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Abstract

The Cauchy problem of the homogenous heat conduction equation leads to a solution which is given by the convolution of the initial data and the well known fundamental solution. In higher dimensions this integral can be evaluated by Quasi Monte Carlo (QMC) methods. A powerful tool to get error estimations for QMC integration is the concept of reproducing kernel Hilbert spaces. These methods can be used to get approximative solution formulas for the heat conduction equation for initial data from a reproducing kernel Hilbert space. Here an estimation for the error is calculated for the special case that the initial data belongs to the Korobow class $K_\alpha([0,1)^s)$.

1 Introduction

At the beginning we recall some facts about the initial value problem of the heat conduction equation:
The Cauchy problem of the homogenous heat conduction equation can be formulated in the following way: Let $x = (x_1, x_2, \ldots, x_s) \in \mathbb{R}^s$ and $t \in \mathbb{R}$. Let $u_0(x)$ be a given function continous on $\mathbb{R}^s$. We are searching for a function $u(x,t) : \mathbb{R}^s \times \mathbb{R} \to \mathbb{R}$ with the following properties:

-) $u(x,t)$ is twice continously differentiable on $\mathbb{R}^s \times \mathbb{R}_+$ and continous on $\mathbb{R}^s \times \mathbb{R}_+^0$
-) $u(x,t)$ satisfies the following equation

$$\frac{\partial u}{\partial t} - \Delta u = 0$$

  for $t > 0$ and $u(x,0) = u_0(x)$.

The symbol Δ denotes the Laplace operator with respect to x:

$$\Delta u = \frac{\partial^2 u}{\partial x_1^2} + \ldots + \frac{\partial^2 u}{\partial x_s^2}$$

To get an integral representation of the solution the fundamental solution can be used:
Theorem 1:(see [1]) The function

$$G(x,t) : \mathbb{R}^s \times \mathbb{R} \to \mathbb{R}$$

$$G(x,t) = \frac{1}{2^s (\pi t)^{\frac{s}{2}}} e^{-\frac{|x|^2}{4t}} \qquad t > 0$$

$$G(x,t) = 0 \qquad t \leq 0$$

fulfills the equation

$$\frac{\partial G}{\partial t} - \Delta G = \delta(x)$$

where $\delta(x)$ denotes the Dirac distribution and the dervatives have to be understood in distributional sense.

With this fundamental solution the solution of the Cauchy problem is given by the convolution of the fundamental solution and the initial data $u_0(x)$**:**

Theorem 2: Let $u_0(x)$ be a continous and bounded function on $\mathbb{R}^s$. The solution of the Cauchyproblem of the homogenous heat conduction equation with initial condition $u(x,0) = u_0(x)$ is given by

$$u(x,t) = \frac{1}{2^s \pi^{\frac{s}{2}} t^{\frac{s}{2}}} \int_{\mathbb{R}^s} u_0(y) e^{-\frac{|x-y|^2}{4t}} dy \tag{1}$$

for $t > 0$. This solution is unique.

Remark: The uniqueness of the solution in Theorem 2 follows from the estimation

$$|u(x,t)| \leq A e^{B|x|^2}$$

and a Theorem from [1]:

Theorem 2a: Let $u(x,t)$ be continous for $x \in \mathbb{R}^s$ and $0 \leq t \leq T$ and $\frac{\partial u}{\partial t}, \frac{\partial^2 u}{\partial x_i \partial x_j}$ exist and be continous for $x \in \mathbb{R}^s$and $0 \leq t \leq T$ and satisfy

$$\frac{\partial u}{\partial t} - \triangle u \leq 0$$

for $x \in \mathbb{R}^s$ and $0 \leq t \leq T$ and $|u(x,t)| \leq A e^{B|x|^2}$ for constants $A, B > 0$ and $u(x,0) = u_0(x)$ for $x \in \mathbb{R}^s$. Then

$$u(x,t) \leq \sup_{y \in \mathbb{R}^s} u_0(y)$$

Due to the fact that we treat the integral (1) by QMC methods and reproducing kernels we recall also some details about these concepts.

In QMC integrals are calculated with the domain $E^s = [0,1)^s$ by formulas of the following form:

$$\int_{E^s} f(x)dx \approx \frac{1}{N}\sum_{k=1}^{N} f(x_k)$$

$\{x_k\}_{k\geq 1} \in E^s$ denotes a sequence of points uniformly distributed in E^s. A sequence of points $\{x_k\}$ is uniformly distributed in E^s if and only if

$$\lim_{N\to\infty} \sup_{J\subset E^s} |\frac{\#(x_k \in J, 1 \leq k \leq N)}{N} - \mu(J)| = 0$$

where $\mu(J) = \int_J dx$ denotes the Lebesgue measure of J. The term

$$D_N := \sup_{J\subset E^s} |\frac{\#(x_k \in J, 1 \leq k \leq N)}{N} - \mu(J)|$$

is called the discrepancy of the sequence $\{x_k\}_{k\geq 1}$. The discrepancy gives one famous error estimation for evaluating integrals by QMC-methods: Let

$$R_N = \int_{E^s} f(x)dx - \frac{1}{N}\sum_{k=1}^{N} f(x_k)$$

the error of the approximative calculation of the integral over $f(x)$. Then we have the following estimation:

$$|R_N| \leq D_N V(f)$$

where $V(f)$ is the total variation. This estimation is called the Hlawka-Koksma inequality. For more detailed regarding discrepancies information refer to [2].

An other error estimation is given by the tool of reproducing kernel Hilbert spaces (see [3]) .We recall some facts about these spaces:

Definition: Let H be a Hilbert space of complex valued functions defined on a set F with inner product $\langle .,. \rangle_H$. If there is a function $K(x,y) : F \times F \to \mathbb{C}$ with the following properties:

-) the functions $g_y(x) := K(x,y)$ are elements of H
-) $K(x,y) = \overline{K(y,x)}$
-) for all $f(x) \in H$ and all $y \in F$ we have $f(y) = \langle f(x), K(x,y)\rangle_H$ (reproducing property)

then H is called a reproducing kernel Hilbert space.

