Splines with Free Knots, the Heat Equation, and the Gauß Transform

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ABSTRACT. The Gauß (or Weierstraß) transform has applications in many fields of applied mathematics. One of its most important properties within approximation theory is the fact that it maps weak Chebychev spaces onto Chebychev spaces. The aim of this paper is twofold. First, after proving some elementary invariance properties of the Gauß transform, necessary and sufficient conditions for best approximation by (Gauß transformed) free knot spline spaces are given. Then, in Section 3, we develop a method for the numerical solution of an initial value problem for the heat equation. The present paper can be viewed as a continuation of two recent publications by Meinardus [5,6].

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1. INTRODUCTION AND PRELIMINARIES

This paper investigates some properties of the *Gauß transform*, defined, for each bounded function $h \in C(\mathbb{R})$, as the mapping

$$h \rightarrow G(h)(x,t) := \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} h(\tau) \cdot \mathrm{e}^{-\frac{(\tau - x)^2}{4t}} \, d\tau , \tag{1.1}$$

with real positive parameter t. This transform has applications in various fields of applied analysis, e.g. probability theory, PDEs, and approximation theory. It is well-known that the image function satisfies the *heat equation*, i.e.,

$$\frac{\partial^2}{\partial x^2} G(h)(x,t) = \frac{\partial}{\partial t} G(h)(x,t) \tag{1.2}$$

for all $x \in \mathbb{R}$ and $t > 0$, and,

$$\lim_{\substack{t \to 0 \\ t > 0}} G(h)(x,t) = h(x) \tag{1.3}$$

for all $x \in \mathbb{R}$.

Recently, Meinardus [5,6] proved some nice results concerning the Gauß transform and its use within constructive approximation. The aim of the present paper is to continue these investigations. We concentrate mainly on best approximation by spline functions with free knots (Section 2), and on the numerical solution of an inital value problem for the heat equation (Section 3).

We first recall some facts from approximation theory which will be needed later. A $k-$ dimensional subspace V of $C[a,b]$ is called a *Chebychev space*, if every nontrivial function $v \in V$ has at most $(k-1)$ zeros in $[a,b]$. The best Chebychev approximation w.r.t. such spaces always exists, is (strongly) unique, and can be computed by the Remez algorithm.

On the other hand, one of the most prominent approximation spaces is that of splines, and spline spaces are *not* Chebychev in general, but "only" weak Chebychev spaces. A $k-$ dimensional subspace W of $C[a,b]$ is called a *weak Chebychev space,* if every nontrivial function $w \in W$ has at most $(k-1)$ sign changes in $[a,b]$. The numerical computation of best approximations becomes much more complicated in weak Chebychev spaces, cf.Nürnberger [9].

Due to Jones & Karlovitz [1], a space $W = \text{span}\{w_1, \ldots, w_k\}$ is a weak Chebychev space if and only if there exists a sequence of Chebychev spaces $V_n = \text{span}\{v_{1,n}, \ldots, v_{k,n}\}$ such that

$$\lim_{n \to \infty} \|v_{i,n} - w_i\|_\infty = 0 \quad \text{for } i = 1, \ldots, k . \tag{1.4a}$$

One possibility to find the sequences $\{v_{i,n}\}$ is to set

$$v_{i,n}(x) \;:=\; G(w_i)(x, t_n) \tag{1.4b}$$

for each i, where $\{t_n\}$ is a sequence of numbers converging to zero. In particular, it follows from (1.4) that the Gauß transform provides an easy method to construct a sequence of Chebychev spaces, which come arbitarily close to a given weak Chebychev space.

Although this was known since many years, it seems that Meinardus in 1989 was the first one who succeeded in using this construction numerically, see [5,6]. In particular, it was shown that if one chooses a B-spline basis $\{B_i\}$ of the given spline space, then the Gauß transforms $\{G(B_i)\}$ of this basis, which span for all $t > 0$ a Chebychev space, can be computed by an easy recursion formula. This was used, among other things, to establish an algorithm for best approximation by fixed knot splines in the following way: Compute, using the Remez algorithm, the best approximation $\sum a_i G(B_i)$ w.r.t. the Chebychev space $\operatorname{span}\{G(B_i)\}$. Then, take the spline function $\sum a_i B_i$ as (nearly) best spline approximation; see [5,6,11] for details. A large number of numerical results in [11] illustrate the efficiency of this algorithm.

