Zeitschrift für Analysis und ihre Anwendungen
Journal for Analysis and its Applications
Volume 15 (1996), No. 4, 1015–1023

On the Uncertainty Principle for Positive Definite Densities

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Abstract. The products of variances of adjoint positive definite densities have a greatest lower bound Λ. We improve the known estimates of Λ showing $0.527 < \Lambda \leq 0.8609\ldots$.

Keywords: *Uncertainty principle, positive definite probability density*

AMS subject classification: 60 E 10, 60 E 99

1. Introduction

Recall that a function $p : \mathbb{R} \to \mathbb{C}$ is called *positive definite* if

$$\sum_{i=1}^{n}\sum_{j=1}^{n} p(x_j - x_i)\, c_i \bar{c_j} \geq 0$$

for all $x_i \in \mathbb{R}$ and $c_i \in \mathbb{C}$ $(i = 1, \ldots, n)$ and for each $n \in \mathbb{N}$. In the sequel, when writing a positive definite density, we mean a density that is positive definite and continuous. The density of the normal distribution with mean zero and variance σ^2 is an example of a positive definite density.

By Bochner's Theorem (see [4: Theorem 1.9.6]) we know that a function f is a characteristic function if and only if f is positive definite, continuous and $f(0) = 1$. Now let p be a positive definite probability density. Then its characteristic function f is integrable and non-negative (see [4: Theorem 1.9.8]). Therefore the function

$$\tilde{p}(x) = \left(\int_{-\infty}^{+\infty} f(x)\, dx \right)^{-1} f(x) \qquad (x \in \mathbb{R})$$

is also a positive definite density. It is called the *adjoint* density of p. A density p is said to be *selfadjoint* if $f = \sqrt{2\pi} p$. Note that p is selfadjoint if and only if $p = \tilde{p}$.

Denoting by σ^2 and $\tilde{\sigma}^2$ the variances of p and $\tilde{p}$, respectively, the product $\sigma^2\tilde{\sigma}^2$ cannot be arbitrarily small. This fact is closely related to the uncertainty principles investigated in harmonic analysis and physics (see [1]). Roughly speaking, it is impossible for a non-zero function and its Fourier transform to be simultaneously very small.

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ISSN 0232-2064 / \$ 2.50

We denote by Λ the greatest lower bound for all products of variances $\sigma^2\tilde{\sigma}^2$ of adjoint densities. It is known that $0.454 < \Lambda < 0.8907$. The lower bound can be found in [3: p. 365] and the upper bound in [2: Resultat 3.12]. From [2: Satz 3.7] it is also known that there is a selfadjoint positive definite density such that its product of variances is $\sigma^4 = \Lambda$. In this note we will improve the lower and upper estimates for Λ showing $0.527 < \Lambda \leq 0.8609\ldots$.

2. The upper estimate for Λ

In this section we give an upper estimation for Λ by considering special selfadjoint densities. These densities are of the form

$$\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \sum_{k=0}^{n} a_k \frac{(2k)!}{(4k)!} H_{4k}(x) \qquad (n \geq 0)$$

where the H_k are Hermite polynomials defined by

$$H_k(x) = (-1)^k e^{x^2} \frac{d^k}{dx^k}(e^{-x^2}) \qquad (k \geq 0).$$

Note that every selfadjoint density p satisfying $\int_{-\infty}^{+\infty} |x| p(x)\, dx < \infty$ has the form

$$p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \sum_{k=0}^{\infty} a_k \frac{(2k)!}{(4k)!} H_{4k}(x)$$

with pointwise convergence (see [2: Satz 1.13]). If the conditions

$$\sum_{k=0}^{n} a_k = 1 \tag{1}$$

and

$$\sum_{k=0}^{n} a_k \frac{(2k)!}{(4k)!} H_{4k}(x) \geq 0 \qquad (x \in \mathbb{R}) \tag{2}$$

are satisfied, then

$$p_n(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \sum_{k=0}^{n} a_k \frac{(2k)!}{(4k)!} H_{4k}(x) \qquad (n \geq 0)$$

is a selfadjoint density. This can be proved using the equality

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-itx} e^{-\frac{x^2}{2}} H_k(x)\, dx = i^k e^{-\frac{t^2}{2}} H_k(t) \qquad (t \in \mathbb{R};\ k \geq 0)$$