The function $K(x,y)$ is always unique and positive definite in the following sense: For all $N \geq 1; \xi_1, \xi_2, \ldots \xi_N \in \mathbb{C}; x_1, x_2, \ldots, x_N \in F$ we have

$$\sum_{i,j=1}^{N} \xi_i \overline{\xi_j} K(x_i, x_j) \geq 0 \tag{2}$$

A special type of reproducing kernels are the Hilbert-Schmidt type kernels: Let $g_k(x)$ be a complete orthonormal system in H. Then the function $K(x,y)$: $F \times F \to \mathbb{C}$ with

$$K(x,y) = \sum_k g_k(x)\overline{g_k(y)}$$

is a reproducing kernel of H.
A well known example of a reproducing kernel Hilbert space with a Hilbert Schmidt kernel is the following: Consider the Korobow-class $K_\alpha([0,1]^s)$ defined by

$$K_\alpha([0,1]^s) =$$

$$= \{f(x_1,\ldots,x_s) | f(x_1,\ldots,x_s) = \sum_{n_1,n_2,\ldots,n_s=-\infty}^{\infty} \frac{a_{n_1,n_2,\ldots n_s}}{\overline{(n_1 n_2 \ldots n_s)}^{\alpha}} e^{2\pi i(n_1x_1+\ldots+n_sx_s)},$$

$$\sum_{n_1,n_2\ldots,n_s=-\infty}^{\infty} |a_{n_1,n_2,\ldots,n_s}|^2 < \infty\}$$

for some $\alpha > 1$ and . $\overline{n}$ is defined by $\overline{n} := \max(1,|n|)$. Now define a Hermitian scalar product on the basis functions $\varphi_\nu(x) := \frac{e^{2\pi i \nu x}}{\overline{\nu}^\alpha}$ in the following way:

$$\langle \varphi_\nu(x), \varphi_\mu(x) \rangle = \langle \frac{e^{2\pi i(n_1x_1+n_2x_2+\ldots+n_sx_s)}}{(\overline{n_1 n_2} \ldots \overline{n_s})^{\alpha}}, \frac{e^{2\pi i(m_1x_1+m_2x_2+\ldots+m_sx_s)}}{(\overline{m_1 m_2} \ldots \overline{nm_s})^{\alpha}} \rangle =$$

$$= \delta_{n_1m_1}\delta_{n_2m_2}\ldots\delta_{n_sm_s} \tag{3}$$

Consider now the Hilbert Schmidt type kernel $K(x,y) : \mathbb{R}^s \times \mathbb{R}^s \to \mathbb{C}$ with

$$K(x,y) = \sum_{\nu\in\mathbb{Z}} \varphi_\nu(x)\overline{\varphi_\nu(y)} = \sum_{\nu\in\mathbb{Z}^s} \frac{e^{2\pi i(n_1(x_1-y_1)+n_2(x_2-y_2)+\ldots+n_s(x_s-y_s))}}{(\overline{n_1 n_2} \ldots \overline{n_s})^{2\alpha}} =$$

$$= \prod_{j=1}^{s} \left(\sum_{n_j\in\mathbb{Z}} \frac{e^{2\pi i n_j(x_j-y_j)}}{\overline{n_j}^{2\alpha}} \right) \tag{4}$$

With Hurwitz' Fourier series of Bernoulli polynomials this kernel can be written in closed form for $\alpha \in \mathbb{N}$. The n-th Bernoulli polynomial $B_n(x)$ for $0 < x < 1$ has the Fourier series

$$B_n(x) = -\frac{n!}{(2\pi i)^n} \sum_{k\in\mathbb{Z},k\neq 0} \frac{e^{2\pi i k x}}{k^n}$$

This means, $K(x,y)$ is equal to

$$K(x,y) = \prod_{j=1}^{s} \left(1 + (-1)^{\alpha} \frac{(2\pi)^{2\alpha}}{(2\alpha)!} B_{2\alpha}(\{x_j - y_j\})\right) \tag{5}$$

If the integrand $f(x)$ is now an element of a reproducing kernel Hilbert space we have another error estimation for R_N: This estimation is called the diaphony of the sequence $\{x_k\}$: We want to calculate the integration error

$$R_N = \int_{E^s} f(x)dx - \frac{1}{N}\sum_{k=1}^{N} f(x_k)$$

for $f(x) \in H$ where H is the reproducing kernel Hilbert space with basis (**??**rkhs}). So $f(x)$ has a series expansion of the form

$$f(x) = \sum_{\nu \in Z^s} \frac{a_\nu}{\overline{\nu}^{\alpha}} e^{2\pi i \nu x}$$

and the integral can be calculated to

$$\int_{E^s} f(x)dx = a_0 = \langle f, 1 \rangle$$

By the reproducing property we can write

$$\frac{1}{N}\sum_{k=1}^{N} f(x_k) = \frac{1}{N}\sum_{k=1}^{N} \langle f(y), K(y, x_k)\rangle =$$

$$= \langle f(y), \frac{1}{N}\sum_{k=1}^{N} K(y, x_k)\rangle$$

So the integration error can be written as a scalar product:

$$R_N = \langle f(y), \frac{1}{N}\sum_{k=1}^{N} K(y, x_k) - 1\rangle$$

The factor

$$r_N := \| \frac{1}{N}\sum_{k=1}^{N} K(y, x_k) - 1\|$$

is called the diaphony (see [4]) of the sequence $\{x_k\}_{k\geq 1}$. If the integral can be written as the scalar product with an arbitrary element $g \in H$, i.e.

$$\int_{E^s} f(x)dx = \langle f, g\rangle$$

the integration error is written in the form

$$R_N = \langle f(y), \frac{1}{N}\sum_{k=1}^{N} K(y, x_k) - g\rangle$$

The factor

$$r_{g,N} := \|\frac{1}{N}\sum_{k=1}^{N} K(y, x_k) - g\|$$

is called the g-diaphony (see [4]).
The modulus of the integration error is now given by Cauchy-Schwartz inequality:

$$|R_N| \leq r_N \|f\| \tag{6}$$

resp.

$$|R| \leq r_{g,N} \|f\| \tag{7}$$

2 Application of QMC methods to the solution of the homogenous heat equation

We consider now the Cauchy problem of the homogenous heat equation with initial data $u_0(x) \in K_\alpha([0,1]^s)$. To apply QMC-methods we transform the integral (**??**waerme}) into an integral over the s-dimensional unitcube. Therefor we fix the values for $x = (x_1, x_2, \ldots, x_s)$ and t and use the following substitution: For $i = 1, 2, \ldots, s$ set

$$v_i = F_{x_i,t}(y_i) = \frac{1}{2\pi^{\frac{1}{2}} t^{\frac{1}{2}}} \int_{-\infty}^{y_i} e^{-\frac{(x_i-w)^2}{4t}} dw \tag{8}$$

The following lemma is a simple consequence of the properties of Gauss normal distribution function:
Lemma: For $i = 1, 2, \ldots, s$ and all $x_i \in \mathbb{R}, t > 0$ the transformation (**??**waerme}) has the following properties:

1. $F_{x_i,t}(-\infty) = 0$
2. $F_{x_i,t}(y)$ is monotone increasing
3. $F_{x_i,t}(+\infty) = 1$

This substitution transforms the integral (**??**waerme}) in the following way:

$$u(x,t) =$$

$$= \frac{1}{2^s \pi^{\frac{s}{2}} t^{\frac{s}{2}}} \int_{\mathbb{R}^s} u_0(y_1, y_2, \ldots, y_s) e^{-\frac{(x_1-y_1)^2}{4t} - \cdots - \frac{(x_s-y_s)^2}{4t}} dy_1 dy_2 \ldots dy_s =$$

$$= \int_{(0,1)^s} u_0(F^{-1}_{x_1,t}(q_1), F^{-1}_{x_2,t}(q_2), \ldots, F^{-1}_{x_s,t}(q_s)) dq_1 dq_2 \ldots dq_s \tag{9}$$

For $\alpha > 1$ the series expansion of $u_0(x)$ is uniform convergent and therefor $u_0(x)$ is continous. The Gauss distribution function is also continous and strictly monotone, so the inverse is also continous. As a composition of continous functions

$$u_0(F_{x_1,t}^{-1}(q_1), F_{x_2,t}^{-1}(q_2), \dots, F_{x_s,t}^{-1}(q_s))$$

is also continous on $(0,1)^s$. By a theorem of uniform distributed sequences (see [2]) the following holds: Let $\{y_k\}_{k\geq 1} = \{(y_k^{(1)}, y_k^{(2)}, \dots, y_k^{(s)})\}_{k\geq 1}$be a uniform distributed sequence (mod 1). Then we have

$$\int_{(0,1)^s} u_0(F_{x_1,t}^{-1}(q_1), F_{x_2,t}^{-1}(q_2), \dots, F_{x_s,t}^{-1}(q_s)) dq_1 dq_2 \dots dq_s =$$

$$= \lim_{N\to\infty} \sum_{k=1}^{N} u_0(F_{x_1,t}^{-1}(y_k^{(1)}), F_{x_2,t}^{-1}(y_k^{(2)}), \dots, F_{x_s,t}^{-1}(y_k^{(s)})) \tag{10}$$

It is not practicable to invert a Gauss distribution function for each x and t. Therefor we use a slight modification of (**??**waerme}): Recall the original substitution

$$q_i = F_{x_i,t}(y_i) = \frac{1}{2\pi^{\frac{1}{2}} t^{\frac{1}{2}}} \int_{-\infty}^{y_i} e^{-\frac{(x_i-w)^2}{4t}} dw$$

We modify this in the following way:

$$q_i = F_{x_i,t}(y_i) = \frac{1}{2\pi^{\frac{1}{2}} t^{\frac{1}{2}}} \int_{-\infty}^{y_i} e^{-\frac{(x_i-w)^2}{4t}} dw = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\frac{y_i - x_i}{2\sqrt{t}}} e^{-w^2} dw \tag{11}$$

We introduce the function

$$\Phi(y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{y} e^{-w^2} dw$$

So we can write the substitution (**??**neu}) in the form

$$q_i = \Phi\left(\frac{y_i - x_i}{2\sqrt{t}}\right)$$

With this substitution the integral (9) is written as

$$u(x,t) = \frac{1}{2^s \pi^{\frac{s}{2}} t^{\frac{s}{2}}} \int_{\mathbb{R}^s} u_0(y_1, y_2, \dots, y_s) e^{-\frac{(x_1-y_1)^2}{4t} - \dots - \frac{(x_s-y_s)^2}{4t}} dy_1 dy_2 \dots dy_s =$$

$$= \int_{(0,1)^s} u_0(2\sqrt{t}\Phi^{-1}(q_1) + x_1, \dots, 2\sqrt{t}\Phi^{-1}(q_s) + x_s) dq_1 \dots dq_s \tag{12}$$

Formula (10) can now be written in the form

$$\int_{(0,1)^s} u_0(2\sqrt{t}\Phi^{-1}(q_1) + x_1, \dots, 2\sqrt{t}\Phi^{-1}(q_s) + x_s) dq_1 \dots dq_s =$$

$$= \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} u_0(2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s) \tag{13}$$

This leads us to an approxiative solution :

$$u_{approx}(x,t) = \frac{1}{N} \sum_{k=1}^{N} u_0(2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s) \tag{14}$$

$\{y_k\}_{k\geq 1}$ denotes a uniform distributed sequence in $(0,1)^s$.

Remark: If we transform the integration domain in formula (13) back to R^s we have the following:

$$\frac{1}{\sqrt{\pi}^s} \int_{R^s} u_0(2\sqrt{t}y_1 + x_1, \ldots 2\sqrt{t}y_s + x_s) e^{-y_1^2 - y_2^2 - \ldots - y_s^2} dy_1 \ldots dy_s =$$

$$= \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} u_0(2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s) \tag{15}$$

This formula is valid for all continous functions $u_0(x)$.

Formula (10) resp. (13) does not deliver any estimation of the integration error. In the next section we use the fact that $K_\alpha([0,1]^s)$ forms a RKHS to get an estimation of the error.

3 Estimation of the integration error

The set $K_\alpha([0,1)^s]$ forms a RKHS. We will discover that the solution of the heat conduction equation is also in $K_\alpha([0,1]^s)$ for $u_0 \in K_\alpha([0,1]^s)$.
We start with an initial condition

$$u_0(x) = \sum_{\nu \in Z^s} \frac{a_\nu}{\overline{\nu}^\alpha} e^{2\pi i \nu x} \tag{16}$$

By calculating the integral (1) for an initial condition of the form (16) the following lemma can be verified:
Lemma: For $u_0(x)$ of the form (16) the solution (1) is given by

$$u_{exact}(x,t) = \sum_{\nu \in \mathbb{Z}^s} \frac{a_\nu}{\overline{\nu}^\alpha} e^{2\pi i \nu x} e^{-4t\pi^2 |\nu|^2} \tag{17}$$