A first obvious generalization of this approach would be to consider best approximation by *non-polynomial* spline spaces. However, we think that the theoretical insight of such investigations would not be too big, and so we concentrate on the two other aspects mentioned above.

We close this introductory section with the following theorem, which collects some invariance properties of the Gauß transform.

Theorem 1.1: *a) If the function h is nonnegative everywhere, then so is $G(h)$.*
b) If $\{h_\nu\}$ is a set of functions such that

$$\sum_\nu h_\nu(x) \;\equiv\; 1 \;\;\forall\, x \in I\!R,$$

then

$$\sum_\nu G(h_\nu)(x,t) \;\equiv\; 1 \;\;\forall\, x \in I\!R \text{ and } t > 0.$$

c) If h is periodic with period p, then $G(h)$, considered as a function of x, is periodic with period p.
d) If h is odd (resp. even), then $G(h)$, considered as a function of x, is odd (resp. even).
e) If h is a polynomial of degree n, then $G(h)$, considered as a function of x, is a polynomial of degree n, i.e., the Gauß transform maps the space Π_n of polynomials of degree n onto itself.

Proof. Statement a) is obvious from the definition of the Gauß transform. To prove b), we use the fact that

$$\frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(\tau-x)^2}{4t}} \, d\tau \;=\; \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-z^2} \, dz \;=\; 1 \, ,$$

and obtain

$$\begin{aligned} 1 \;&=\; \frac{1}{\sqrt{4\pi t}} \int\limits_{-\infty}^{\infty} \sum_{\nu} h_\nu(\tau) \cdot e^{-\frac{(\tau-x)^2}{4t}} \, d\tau \\ &=\; \sum_{\nu} \frac{1}{\sqrt{4\pi t}} \int\limits_{-\infty}^{\infty} h_\nu(\tau) \cdot e^{-\frac{(\tau-x)^2}{4t}} \, d\tau \;=\; \sum_{\nu} G(h_\nu)(x,t) \, . \end{aligned}$$

Statements c) and d) can be verified by straightforward calculations, so we are left to prove e). Do to linearity, it suffices to do this for a basis of Π_n , say $\{1, x, \cdots, x^n\}$, so let $h(x) := x^j$, $j \in \{0, \ldots, n\}$. Then

$$\begin{aligned} G(h) \;&=\; \frac{1}{\sqrt{4\pi t}} \int\limits_{-\infty}^{\infty} \tau^j \cdot e^{-\frac{(\tau-x)^2}{4t}} \, d\tau \\ &=\; \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{\infty} (x + 2z\sqrt{t})^j \cdot e^{-z^2} \, dz \, , \end{aligned}$$

which is a polynomial of degree j in x . This completes the proof of Theorem 1.1. □

These properties show that the Gauß transform carries over a lot of nice properties of the spaces to be transformed and therefore, as mentioned at the beginning, possesses widespread applications. As a first example, think of curve design problems, where the *convex hull property* is needed; statements a) and b) imply that the Gauß transform preserves this property. Another implication is derived from statement c), namely the fact that the Gauß transform maps the space of periodic splines onto a periodic space.

2. APPROXIMATION BY SPLINES WITH FREE KNOTS

In this section, we investigate best approximation by splines with free knots. These are non-linear approximation problems, and characterizations of best approximations cannot be given in general, see e.g. [2,9]. In the following, it will be shown that the Gauß transform can be used to derive necessary and sufficient conditions, which in some cases coincide and thus provide a characterization.

We first need a result on the tangent space of the Gauß transform. Let Φ denote a set of functions, which depend on a parameter vector $a = (a_1, \ldots, a_l) \in I\!R^l$. Then, for each $\varphi \in \Phi$, the *tangent space* of φ is defined as

$$T(\varphi) \;:=\; \operatorname{span}\left\{ \tfrac{\partial}{\partial a_1}\varphi(\,\cdot\,,a), \ldots, \tfrac{\partial}{\partial a_l}\varphi(\,\cdot\,,a) \right\}, \tag{2.1}$$

provided that these derivatives exist.

Theorem 2.1: *Let $\varphi = \varphi(\,\cdot\,,a) \in \Phi$ depend continuously differentiable on the parameter a. Then*

$$G(T(\varphi)) \;=\; T(G(\varphi)), \tag{2.2}$$

i.e., the Gauß transform of the tangent space of φ is identical with the tangent space of the Gauß transform of φ.