(see [5: Theorem 57]). The variance of this density is given by $1 + 8\sum_{k=1}^{n} k\, a_k$ (see [2: p. 49]). Hence the product of variances, denoted by λ_n, is

$$\lambda_n(a_1, \dots, a_n) = \left(1 + 8\sum_{k=1}^{n} k\, a_k\right)^2 \qquad (n \geq 1).$$

We search for coefficents $a_0, \dots, a_n$ such that the conditions (1) and (2) are satisfied and the product of variances is as low as possible. Because the coefficient of x^n in the Hermite polynomial H_n is positive condition (2) implies that a_n is non-negative. If the product of variances is lower than 1, then at least one a_k $(k = 1, \dots, n-1)$ is negative. Therefore we consider the case $n \geq 2$. Obviously the conditions (1) and (2) are equivalent to the conditions

$$1 + \sum_{k=1}^{n} G_{4k}(x)\, a_k \geq 0 \qquad (n \geq 2) \tag{3}$$

where

$$G_{4k}(x) = \frac{(2k)!}{(4k)!} H_{4k}(x) - 1 \qquad (x \in \mathbb{R};\ k \geq 1)$$

and

$$a_0 = 1 - \sum_{k=1}^{n} a_k \qquad (n \geq 2).$$

The product of variances is minimal if and only if the value $c_n = \sum_{k=1}^{n} k\, a_k$ is minimal. So we search for a point $\tilde{\mathrm{a}} \in \mathbb{R}^n$ such that

$$\tilde{\mathrm{a}} \in P_n = \left\{ \mathrm{a} \in \mathbb{R}^n \,\middle|\, a_1 \geq -\sum_{k=2}^{n} \frac{G_{4k}(x)}{G_4(x)}\, a_k - \frac{1}{G_4(x)} \quad (x > \sqrt{3}) \right\}$$

$$\tilde{\mathrm{a}} \in \tilde{P}_n = \left\{ \mathrm{a} \in \mathbb{R}^n \,\middle|\, a_1 \leq -\sum_{k=2}^{n} \frac{G_{4k}(x)}{G_4(x)}\, a_k - \frac{1}{G_4(x)} \quad (0 < x < \sqrt{3}) \right\}$$

and

$$\sum_{k=1}^{n} k\, \tilde{a}_k \longrightarrow \min.$$

Note that the function G_4 has its only zero in $(0, +\infty)$ at $\sqrt{3}$.

Now we consider the case $n = 2$.

Theorem 2.1. *There are coefficents $\tilde{a}_0, \tilde{a}_1$ and $\tilde{a}_2$ such that the conditions* (1) *and* (2) *are satisfied and*

$$\lambda_2(\tilde{a}_1, \tilde{a}_2) = \min_{(a_1, a_2) \in P_2 \cap \tilde{P}_2} \lambda_2(a_1, a_2) = 0.8609\dots$$

holds.

Proof. First we minimize $c_2 = a_1 + 2a_2$ in the set P_2. For each $x \in (\sqrt{3}, +\infty)$

$$u = -\frac{G_8(x)}{G_4(x)} v - \frac{1}{G_4(x)}$$

is a straight line in the Cartesian coordinate system (v, u). In the sequel we exchange the coordinates writing (u, v). A point (a_1, a_2) is in the set P_2 if it is above all lines of the form

$$u = -\frac{G_8(x)}{G_4(x)} v - \frac{1}{G_4(x)} \qquad (x > \sqrt{3}). \tag{4}$$

In the line $a_1 = -2a_2 + c_2$ the value c_2 is to minimize. We shift this line downwards within the set P_2. So the line $a_1 = -2a_2 + c_2$ is one of the lines which limit the set P_2, that is there is an $x_s \in (\sqrt{3}, +\infty)$ such that the corresponding line (4) has the slope -2. We denote the obtained point by $(\tilde{a}_1, \tilde{a}_2)$. First we calculate the product of variances $\lambda_2(\tilde{a}_1, \tilde{a}_2)$. Then we prove that the point $(\tilde{a}_1, \tilde{a}_2)$ is in the sets $\tilde{P}_2$ and P_2. Last we show that the obtained product of variances is minimal.