The next step is to write (17) as a scalar product from $u_0(x)$ and another element of $K_\alpha([0,1]^s)$. From the scalar product in $K_\alpha([0,1]^s)$ we know that

$$a_\nu = \langle u_0(y), \frac{e^{2\pi i \nu y}}{\overline{\nu}^\alpha} \rangle$$

and therefor

$$u(x,t) = \sum_{\nu \in Z^s} \langle u_0(y), \frac{e^{2\pi i \nu y}}{\overline{\nu}^\alpha} \rangle \frac{e^{2\pi i \nu x}}{\overline{\nu}^\alpha} e^{-4t\pi^2|\nu|^2} =$$

$$= \langle u_0(y), \sum_{\nu \in Z^s} \frac{e^{2\pi i \nu y} e^{-2\pi i \nu x}}{\overline{\nu}^{2\alpha}} e^{-4t\pi^2|\nu|^2} \rangle =$$

$$= \langle u_0(y), g_{x,t}(y) \rangle$$

with

$$g_{x,t}(y) := \sum_{\nu \in Z^s} \frac{e^{2\pi i \nu y} e^{-2\pi i \nu x}}{\overline{\nu}^{2\alpha}} e^{-4t\pi^2|\nu|^2}$$

It is easily seen that $g_{x,t}(y)$ is an element of $K_\alpha([0,1]^s)$.
The next step is to write $u_{approx}(x,t)$ as a scalar product. By the reproducing property we get

$$u_{approx}(x,t) = \frac{1}{N} \sum_{k=1}^{N} u_0(2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s) =$$

$$= \frac{1}{N} \sum_{k=1}^{N} \langle u_0(z_1, z_2, \ldots, z_s), K((z_1, \ldots z_s), (2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s)) \rangle =$$

$$= \langle u_0(z_1, \ldots, z_s), \frac{1}{N} \sum_{k=1}^{N} K((z_1, \ldots z_s), (2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s)) \rangle$$

Collecting these facts we can write the difference $u_{approx}(x,t) - u_{exact}(x,t)$ as a scalar product:

$$u_{approx}(x,t) - u_{exact}(x,t) =$$

$$= \langle u_0(z_1, \ldots, z_s), \frac{1}{N} \sum_{k=1}^{N} K((z_1, \ldots z_s), (2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s)) - g_{x,t}(z_1, \ldots, z_s) \rangle$$

Application of Cauchy-Schwartz inequality deliveres an estimation of the error:

$$|u_{approx}(x,t) - u_{exact}(x,t)| \leq$$

$$\leq \|u_0\| \quad \| \frac{1}{N} \sum_{k=1}^{N} K((z_1, \ldots z_s), (2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s)) - g_{x,t}(z_1, \ldots, z_s) \|$$

$\|.\|$ denotes the norm induced by the scalar product $\langle ., . \rangle$and is calculated with respect to $(z_1, \ldots, z_s)$. This error estimation has the same form as (7).
The term

$$R_N(x,t) := \| \frac{1}{N} \sum_{k=1}^{N} K((z_1, \ldots z_s), (2\sqrt{t}\Phi^{-1}(y_k^{(1)}) + x_1, \ldots, 2\sqrt{t}\Phi^{-1}(y_k^{(s)}) + x_s)) - g_{x,t}(z_1, \ldots, z_s) \|^2$$

can be simplified. Calculation of the norm showes that

$$R_N(x,t) = \frac{1}{N^2}\sum_{k,l=1}^{N} K\left(\left(2\sqrt{t}\Phi^{-1}(y_k^{(1)}),\dots,2\sqrt{t}\Phi^{-1}(y_k^{(s)})\right),\left(2\sqrt{t}\Phi^{-1}(y_l^{(1)}),\dots,2\sqrt{t}\Phi^{-1}(y_l^{(s)})\right)\right) -$$

$$-\frac{2}{N}\sum_{\nu\in\mathbb{Z}^s}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1\Phi^{-1}(y_k^{(1)})+\dots+n_s\Phi^{-1}(y_k^{(s)})\right)+\sum_{\nu\in\mathbb{Z}^s}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}$$

This error term does not depend on the spatial coordinate, only on the "time"-coordinate.

We state the following definition:
Definition: Let $(y_n) = (y_n^{(1)}, y_n^{(2)}, \dots, y_n^{(s)})$, $y_n \in (0,1)^s$ a uniform distributed sequence. Let $F_i(x)$, $i = 1,2,\dots,s$ be probability distribution functions on $(-\infty,+\infty)$. We call a sequence $(x_n) = \left(F_1^{-1}(y_n^{(1)}), F_2^{-1}(y_n^{(2)}),\dots,F_s^{-1}(y_n^{(s)})\right)$ uniform ditributed with respect to the s-dimensional distribution function $F(x) = F(x_1,x_2,\dots,x_s) = F_1(x_1)F_2(x_2)\dots F_s(x_s)$.

We can state the following
Theorem: For a uniform distributed sequence $(y_n) = (y_n^{(1)},\dots,y_n^{(s)})$ with respect to the s-dimensional distribution function $F(x) = \Phi(x_1)\Phi(x_2)\dots\Phi(x_2)$ the error expression $R_N(x,t) \to 0$ as $N \to \infty$.

Proof: From formula (15) we know that

$$\frac{1}{\sqrt{\pi}^s}\int_{R^s} f(x_1,x_2,\dots,x_s)e^{-x_1^2-\dots-x_s^2}dx_1\dots dx_s =$$

$$= \lim_{N\to\infty}\frac{1}{N}\sum_{k=1}^{N} f(y_k^{(1)},\dots,y_k^{(s)})$$

We start our investigation of $R_N(x,t)$ with the term

$$\frac{2}{N}\sum_{\nu\in\mathbb{Z}^s}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1y_k^{(1)}+\dots+n_sy_k^{(s)}\right)$$

We choose an $M > 0$ and define $I_M = \{-M,-M+1,\dots,M-1,M\}^s$. We split the sum over ν into 2 parts:

$$\frac{2}{N}\sum_{\nu\in I_M}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1y_k^{(1)}+\dots+n_sy_k^{(s)}\right)+$$

$$+\frac{2}{N}\sum_{\nu\notin I_M}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1y_k^{(1)}+\dots+n_sy_k^{(s)}\right)$$

For the second part we can find an estimation independant from the node points:

$$\frac{2}{N}\sum_{\nu\notin I_M}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1y_k^{(1)}+\ldots+n_sy_k^{(s)}\right)\leq$$

$$\leq 2\sum_{\nu\notin I_M}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\leq 2\left(\frac{2}{(M+1)^{2\alpha}}\frac{e^{-4t\pi^2M}}{1-e^{-4t\pi^2}}\right)^s$$