Proof. First, we consider for arbitrary index $j \in \{1, \ldots, l\}$, one single partial derivative

$$\tfrac{\partial}{\partial a_j}\varphi(\,\cdot\,,a).$$

It follows that

$$\begin{aligned} G\left(\tfrac{\partial}{\partial a_j}\varphi(\,\cdot\,,a)\right) &= \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \tfrac{\partial}{\partial a_j}\varphi(\,\cdot\,,a) \cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \\ &= \frac{\partial}{\partial a_j} \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \varphi(\,\cdot\,,a) \cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \\ &= \tfrac{\partial}{\partial a_j} G(\varphi(\,\cdot\,,a)), \end{aligned} \tag{2.3}$$

since $\frac{\partial}{\partial a_j}\varphi(\,\cdot\,,a)$ is a continuous function.

Let now σ be an arbitrary element of the tangent space $T(G(\varphi))$. Then there exist coefficients $\gamma_1, \ldots, \gamma_l$, such that

$$\begin{aligned} \sigma &= \sum_{j=1}^{l} \gamma_j \tfrac{\partial}{\partial a_j} G(\varphi(\,\cdot\,,a)) \\ &= \sum_{j=1}^{l} \gamma_j\, G\left(\tfrac{\partial}{\partial a_j}\varphi(\,\cdot\,,a)\right) \;=\; G\left(\sum_{j=1}^{l} \gamma_j \tfrac{\partial}{\partial a_j}\varphi(\,\cdot\,,a)\right), \end{aligned}$$

where we have used (2.3), and thus $\sigma \in G(T(\varphi))$ The inclusion $G(T(\varphi)) \subset T(G(\varphi))$ follows in the same way. $\square$

We now investigate a classical approximation problem, introduced by and usually named after Schoenberg [2], which involves one single B-spline with free knots. Let $\mathcal{B}_m$ denote the set of all B-splines B_m of order m with multiple knots, normalized by

$$\int_{-\infty}^{\infty} B_m(t)\, dt \;=\; 1\,. \tag{2.4}$$

Then, given some Polya frequency function f, we look for a B-spline $B^*_m \in \mathcal{B}_m$, such that

$$\max_{x\in I\!R} \left| \int_{-\infty}^{x} f(\xi)\, d\xi \;-\; \int_{-\infty}^{x} B^*_m(\xi)\, d\xi \right| \;\le\; \max_{x\in I\!R} \left| \int_{-\infty}^{x} f(\xi)\, d\xi \;-\; \int_{-\infty}^{x} B_m(\xi)\, d\xi \right| \tag{2.5}$$

for all $B_m \in \mathcal{B}_m$. If (2.5) holds, we say that B^* is a best approximation of f *in the sense of Schoenberg.* The following sufficient condition for best approximations in this sense was given by Kaiser [2]:

Theorem 2.2: *If the difference function*

$$e(x) \;:=\; \int_{-\infty}^{x} f(\xi)\, d\xi \;-\; \int_{-\infty}^{x} B^*_m(\xi)\, d\xi \tag{2.6}$$

possesses at least $m+2$ *alternating extreme points, then* B^*_m *is a best approximation of* f *in the sense of Schoenberg.*

Establishing necessary conditions and therefore characterizations is difficult. We attack this problem via the Gauß transform, since its tangent space will turn out to be a Chebychev space. It follows from (1.3) that the solution of a best approximation problem in the transformed space for small values of t yields also a good approximation in the original, i.e., the spline space (cf. [5,6,11]).

We need some more detailed notation: Let

$$B_m\left(x \,\middle|\, \begin{matrix} x_0 & x_1 & \cdots\cdots & x_k \\ \rho_0 & \rho_1 & \cdots\cdots & \rho_k \end{matrix} \right) \tag{2.7}$$

denote the B-spline from $\mathcal{B}_m$ with knots $x_0 < x_1 < \cdots < x_k$ of respective multiplicity $\rho_0, \ldots, \rho_k$, where $\rho_0 + \rho_1 + \cdots + \rho_k = m+1$. Moreover, by $\Phi(f)$, we denote the Gauß transform of the function $\int_{-\infty}^{x} f(\xi) d\xi$, i.e.,

$$\Phi(f)(x,t) \;:=\; \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \int_{-\infty}^{\tau} f(\xi) d\xi \cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \tag{2.8}$$

and, analogously, for $B_m \in \mathcal{B}_m$,

$$\Phi(B_m)(x,t) \;:=\; \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \int_{-\infty}^{\tau} B_m\left(\xi \,\middle|\, \begin{matrix} x_0 & x_1 & \cdots\cdots & x_k \\ \rho_0 & \rho_1 & \cdots\cdots & \rho_k \end{matrix}\right) d\xi \cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau\,. \quad (2.9)$$