The equation

$$-2 = -\frac{G_8(x_s)}{G_4(x_s)} \qquad (x_s > \sqrt{3}) \tag{5}$$

holds. We obtain

$$x_{s,1} = \sqrt{7 - \sqrt{14}} \qquad \text{and} \qquad x_{s,2} = \sqrt{7 + \sqrt{14}}.$$

Moreover,

$$-\frac{1}{G_4(x_{s,1})} = -0.890981\ldots \qquad \text{and} \qquad -\frac{1}{G_4(x_{s,2})} = -0.00901895\ldots .$$

Because of the definition of the set P_2, $x_{s,2} = \sqrt{7 + \sqrt{14}}$ is a solution of equation (5). Therefore

$$\tilde{c}_2 := -\frac{1}{G_4(x_{s,2})} = -0.00901895\ldots .$$

For the product of variances we obtain

$$\lambda_2(\tilde{a}_1, \tilde{a}_2) = (1 + 8\tilde{c}_2)^2 = 0.860903\ldots$$

and for the point $\tilde{a}$

$$\tilde{a}_1 = -2\tilde{a}_2 + \tilde{c}_2 = -\frac{G_8(x_{s,2})}{G_4(x_{s,2})} \tilde{a}_2 - \frac{1}{G_4(x_{s,2})}.$$

In view of the above consideration we can suppose that $\tilde{a}_1 < 0$ and $\tilde{a}_2 > 0$. Since $-\frac{G_8}{G_4} > -2$ and $-\frac{1}{G_4} > 0$ on $(0, \sqrt{3})$, we see that

$$\tilde{a}_1 = -2\tilde{a}_2 + \tilde{c}_2 < -\frac{G_8(x)}{G_4(x)}\tilde{a}_2 - \frac{1}{G_4(x)} \qquad (x \in (0, \sqrt{3}))$$

and therefore $\tilde{\mathbf{a}} \in \tilde{P}_2$.

Now we prove that $\tilde{\mathbf{a}} \in P_2$. We show that

$$\tilde{a}_1 = \max_{x>\sqrt{3}} \left(-\frac{G_8(x)}{G_4(x)} \tilde{a}_2 - \frac{1}{G_4(x)} \right).$$

First the functions $-\frac{1}{G_4}$ and $-\frac{G_8}{G_4}$ are considered on the intervall $(\sqrt{3}, +\infty)$. They have the following properties: $-\frac{1}{G_4} < 0$, $-(\frac{1}{G_4})' > 0$, $-(\frac{1}{G_4})'' < 0$, $-(\frac{G_8}{G_4})'$ is strictly decreasing, and there is an $x_0 \in (2,3)$ with $-(\frac{G_8(x_0)}{G_4(x_0)})' = 0$. Up to now it was sufficient to know that $\tilde{a}_1 = -2\tilde{a}_2 + \tilde{c}_2$. Next we show that the coordinate $\tilde{a}_2$ has the value

$$\tilde{a}_2 = -\left(-\frac{1}{G_4(x_{s,2})} \right)' \Big/ \left(-\frac{G_8(x_{s,2})}{G_4(x_{s,2}} \right)'.$$