So we can find an index M so that this term is smaller than any given ϵ. Now we turn to the finite part: An easy calculation showes that

$$\frac{1}{\sqrt{\pi}^s}\int_{R^s}\cos(4\sqrt{t}\pi(n_1x_1+\ldots+n_sx_s))e^{-x_1^2-\ldots-x_s^2}dx_1\ldots dx_s=$$

$$=e^{-4t\pi^2(n_1^2+\ldots+n_s^2)}$$

So we can find an index $N_1(\epsilon,M)$ so

$$|\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\left(n_1y_k^{(1)}+\ldots+n_sy_k^{(s)}\right)-\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}|<\frac{\epsilon}{(2M+1)^s}$$

for $N>N_1(\epsilon,M)$ and all $\nu\in I_M$. Now we investigate the term

$$\frac{1}{N^2}\sum_{k,l=1}^{N}K\left(\left(2\sqrt{t}y_k^{(1)},\ldots,2\sqrt{t}\Phi^{-1}y_k^{(s)}\right),\left(2\sqrt{t}y_l^{(1)},\ldots,2\sqrt{t}y_l^{(s)}\right)\right)\qquad(18)$$

Recall that the kernel function is given by

$$K(x,y)=\sum_{\nu\in Z^s}\frac{e^{2\pi i\nu(x-y)}}{\overline{\nu}^{2\alpha}}$$

So the expression (18) is an infinite sum over ν. We split this infinite sum into 2 parts:

$$\frac{1}{N^2}\sum_{k,l=1}^{N}K\left(\left(2\sqrt{t}y_k^{(1)},\ldots,2\sqrt{t}\Phi^{-1}y_k^{(s)}\right),\left(2\sqrt{t}y_l^{(1)},\ldots,2\sqrt{t}y_l^{(s)}\right)\right)=$$

$$=\frac{1}{N^2}\sum_{\nu\in I_L}\sum_{k,l=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}}+\frac{1}{N^2}\sum_{\nu\notin I_L}\sum_{k,l=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}}$$

Due to the convergence of $\sum\frac{1}{\nu^{2\alpha}}$ we can find an index L_0 (independent from the node points) with

$$|\sum_{\nu\notin I_L}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_L)}}{\overline{\nu}^{2\alpha}}|<\epsilon$$

for all $L > L_0$. So we have

$$|\frac{1}{N^2}\sum_{\nu\notin I_L}\sum_{k,l=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}}| < \epsilon$$

for all $L > L_0$. We can write the finite part in the form

$$\frac{1}{N^2}\sum_{\nu\in I_L}\sum_{k,l=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}} = \sum_{\nu\in I_L}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right)\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right) \tag{19}$$

We can find indices $N_2(\epsilon, L)$ and $N_3(\epsilon, L)$ with

$$|\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}| < \frac{\epsilon}{(2L+1)^{\frac{s}{2}}}$$

for all $\nu \in I_L$ and $N > N_2(\epsilon, L)$ and

$$|\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}| < \frac{\epsilon}{(2L+1)^{\frac{s}{2}}}$$

for all $N > N_3(\epsilon)$. So we get from term (19)

$$\sum_{\nu\in I_L}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right)\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right) - \sum_{\nu\in I_L}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} =$$

$$= \sum_{\nu\in I_L}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}\right)\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}|\right) +$$

$$-\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}\right) -$$

$$-\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}} - \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{\alpha}}\right)$$

So we have for $N > \max(N_2(\epsilon), N_3(\epsilon))$

$$|\sum_{\nu\in I_L}\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right)\left(\frac{1}{N}\sum_{k=1}^{N}\frac{e^{-4\sqrt{t}\pi i\nu y_k}}{\overline{\nu}^{\alpha}}\right) - \sum_{\nu\in I_L}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}| <$$

$$< \epsilon^2 + \frac{\epsilon}{(2L+1)^{\frac{s}{2}}} + \frac{\epsilon}{(2L+1)^{\frac{s}{2}}}$$

Let $P = \max(L, M)$. To use these results we write

$$R_N(x,t) = \frac{1}{N^2}\sum_{k,l=1}^{N}\sum_{\nu\in I_P}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}} - \sum_{\nu\in I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} -$$

$$-2\left(\frac{1}{N}\sum_{\nu\in I_p}\sum_{k=1}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\nu y_k - \sum_{\nu\in I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\right) + \sum_{\nu\notin I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} +$$

$$+\frac{1}{N^2}\sum_{k,l=1}^{N}\sum_{\nu\notin I_P}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}} - \frac{2}{N}\sum_{\nu\notin I_p}\sum_{k=1}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\nu y_k$$

So we get the estimation

$$|R_N(x,t)| \leq$$

$$\leq |\frac{1}{N^2}\sum_{k,l=1}^{N}\sum_{\nu\in I_P}\frac{e^{4\sqrt{t}\pi i\nu(y_k-y_l)}}{\overline{\nu}^{2\alpha}} - \sum_{\nu\in I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}|+$$

$$+2|\frac{1}{N}\sum_{\nu\in I_p}\sum_{k=1}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}\cos 4\sqrt{t}\pi\nu y_k - \sum_{\nu\in I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}|+$$

$$+\sum_{\nu\notin I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} + \sum_{\nu\notin I_P}\frac{1}{\overline{\nu}^{2\alpha}} + 2\sum_{\nu\notin I_P}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} <$$

$$< \epsilon^2 + \frac{\epsilon}{(2P+1)^{\frac{s}{2}}} + \frac{\epsilon}{(2P+1)^{\frac{s}{2}}} + 2\epsilon + \epsilon + 2\epsilon + \sum_{\nu\notin I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}$$

The sum

$$\sum_{\nu\notin I_P}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}$$

can be majorized by

$$\sum_{\nu\notin I_P}\frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}$$