The approximation problem consists now in finding, for given f , a B-spline $B_m^* \in \mathcal{B}_m$ (i.e., a set of knots and respective multiplicities), such that the image function $\Phi(B_m^*)$ is a best approximation of $\Phi(f)$.

Theorem 2.3: *For given Polya frequency function f we define, for fixed t , the difference function E as*

$$E(x,t) \;:=\; \Phi(f)(x,t) - \Phi(B_m)(x,t)\,.$$

Then the following statements hold:
(i) If E has at least $m+2$ alternating extreme points, then $\Phi(B_m)$ is a best approximation of $\Phi(f)$.
(ii) If $\Phi(B_m)$ is a best approximation of $\Phi(f)$, then E has at least $k+2$ alternating extreme points.

Corollary 2.4: *If all knots of B_m are simple, then $\Phi(B_m)$ is a best approximation of $\Phi(f)$ if and only if E has $m+2$ alternating extreme points.*

Proof of Theorem 2.3. We first proof *(i)*. Assume that there is a better approximation, say $\Phi(\widetilde{B}_m)$ with knots $\widetilde{x}_\nu$ and error function $\widetilde{E}$. Then there is a sign $\sigma \in \{-1,1\}$ such that

$$\begin{aligned} &\sigma \cdot (-1)^j \cdot (E(\eta_j) - \widetilde{E}(\eta_j)) \\ &\qquad = \sigma \cdot (-1)^{j+1} \cdot (T(\eta_j) - \widetilde{T}(\eta_j)) \;<\; 0 \end{aligned} \quad (2.10)$$

for $j = 1, \ldots, m+2$, where $\{\eta_j\}$ is the set of alternating extreme points of E .

This implies that the function

$$T \;-\; \widetilde{T} \quad \text{has at least } m+1 \text{ zeros (with sign changes)} \quad (2.11)$$

in the interval (η_1, η_{m+2}) .

$T - \widetilde{T}$ is the Gauß transform of the function

$$d(x) \;:=\; \int_{-\infty}^{x} \widetilde{B}_m(\xi)\, d\xi \;-\; \int_{-\infty}^{x} B_m(\xi)\, d\xi\,. \quad (2.12)$$

Since the kernel function $\mathrm{e}^{-\frac{(x-\tau)^2}{4t}}$ is totally positive, it follows that the Gauß transformation is variation diminishing (cf. [3]), and so, from (2.11), that d has at least $m+1$ zeros in (η_1, η_{m+2}). Moreover, due to the finite-support property of the B-splines, there are two additional zeros of d in $\alpha := \min\{x_0, \widetilde{x}_0\}$ and $\beta := \max\{x_k, \widetilde{x}_k\}$, such that d has a total of $m+3$ zeros in the interval $[\alpha, \beta]$.

Since d is a (continuous) spline function, Rolle's theorem for splines implies that the derivative $d'(x) = \widetilde{B}_m(x) - B_m(x)$ has at least $m+2$ zeros, which is not possible (cf. e.g. [2]). This contradiction proves statement *(i)*.

To show *(ii)*, we use the following result (cf. [2]), which can be proved by straightforward calculations, using the well-known contour-integral representation of B-splines (cf. e.g. [2,7]): The tangent space of the function

$$\int_{-\infty}^{x} B_m\left(\xi \,\middle|\, \begin{matrix} x_0 & x_1 & \cdots\cdots & x_k \\ \rho_0 & \rho_1 & \cdots\cdots & \rho_k \end{matrix}\right) d\xi \tag{2.13}$$

is the $(k+1)$-dimensional spline space

$$\operatorname{span}\left\{B_{m+1}\left(x \,\middle|\, \begin{matrix} x_0 & \cdots & x_j & \cdots & x_k \\ \rho_0 & \cdots & \rho_j+1 & \cdots & \rho_k \end{matrix}\right), j=0,\ldots,k\right\}. \tag{2.14}$$