Obviously $x_{s,2} \doteq 3.2774\ldots > x_0$. Therefore $\tilde{a}_2 > 0$ and the function $-\frac{G_8}{G_4}\tilde{a}_2 - \frac{1}{G_4}$ has a local maximum at $x_{s,2}$. Now we suppose that there is another extremum at $x_w \neq x_{s,2}$. So

$$\tilde{a}_2 = -\left(-\frac{1}{G_4(x_w)} \right)' \Big/ \left(-\frac{G_8(x_w)}{G_4(x_w)} \right)'$$

follows. It is clear that also x_w must be greater than x_0. Furthermore the derivative of the function $-(-\frac{1}{G_4})'/(-\frac{G_8}{G_4})'$ must have a zero x_d between x_w and $x_{s,2}$. Hence

$$\left(-\frac{1}{G_4(x_d)} \right)'' \left(-\frac{G_8(x_d)}{G_4(x_d)} \right)' = \left(-\frac{1}{G_4(x_d)} \right)' \left(-\frac{G_8(x_d)}{G_4(x_d)} \right)''$$

but this is not possible because the left side is positive and the right side is negative on the interval $(x_0, +\infty)$. Applying

$$\lim_{x \downarrow \sqrt{3}} \left(-\frac{G_8(x)}{G_4(x)} \tilde{a}_2 - \frac{1}{G_4(x)} \right) = \lim_{x \to \infty} \left(-\frac{G_8(x)}{G_4(x)} \tilde{a}_2 - \frac{1}{G_4(x)} \right) = -\infty$$

it follows that

$$\tilde{a}_1 = -\frac{G_8(x_{s,2})}{G_4(x_{s,2})} \tilde{a}_2 - \frac{1}{G_4(x_{s,2})} = \max_{x>\sqrt{3}} \left(-\frac{G_8(x)}{G_4(x)} \tilde{a}_2 - \frac{1}{G_4(x)} \right)$$

and also $\tilde{\mathbf{a}} \in P_2$. [1)] Obviously the point $\tilde{\mathbf{a}}$ is in the boundary ∂P_2 of the set P_2. So the product of variances is minimal.

Now we have found a point $\tilde{\mathbf{a}} \in \partial P_2 \cap \tilde{P}_2$, that is, $\tilde{\mathbf{a}}$ satisfies condition (3). Hence

$$p_2(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \sum_{k=0}^{2} a_k \frac{(2k)!}{(4k)!} H_{4k}(x)$$

with coeffients $a_0 = 1 - \tilde{a}_1 - \tilde{a}_2$, $a_1 = \tilde{a}_1$ and $a_2 = \tilde{a}_2$ is a selfadjoint positive definite density with product of variances

$$\lambda_2(\tilde{a}_1, \tilde{a}_2) = \min_{(a_1,a_2) \in P_2 \cap \tilde{P}_2} \lambda_2(a_1, a_2) = 0.8609\ldots .$$

Thus the assertion is proved ∎

Collorary 2.2. *The inequality* $\Lambda \leq 0.8609\ldots$ *holds.*

[1)] We note that $\tilde{a}_1 = -0.0123976\ldots$ and $\tilde{a}_2 = 0.0016893\ldots$.

3. The lower estimate for Λ

In this section we give a lower estimation for Λ. First we prove that the set of all products of variances is an interval.

Lemma 3.1. *The set of all products of variances $\sigma^2\tilde{\sigma}^2$ of adjoint positive definite densities is the interval $[\Lambda, +\infty)$.*

Proof. Let $(p_1, \tilde{p_1})$ and $(p_2, \tilde{p_2})$ be pairs of adjoint positive definite densities with products of variances $\lambda_1 = \sigma_1^2\tilde{\sigma_1}^2$ and $\lambda_2 = \sigma_2^2\tilde{\sigma_2}^2$, and for $\beta \in [0,1]$ let p be the positive definite density given by

$$p(x) = \beta\, p_1(x) + (1-\beta)\, p_2(x) \qquad (x \in \mathbb{R}).$$

We denote the variance of p by σ^2, the characteristic function by f and the variance of the adjoint positive definite density $\tilde{p}$ by $\tilde{\sigma}^2$. We have $\sigma^2 = \beta\,\sigma_1^2 + (1-\beta)\,\sigma_2^2$ and

$$\tilde{\sigma}^2 = \frac{\int t^2 f(t)\,dt}{\int f(t)\,dt} = \frac{\dfrac{\beta}{\tilde{p}_1(0)}\,\tilde{\sigma_1}^2 + \dfrac{1-\beta}{\tilde{p}_2(0)}\,\tilde{\sigma_2}^2}{\dfrac{1}{\tilde{p}(0)}}.$$