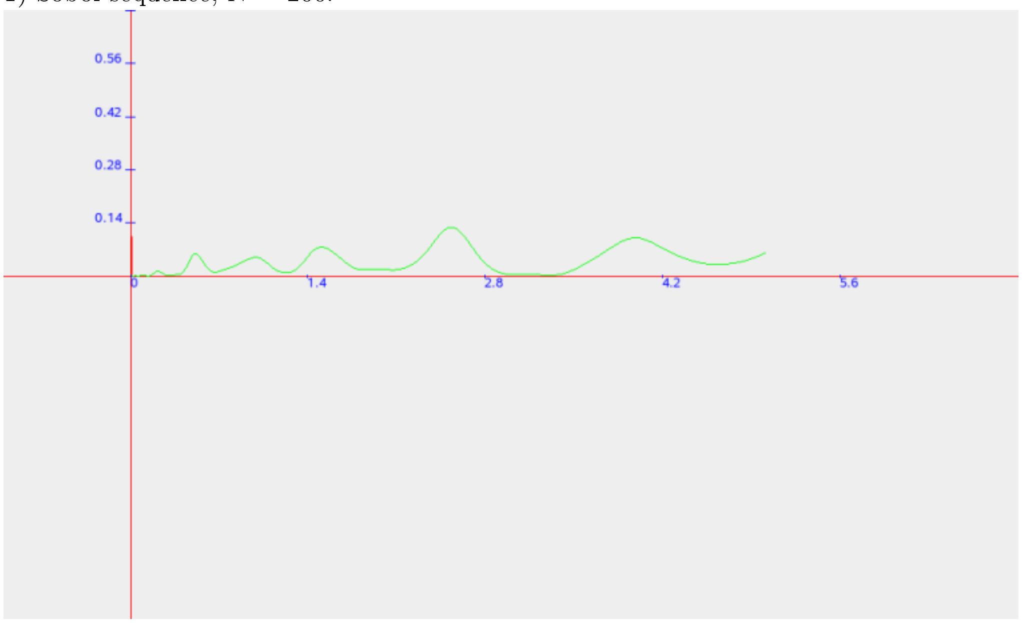
This sum is smaller than ϵ due to the fact that $P = \max(L, M)$. So

$$|R_N(x,t)| < \epsilon\left(\frac{2}{(2P+1)^{\frac{s}{2}}} + 6\right) + \epsilon^2$$

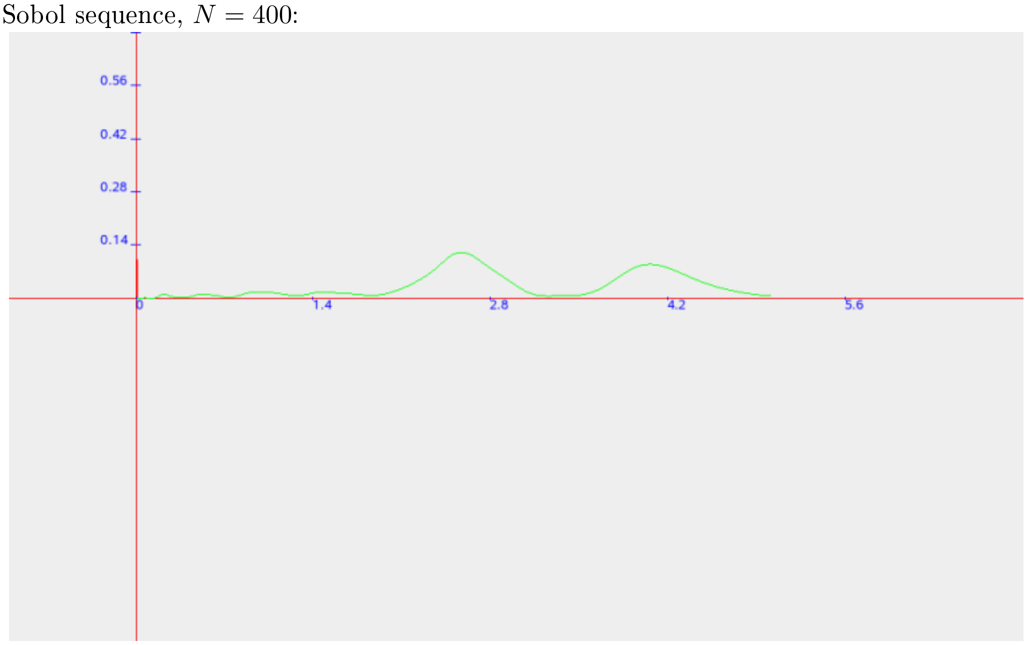
for $N > \max(N_1(\epsilon, P), N_2(\epsilon, P), N_3(\epsilon, P))$. So the theorem is proved.

In the following there are some graphs for $s = 2$ of the function $h(t) := R_N(t)$ for different values of N and different sequences:

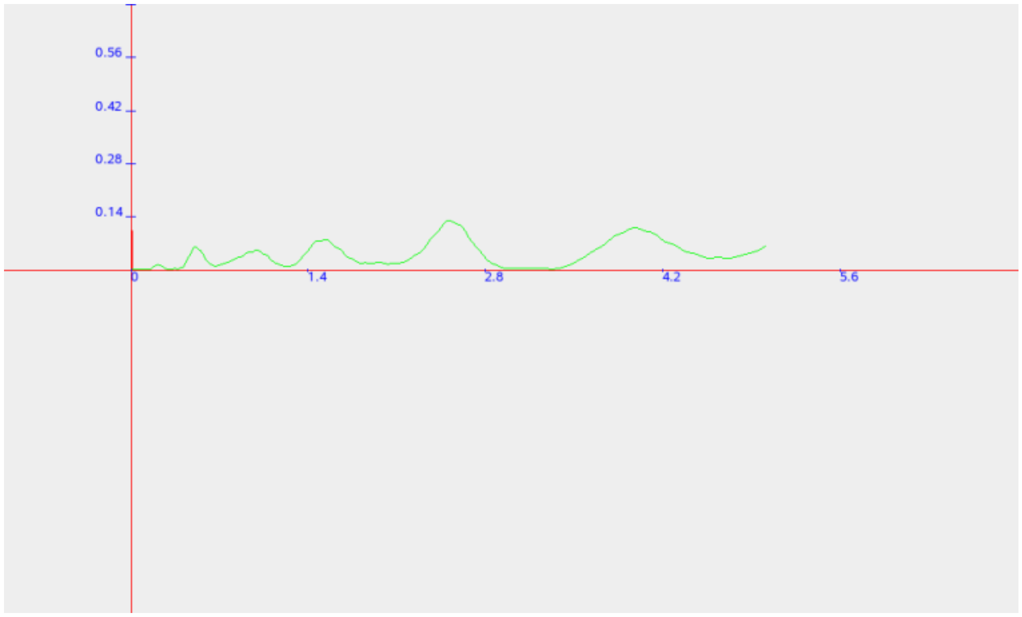
1) Sobol-sequence, $N = 200$:



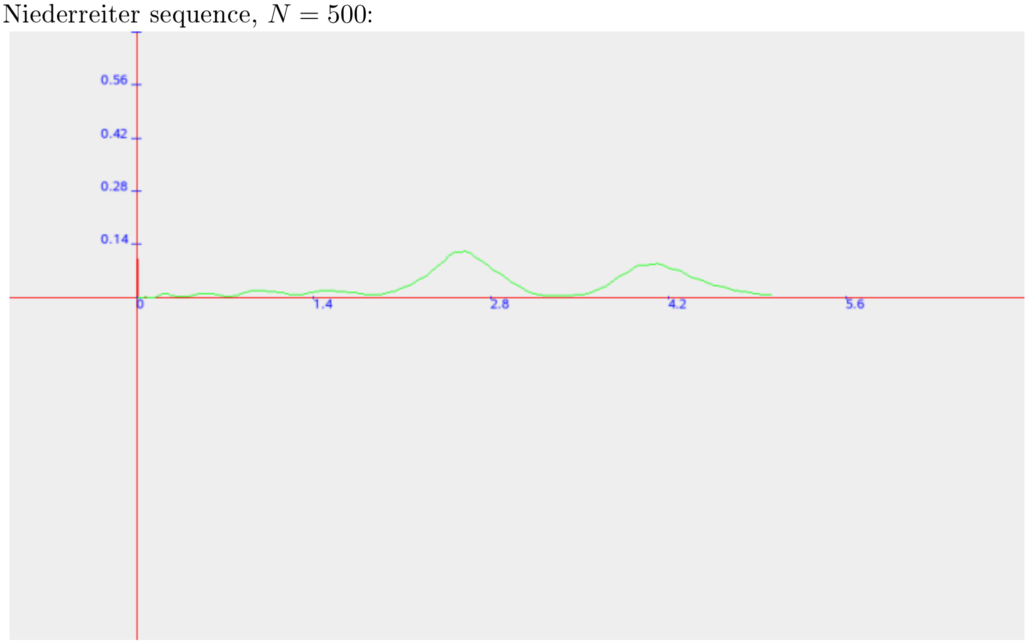
2) Sobol sequence, $N = 400$:



3) Niederreiter-Sequence, N=200:



4) Niederreiter sequence, $N = 500$:



4 A "weighted" form of $R_N(x,t)$

The algorithm can be modified. We return to the Poisson integral (**??**waerme}):

$$u(x,t) = \frac{1}{2^s \pi^{\frac{s}{2}} t^{\frac{s}{2}}} \int_{\mathbb{R}^s} u_0(y) e^{-\frac{|x-y|^2}{4t}} dy$$

At first we use the transformation

$$w_i = \frac{y_i - x_i}{2\sqrt{t}} \qquad i = 1, 2, \dots s$$

and we get

$$u(x,t) = \frac{1}{\sqrt{\pi}^s} \int_{R^s} u_0(2\sqrt{t}w_1 + x_1, \dots 2\sqrt{t}w_s + x_s) e^{-|w|^2} dw$$

Now let $\beta = (b_1, \dots, b_s)$ with $0 < b_i < 1$ for $i = 1, 2, \dots, s$. Then we can write

$$u(x,t) = \frac{1}{\pi^{\frac{s}{2}}} \int_{\mathbb{R}^s} u_0(2\sqrt{t}w_1 + x_1, \dots, 2\sqrt{t}w_s + x_s) e^{-b_1 w_1^2 - \dots - b_s w_s^2} e^{-(1-b_1)w_1^2 - (1-b_s)w_s^2} dw \tag{20}$$

Now we use the substitution

$$q_i = \Phi\left(\sqrt{1-b_i}w_i\right) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\sqrt{1-b_i}w_i} e^{-u^2} du$$

and we get from (20)

$$u(x,t) = \frac{1}{\sqrt{\prod_{i=1}^s (1-b_i)}} \int_{E^s} u_0\left(2\sqrt{t}\frac{\Phi^{-1}(q)}{\sqrt{1-b}} + x\right) e^{-\frac{b}{1-b}\left(\Phi^{-1}(q)\right)^2} dq \tag{21}$$

Of course,

$$u_0\left(2\sqrt{t}\frac{\Phi^{-1}(q)}{\sqrt{1-b}} + x\right)$$

stands for

$$u_0\left(2\sqrt{t}\frac{\Phi^{-1}(q_1)}{\sqrt{1-b_1}} + x_1, \dots 2\sqrt{t}\frac{\Phi^{-1}(q_s)}{\sqrt{1-b_s}} + x_s\right)$$

and

$$e^{-\frac{b}{1-b}\left(\Phi^{-1}(q)\right)^2}$$

is an abbrevation for

$$e^{-\frac{b_1}{1-b_1}\left(\Phi^{-1}(q_1)\right)^2 - \dots - \frac{b_s}{1-b_s}\left(\Phi^{-1}(q_s)\right)^2}$$

Evaluation of (21) leads us to an approximative solution of the IVP :

$$u_{approx}^{(w)} = \frac{1}{N} \sum_{k=1}^{N} \frac{e^{-\frac{b}{1-b}\left(\Phi^{-1}(q^{(k)})\right)^2}}{\sqrt{\prod_{i=1}^s (1-b_i)}} u_0\left(2\sqrt{t}\frac{\Phi^{-1}(q^{(k)})}{\sqrt{1-b}} + x\right)$$

We can interpret the numbers

$$w_k := \frac{e^{-\frac{b}{1-b}\left(\Phi^{-1}(q^{(k)})\right)^2}}{\sqrt{\prod_{i=1}^{s}(1-b_i)}}$$

as "weights" of the quadrature formula. By use of the scalar product in the RKHS we get again an error estimation in the form of a diaphony:

$$|u_{exact}(x,t) - u_{approx}^{(w)}(x,t)| \leq R_N^{(w)}(x,t)\|u_0\|$$

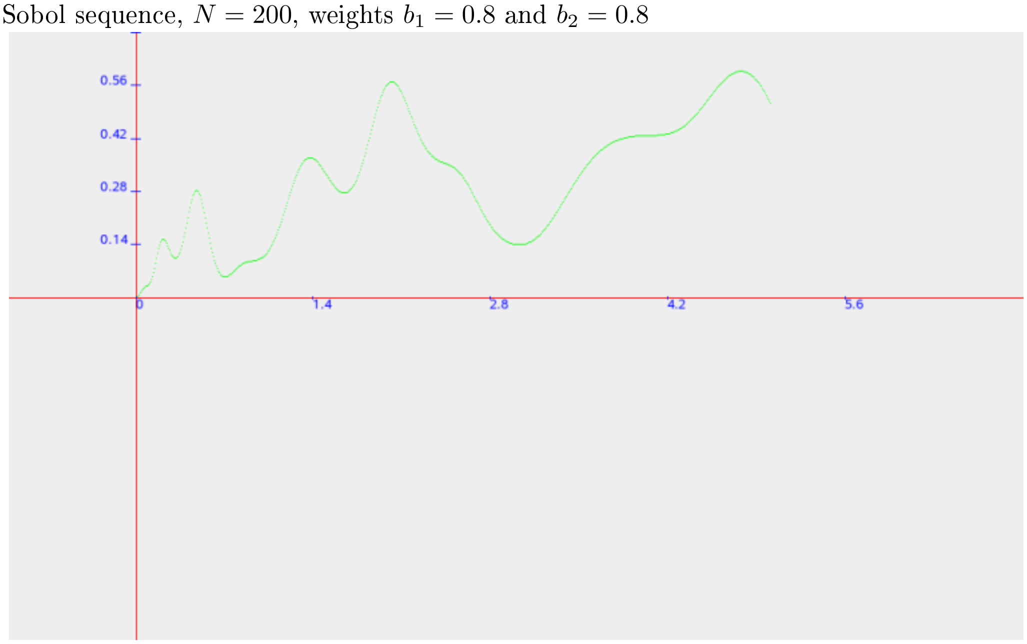
with

$$\left(R_N^{(w)}(x,t)\right)^2 = \frac{1}{N^2}\sum_{k,l=1}^{N} w_k w_l K\left(2\sqrt{t}\frac{\Phi^{-1}(q^{(k)})}{\sqrt{1-b}}, 2\sqrt{t}\frac{\Phi^{-1}(q^{(l)})}{\sqrt{1-b}}\right) -$$

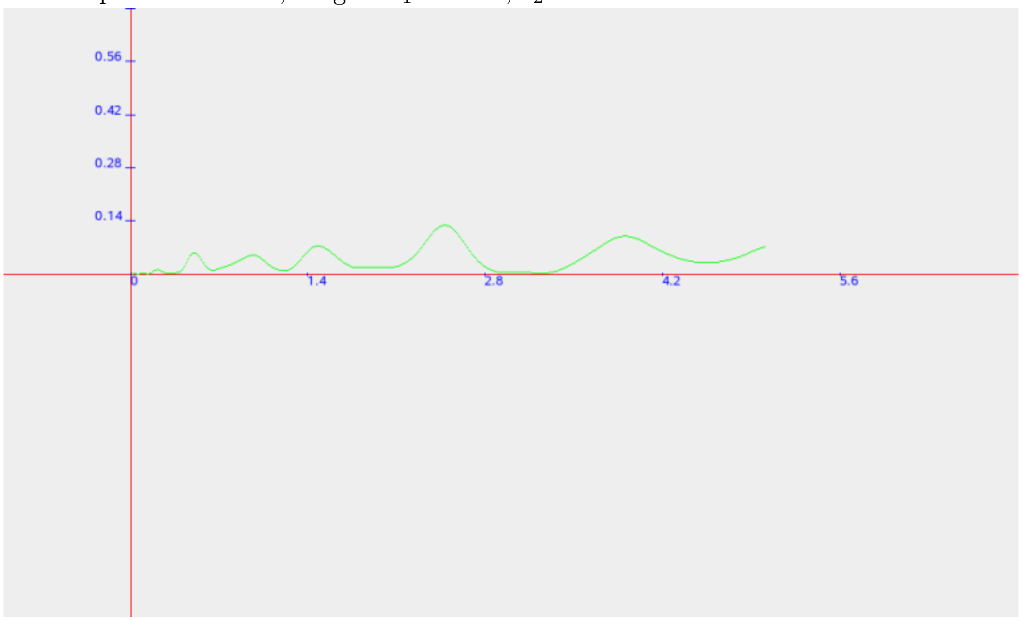
$$-\frac{2}{N}\sum_{k=1}^{N} w_k \sum_{\nu\in Z^s} \frac{e^{-4t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}} \cos 4\sqrt{t}\pi\nu\frac{\Phi^{-1}(q^{(k)})}{\sqrt{1-b}} +$$

$$+\sum_{\nu\in Z^s}\frac{e^{-8t\pi^2|\nu|^2}}{\overline{\nu}^{2\alpha}}$$

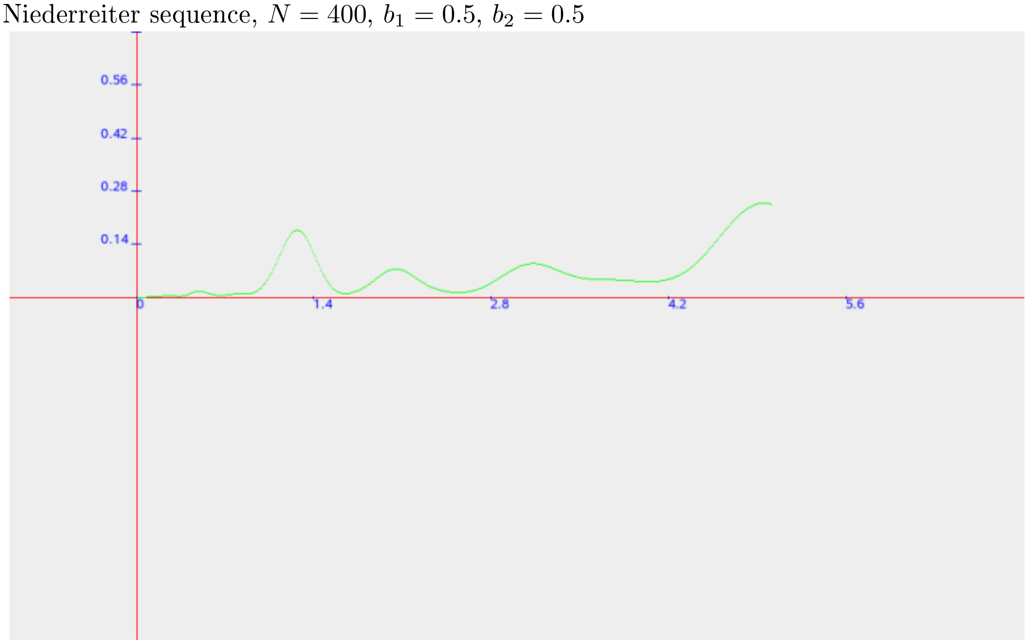
The term $R_N^{(w)}(x,t)$ is the "weighted" form of $R_N(x,t)$.
In the following there are some graphs for $s = 2$ of $h(t) := R_N^{(w)}(t)$ for different sequences and different weights:
1) Sobol sequence, $N = 200$, weights $b_1 = 0.8$ and $b_2 = 0.8$



2) Sobol sequence $N = 200$, weights $b_1 = 0.02$, $b_2 = 0.02$:



3) Niederreiter sequence, $N = 400$, $b_1 = 0.5$, $b_2 = 0.5$



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