Since the function $\Phi(B_m)$ is the Gauß transform of the function in (2.13), it follows from Theorem 2.1 that the tangent space of the functions $\Phi(B_m)$ is the space

$$\Sigma := \operatorname{span}\left\{G\left(B_{m+1}\left(x \,\middle|\, \begin{matrix} x_0 & \cdots & x_j & \cdots & x_k \\ \rho_0 & \cdots & \rho_j+1 & \cdots & \rho_k \end{matrix}\right)\right), j=0,\ldots,k\right\}.$$

This is a $(k+1)$-dimensional Chebychev space, and thus the space of approximation functions (2.9) satisfies the local Haar condition (cf.[4]). This implies the existence of $(\dim \Sigma + 1)$ alternating extreme points of the best approximation, and so the proof of statement *(ii)* is complete. □

We can now also derive a necessary condition for the general problem of approximation by splines with free knots. On a given interval $[a, b]$, we consider the space

$$S_m\begin{pmatrix} x_1 & \cdots\cdots & x_r \\ \rho_1 & \cdots\cdots & \rho_r \end{pmatrix}$$

of splines of order m with fixed inner knots $x_1 < \cdots < x_r$ and corresponding multiplicities $\rho_1, \ldots \rho_r$. The dimension of this space is

$$\dim S_m = m + \sum_{j=1}^{r} \rho_j .$$

Moreover, by $S_{m,n}$ we denote the space of splines of order m with n free knots, i.e.

$$S_{m,n} = \bigcup_{\substack{r\in\{1,\ldots,n\} \\ x_1<\cdots<x_r \\ \rho_1+\cdots+\rho_r\le n}} S_m\begin{pmatrix} x_1 & \cdots\cdots & x_r \\ \rho_1 & \cdots\cdots & \rho_r \end{pmatrix}.$$

It is well-known [9,10] that the tangent space $T(s)$ for each $s \in S_{m,n}$ is the spline space with fixed knots

$$T(s) = S_m \begin{pmatrix} x_1 & \cdots\cdots & x_r \\ \rho_1 + 1 & \cdots\cdots & \rho_r + 1 \end{pmatrix}$$

of dimension

$$\dim T(s) = m + r + \sum_{j=1}^{r} \rho_j .$$

This means that we are in a situation very similar to that in the proof of Theorem 2.3, and so the following necessary condition for a best approximation can be proved by the same arguments as used in the second part of the proof above.

Theorem 2.5: *For given $f \in C[a,b]$ and arbitrary fixed $t > 0$, we consider best approximation w.r.t. the set Γ of Gauß transforms of the free knot spline space $S_{m,n}$, i.e.,*

$$\Gamma = \{g \in C[a,b] ; \; g(x) = G(s)(x,t) ; \; s \in S_{m,n}\} .$$

Then the following necessary condition holds: If $g \in \Gamma$ is a best approximation of f, then the difference function $(g-f)(x)$ has at least

$$m + r - 1 + \sum_{j=1}^{r} \rho_j$$

alternating extreme points in $[a,b]$.

3. NUMERICAL SOLUTION OF A HEAT EQUATION PROBLEM

In this section we consider the following initial-boundary value problem for the heat equation on the region

$$R := \{(x,t) \in \mathbb{R}^2 ; \; 0 < x < 1 , \, 0 < t < \infty\} :$$

Given a univariate function $f \in C[0,1]$ with zeros of order one at least in the points 0 and 1, find a function $u \in C^2(R) \cap C(\overline{R})$, which satisfies

$$u_t = x_{xx} \tag{3.1a}$$

everywhere in R, and takes the boundary values

$$u(x,0) = f(x) \quad \text{for} \quad 0 \le x \le 1 , \tag{3.1b}$$

and

$$u(0,1) = u(1,t) = 0 \quad \text{for} \quad 0 \le t < \infty . \tag{3.1c}$$

We define the function $\widehat{f} \in C(\mathbb{R})$ as the odd periodic continuation with period 2 of f to the real line, i.e., for each $\mu \in \mathbb{N}_0$,

$$\widehat{f}(x) := \begin{cases} f(x-2\mu), & \text{if } x \in [2\mu, 2\mu+1], \\ -f(2\mu+2-x), & \text{if } x \in [2\mu+1, 2\mu+2]. \end{cases} \tag{3.2}$$

Then, as it is well-known, a solution of the above problem is given by the Gauß transform of the function $\widehat{f}$, i.e.,

$$u(x,t) := G(\widehat{f})(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \widehat{f}(\tau) \cdot e^{-\frac{(\tau-x)^2}{4t}} \, d\tau \tag{3.3}$$

satisfies (3.1). However, in practice the problem arises that the integration in (3.3) may cause numerical problems, and so one would like to approximate the function $\widehat{f}$ (resp. f) first by another function, such that the integration in (3.3) can be replaced by an easier process.