Hence

$$\lambda(\beta) := \sigma^2\tilde{\sigma}^2 = \frac{\left(\beta\,\sigma_1^2 + (1-\beta)\,\sigma_2^2\right)\left(\dfrac{\beta}{\tilde{p}_1(0)}\,\tilde{\sigma_1}^2 + \dfrac{1-\beta}{\tilde{p}_2(0)}\,\tilde{\sigma_2}^2\right)}{\dfrac{1}{\tilde{p}(0)}}.$$

Since λ is a continuous function of β, and since $\lambda(0) = \lambda_2$ and $\lambda(1) = \lambda_1$ we see that the set of products of variances is an interval I. By [2: Satz 3.7] Λ is the lower end point of the interval I.

To show that the product of variances can be arbitrarily large we give a simple example. Let p_ϕ be the density of the standard normal distribution. Then the characteristic function f_ϕ is given by $f_\phi(t) = e^{-\frac{t^2}{2}}$, and the variance is $\sigma_\phi^2 = 1$. We define for $y \geq 0$ a new density by

$$p(x) = \frac{1}{2}\,p_\phi(x) + \frac{1}{4}\left(p_\phi(x-y) + p_\phi(x+y)\right).$$

The characteristic function is given by

$$f(t) = \frac{1}{2}(1 + \cos yt)e^{-\frac{t^2}{2}}.$$

Since f is integrable and non-negative the density p is positive definite. Recall that the variance σ^2 of the density p is $-f''(0)$, where f is the corresponding characteristic function. Since the adjoint density $\tilde{p}$ of p is $\left(\int f(x)\,dx\right)^{-1} f$ the variance $\tilde{\sigma}^2$ of $\tilde{p}$ is given by $\tilde{\sigma}^2 = \left(\int x^2 f(x)\,dx\right) / \left(\int f(x)\,dx\right)$. We obtain for the product of variances λ of the adjoint densities p and $\tilde{p}$

$$\lambda(y) = \frac{-f''(0)\int t^2 f(t)\,dt}{\int f(t)\,dt} = \frac{\left(\frac{1}{2}y^2 + 1\right)\left(e^{\frac{y^2}{2}} - y^2 + 1\right)}{e^{\frac{y^2}{2}} + 1}.$$

Since $\lim_{y\to\infty} \lambda(y) = +\infty$ the set of products of variances is the interval $[\Lambda, +\infty)$ ∎

Now let p be a selfadjoint density with characteristic function f. Then

$$f(x) = \sqrt{2\pi}\, p(x). \tag{5}$$

We will use the inequality

$$f(x) > \cos\sigma x + 2J\left(\frac{x}{2}\right) \qquad \left(0 < |x\sigma| < \frac{\pi}{2}\right) \tag{6}$$

where

$$J(x) = \int_{-\infty}^{+\infty} (\cos tx - \cos\sigma x)^2 p(t)\, dt$$

(see [3: Satz 3/p. 348]).

Lemma 3.2. *The inequality*

$$J(x) > \frac{2}{\sqrt{2\pi}\sigma} \int_0^{\pi/2} \left(\cos\frac{xt}{\sigma} - \cos x\sigma\right)^2 \left(2J\left(\frac{t}{2\sigma}\right) + \cos t\right) dt \qquad (x \in \mathbb{R})$$

holds.

