of Mathematics
University of Lübeck
Wallstraße 40
D-23560 Lübeck
GERMANY
E-mail: fernande@math.uni-luebeck.de

Jürgen Prestin

Institute of Mathematics
University of Lübeck
Wallstraße 40
D-23560 Lübeck
GERMANY
E-mail: prestin@math.uni-luebeck.de