This is an approximation problem with constraints: Given f and a suitable function class $B \subset C[0,1]$, determine a $b_f \in B$, such that

$$\|b_f - f\|_{[0,1]} \text{ is relatively small,} \tag{3.4a}$$

and, in addition,

$$b_f(0) = b_f(1) = 0. \tag{3.4b}$$

Here, $\|\cdot\|_{[0,1]}$ denotes the maximum norm on $[0,1]$.

In [5], it was suggested to use as approximation class B a space of periodic splines. Since the approximation of functions by periodic splines is still a difficult problem (see e.g. Zeilfelder [12]), we propose another method, to be developed now. For $n \in \mathbb{N}$ and $0 \le \nu \le n$, we denote by β_ν^n the ν^{th} Bernstein basis polynomial of degree n, i.e.,

$$\beta_\nu^n(x) = \binom{n}{\nu} x^\nu (1-x)^{n-\nu}. \tag{3.5}$$

Moreover, it is convenient to define $\beta_\nu^n(x) :\equiv 0$, if $\nu < 0$ or $\nu > n$. The following result on the structure of the linear space

$$B_n = \operatorname{span}\{\beta_1^n, \dots, \beta_{n-1}^n\} \tag{3.6}$$

holds.

Lemma 3.1: *a) It is*

$$B_n \equiv x(1-x)\,\Pi_{n-2}. \tag{3.7}$$

In particular, each $b \in B_n$ satisfies (3.4b).
b) The space B_n is a Chebychev space on the open interval $(0,1)$, and a weak Chebychev space on the closed interval $[0,1]$.

Proof. Each element $p \in B_n$ is a polynomial of degree n, which vanishes at the points 0 and 1. Hence B_n is a subspace of $x(1-x)\Pi_{n-2}$. Since the dimension of B_n equals $(n-1)$, the identity (3.7) is proved.

To prove statement b), we use the fact that Π_{n-2} is a Chebychev space everywhere in $\mathbb{R}$. Since the weight function $x(1-x)$ has no zero in $(0,1)$, B_n is also Chebychev on this interval. This implies b). □

Since B_n is no Chebychev space on $[0,1]$, good approximations (i.e., via interpolation), are hard to determine directly. However, the following result implies methods for this by using the strong connection of B_n with the space Π_{n-2}.

We define the function g_f by

$$g_f(x) \;:=\; \frac{f(x)}{x\,(1-x)} \tag{3.8}$$

for all $x \in [0,1]$. Note that g_f is still bounded on $[0,1]$.

Theorem 3.2: *Let $p \in \Pi_{n-2}$ be an approximation of g_f with error ϱ, given in Bernstein form*

$$p(x) \;=\; \sum_{\nu=0}^{n-2} \alpha_\nu \beta_\nu^{n-2}(x)\,.$$

Then the function $b_f \in B_n$, defined as

$$b_f(x) \;:=\; \sum_{\nu=1}^{n-1} \gamma_\nu \beta_\nu^{n}(x) \tag{3.9a}$$

with

$$\gamma_\nu \;=\; \binom{n-2}{\nu-1} \cdot \alpha_{\nu-1} \tag{3.9b}$$

is an approximation of f w.r.t. B_n, with approximation error

$$\|b_f - f\|_{[0,1]} \;\le\; \frac{\varrho}{4}\,. \tag{3.10}$$

Remark. Since Π_{n-2} is a Chebychev space on $[0,1]$, many types of good approximations, e.g. the polynomial of best approximation as well as the interpolating polynomial, are very easy to compute. Thus, Theorem 3.2 opens many possibilities to compute good approximations w.r.t. B_n.