Proof. Applying (5) and (6) we obtain

$$\begin{aligned} J(x) &= \frac{2}{\sqrt{2\pi}} \int_0^{+\infty} (\cos xt - \cos\sigma x)^2 f(t)\, dt \\ &\geq \frac{2}{\sqrt{2\pi}} \int_0^{\pi/2\sigma} (\cos xt - \cos\sigma x)^2 f(t)\, dt \\ &> \frac{2}{\sqrt{2\pi}} \int_0^{\pi/2\sigma} (\cos xt - \cos\sigma x)^2 \left(2J\left(\frac{t}{2}\right) + \cos t\sigma\right) dt \end{aligned}$$

and the assertion is proved ∎

We define $J_0 = 0$ and

$$J_n(x) = \frac{2}{\sqrt{2\pi}\sigma} \int_0^{\pi/2} \left(\cos\frac{tx}{\sigma} - \cos\sigma x\right)^2 \left(2J_{n-1}\left(\frac{t}{2\sigma}\right) + \cos t\right) dt$$

for all $x \in \mathbb{R}$ and $n \geq 1$. It is clear that J and J_n $(n \geq 1)$ are strictly positive and that the inequalities

$$J > J_n \qquad (n \geq 0) \tag{7}$$

hold.

Lemma 3.3. *If σ^2 is the variance of a selfadjoint density, then*

$$F_n(\sigma) := \sigma^2 - \frac{\pi^2 - 8}{2\sqrt{2\pi\sigma^3}} - K_n(\sigma) > 0$$

where

$$K_n(\sigma) = \frac{4}{\sqrt{2\pi\sigma^3}} \int_0^{\pi/2} J_n\left(\frac{x}{2\sigma}\right) x^2\, dx \qquad (n \geq 0).$$

Proof. Applying (5) - (7) we obtain

$$\begin{aligned}
\sigma^2 &= \int_{-\infty}^{+\infty} x^2 p(x)\, dx \\
&\geq \frac{2}{\sqrt{2\pi\sigma^3}} \int_0^{\pi/2} x^2 f\left(\frac{x}{\sigma}\right) dx \\
&> \frac{2}{\sqrt{2\pi\sigma^3}} \int_0^{\pi/2} x^2 \cos x\, dx + \frac{4}{\sqrt{2\pi\sigma^3}} \int_0^{\pi/2} J\left(\frac{x}{2\sigma}\right) x^2\, dx \\
&= \frac{\pi^2 - 8}{2\sqrt{2\pi\sigma^3}} + \frac{4}{\sqrt{2\pi\sigma^3}} \int_0^{\pi/2} J\left(\frac{x}{2\sigma}\right) x^2\, dx \\
&> \frac{\pi^2 - 8}{2\sqrt{2\pi\sigma^3}} + K_n(\sigma) \quad (n \geq 0)
\end{aligned}$$

and the assertion is proved ∎

Theorem 3.4. *The inequality $\Lambda > 0.5276\ldots$ holds.*

Proof. From [3: Satz 5/p. 364] we know that if p and $\tilde{p}$ are adjoint densities with product of variances λ, then there is a selfadjoint density with the same product of variances. Therefore it is sufficient to consider only selfadjoint desities. By Lemma 3.3, the inequalities $F_n(\sigma) > 0$ $(n \geq 0)$ hold for σ if σ^2 is the variance of a selfadjoint density. Hence σ^4 cannot be contained in the interval $[\Lambda, +\infty)$ if $F_n(\sigma) \leq 0$. We computed the following values with the program Mathematica:

n	σ	$F_n(\sigma)$	σ^4
0	0.8207	−0.0010983517...	0.453667568...
1	0.8464	−0.0012940136...	0.513218873...
2	0.8511	−0.0011355911...	0.524713649...
3	0.852	−0.0015642939...	0.526936617...
4	0.8523	−0.0011071585...	0.527679173...

Hence $\Lambda > 0.5276\ldots$ ∎

Acknowledgement. The author's research is sponsored by Claussen- Stiftung. The author would also like to acknowledge helpful discussions with Prof. Zoltán Sasvári and Dr. Matthias Weber.

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Received 08.02.1996