Proof of Theorem 3.2. We first show that

$$b_f(x) = x(1-x)\,p(x)$$

by the following equations:

$$\begin{aligned} x(1-x)\,p(x) &= \sum_{\nu=0}^{n-2} \alpha_\nu\, x(1-x)\,\beta_\nu^{n-2}(x) \\ &= \sum_{\nu=0}^{n-2} \alpha_\nu \binom{n-2}{\nu} x^{\nu+1}(1-x)^{n-1-\nu} \\ &= \sum_{\nu=1}^{n-1} \alpha_{\nu-1} \binom{n-2}{\nu-1} x^{\nu}(1-x)^{n-\nu} = b_f(x)\,. \end{aligned}$$

Then it follows that

$$\begin{aligned} \|b_f - f\|_{[0,1]} &= \max_{x\in[0,1]} \{|b_f(x) - f(x)|\} \\ &= \max_{x\in[0,1]} \{|x(1-x)| \cdot |p_f(x) - g_f(x)|\} \\ &\le \max_{x\in[0,1]} \{|x(1-x)|\} \cdot \max_{x\in[0,1]} \{|p_f(x) - g_f(x)|\} \le \frac{1}{4} \cdot \varrho\,, \end{aligned}$$

and so the proof is complete. $\square$

Given any function $b \in B_n$, we define, in analogy to (3.2), the odd periodic continuation $\widehat{b}$ of b by

$$\widehat{b}(x) := \begin{cases} b(x-2\mu), & \text{if } x \in [2\mu, 2\mu+1]\,, \\ -b(2\mu+2-x), & \text{if } x \in [2\mu+1, 2\mu+2]\,. \end{cases} \tag{3.11}$$

For formal reasons, we set in addition

$$\widetilde{b}(x) := \begin{cases} b(x), & \text{if } x \in [0,1]\,, \\ 0, & \text{elsewhere.} \end{cases} \tag{3.12}$$

Note that both functions are continuous everywhere on $\mathbb{R}$. We consider now the Gauß transform of a function $b = b_f \in B_n$, which is supposed to be an approximation to the initial value function f.

Theorem 3.3: *Let $b \in B_n$. Then the Gauß transform of the function $\widehat{b}$, defined in (3.11), is an odd periodic function (w.r.t. x), and possesses the representation*

$$G(\widehat{b})(x,t) = \sum_{\mu\in\mathbb{Z}} \left(G(\widetilde{b})(x-2\mu,t) - G(\widetilde{b})(2\mu-x,t)\right), \tag{3.13}$$

valid for all $(x,t) \in R$

Proof. Since $\widehat{b}$ is an odd periodic function, the same is true for its Gauß transform, due to Theorem 1.1.

In order to prove (3.13), we use the identity

$$\widehat{b}(\tau) \;=\; \sum_{\mu\in\mathbb{Z}} \left(\widetilde{b}(\tau-2\mu) - \widetilde{b}(2\mu-\tau)\right), \tag{3.14}$$

valid for each $\tau \in \mathbb{R}$. Note that no problem with the convergence of the series on the right hand side occurs, since for each $\tau \in \mathbb{R}$ in fact at most one term in this series is different from zero.

From (3.14), we obtain the relation

$$\begin{aligned} G(\widehat{b})(x,t) \;&=\; \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} \widehat{b}(\tau)\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \\ &=\; \frac{1}{\sqrt{4\pi t}} \sum_{\mu\in\mathbb{Z}} \Big(\int_{-\infty}^{\infty} \widetilde{b}(\tau-2\mu)\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \;- \\ &\qquad\qquad - \int_{-\infty}^{\infty} \widetilde{b}(2\mu-\tau)\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \Big) \qquad (3.15) \\ &=\; \sum_{\mu\in\mathbb{Z}} \Big(G\big(\widetilde{b}(\,\cdot\, - 2\mu)\big)(x,t) - G\big(\widetilde{b}(2\mu - \,\cdot\,)\big)(x,t) \Big), \end{aligned}$$

and so, using the fact that the Gauß transform is shift invariant, i.e.,

$$G(\widetilde{b})(x-y,t) \;=\; G\big(\widetilde{b}(\,\cdot\, - y)\big)(x,t)$$

for all $y \in \mathbb{R}$, the second statement of Theorem 3.3 is proved. □

Theorem 3.3 implies that it suffices to investigate the Gauß transform of the function $\widetilde{b}$. Moreover, due to linearity, we may even more concentrate on the Gauß transforms of the basis functions β_ν^n, cf. (3.5). To do this, we introduce the continuations $\widehat{\beta}_\nu^n$ and $\widetilde{\beta}_\nu^n$ of β_ν^n, defined in analogy to (3.11) resp. (3.12).

Theorem 3.4: *Let, for all ν and n under consideration,*

$$G_\nu^n \;:=\; G(\widetilde{\beta}_\nu^n)\,.$$

Then for $n \geq 2$ the recursion formula

$$\begin{aligned} G_\nu^n(x,t) \;&=\; (1-x)\, G_\nu^{n-1}(x,t) \;+\; x\, G_{\nu-1}^{n-1}(x,t) \;+ \\ &\quad +\; 2tn\Big(G_{\nu-2}^{n-2}(x,t) - 2G_{\nu-1}^{n-2}(x,t) + G_\nu^{n-2}(x,t)\Big) \end{aligned} \tag{3.16}$$

is valid.

Proof. The functions $\widetilde{\beta}_\nu^n$ can be interpreted as B-splines with multiple knots at 0 and 1. Hence, the assertion of Theorem 3.4 can be deduced from the corresponding result on B-splines, see Meinardus [5] or Weis [11].

Alternatively, a straightforward but lengthy proof can be given, using integration by parts and the recurrence relations

$$\beta_\nu^n(x) \;=\; (1-x)\,\beta_\nu^{n-1}(x) \;+\; x\,\beta_{\nu-1}^{n-1}(x)$$

and

$$\frac{d}{dx}\,\beta_\nu^n(x) \;=\; n\left(\beta_{\nu-1}^{n-1}(x) - \beta_\nu^{n-1}(x)\right)$$

for Bernstein basis polynomials. □

In order to compute the values of the functions G_ν^n by the recursion (3.16), it is necessary to have approximations for the initial value functions

$$\begin{aligned} G_0^0(x,t) &= \frac{1}{\sqrt{4\pi t}} \int_0^1 \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau\,, \\ G_0^1(x,t) &= \frac{1}{\sqrt{4\pi t}} \int_0^1 (1-\tau)\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau\,, \quad \text{and} \\ G_1^1(x,t) &= \frac{1}{\sqrt{4\pi t}} \int_0^1 \tau\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\, d\tau \end{aligned} \tag{3.17}$$

available. This can easily be done, e.g., via the well-known error function $\operatorname{erf}(z)$, defined as

$$\operatorname{erf}(z) \;=\; \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-\eta^2}\, d\eta\,, \tag{3.18}$$

which in turn can be computed using various types of approximations, see [5,8,11]. The connection between the error function and the desired initial value functions is provided by the following relations.

Lemma 3.5: *It is*

$$G_0^0(x,t) \;=\; \frac{1}{2}\left(\operatorname{erf}\Big(\frac{1-x}{\sqrt{4t}}\Big) \;+\; \operatorname{erf}\Big(\frac{x}{\sqrt{4t}}\Big)\right), \tag{3.19}$$

$$G_1^1(x,t) \;=\; x\,G_0^0(x,t) \;-\; \sqrt{\frac{t}{\pi}}\cdot\left(\mathrm{e}^{-\frac{(1-x)^2}{4t}} \;-\; \mathrm{e}^{-\frac{x^2}{4t}}\right), \quad \textit{and} \tag{3.20}$$

$$G_0^1(x,t) \;=\; G_0^0(x,t) \;-\; G_1^1(x,t)\,. \tag{3.21}$$

Proof. Relation (3.19) follows directly from the definition G_0^0 and (3.18). To prove (3.20), we write $\tau = x + (\tau - x)$ and obtain

$$\begin{aligned} G_1^1(x,t) &= x\,G_0^0(x,t) + \frac{1}{\sqrt{4\pi t}} \int_0^1 (\tau - x)\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\,d\tau \\ &= x\,G_0^0(x,t) - 2t\cdot\frac{1}{\sqrt{4\pi t}} \int_0^1 -\frac{(\tau-x)}{2t}\cdot \mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\,d\tau \\ &= x\,G_0^0(x,t) - \sqrt{\frac{t}{\pi}}\left[\mathrm{e}^{-\frac{(\tau-x)^2}{4t}}\right]_{\tau=0}^{\tau=1}. \end{aligned}$$

Finally, relation (3.21) follows immediately from (3.17). □

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