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QUASI-MONTE CARLO INTEGRATION IN UNANCHORED SOBOLEV SPACES

Jana Fialová

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ABSTRACT. We find a concrete sequence of N points, for which the squared worst-case quasi-Monte Carlo error in the Hilbert space of continuous functions defined on $[0,1]$ with square integrable second derivative is smaller than for the centered regular lattice point set.

1. Introduction

In this article we consider two Hilbert spaces of functions $\mathcal{H}_1, \mathcal{H}_2$ with different degrees of smoothness. They are defined, for example, in [H02: p. 277] and [DP10] also in weighted and multidimensional case. We restrict our attention to the one-dimensional case where the spaces are defined as follows:

$$\mathcal{H}_\alpha = \{f: \ \|f\|_\alpha < \infty\}, \qquad \alpha = 1, 2,$$

where

$$\|f\|_1^2 = \left[\int_0^1 f(x)\,\mathrm{d}x\right]^2 + \int_0^1 \left[f'(x)\right]^2 \mathrm{d}x, \tag{1}$$

$$\|f\|_2^2 = \left[\int_0^1 f(x)\,\mathrm{d}x\right]^2 + \left[\int_0^1 f'(x)\,\mathrm{d}x\right]^2 + \int_0^1 \left[f''(x)\right]^2 \mathrm{d}x, \qquad \text{respectively.}$$

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So $\mathcal{H}_\alpha$ are the spaces of absolutely continuous functions defined on $[0,1]$ for which the derivatives up to order α are square integrable. These Hilbert spaces are also known as *unanchored Sobolev spaces* and have the reproducing kernel

$$K_\alpha(x,y) = \frac{(-1)^{\alpha+1}}{(2\alpha)!} B_{2\alpha}(|x-y|) + \sum_{t=0}^{\alpha} \frac{1}{(t!)^2} B_t(x) B_t(y),$$

where $\alpha = 1,2$ and B_t is the tth Bernoulli polynomial.

The aim of this paper is to consider the integration error in these spaces. We are interested in the squared worst-case error defined as follows

$$\mathrm{e}^2_\alpha(P) = \sup_{\substack{f\in\mathcal{H}_\alpha \\ \|f\|_\alpha \le 1}} \left| \frac{1}{N} \sum_{n=0}^{N-1} f(x_n) - \int_0^1 f(x)\,\mathrm{d}x \right|^2 \tag{2}$$

where $P = (x_n)_{n=0}^{N-1}$ is the given sequence.

The starting sequence is $\left(\frac{n}{N}\right)_{n=0}^{N-1}$ called the regular lattice sequence. This sequence is transformed using uniform distribution preserving functions [SP05: 2.5.1], especially the tent function $\Phi(x) = 1 - |2x-1|$, $x \in [0,1]$ (called also the baker's transformation) and the function $f_\sigma(x) = x + \sigma \mod 1$ where σ is an arbitrary positive real number.

Applying $f_\sigma(x)$ for $\sigma = \frac{1}{2N}$ we have the sequence $\left(\frac{n}{N} + \frac{1}{2N}\right)_{n=0}^{N-1}$, which is called *the centered regular lattice point set.* For example the centered regular lattice of $N = 6$ points is shown in Fig. 1.

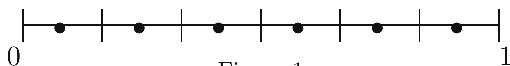

Figure 1

It is known, that this sequence minimizes some errors like the L_2 discrepancy [SP05: 2.22.15] and, based on a result of G. Larcher (see [DP10: p. 10]), it minimizes the integration error for the class of uniformly continuous functions with a fixed modulus of continuity M_f, where

$$M_f(\delta) := \sup_{\substack{x,y\in[0,1] \\ |x-y|\le\delta}} |f(x) - f(y)| \qquad \text{for} \quad \delta \ge 0.$$

In [CDLP] the authors study the squared worst-case error $\mathrm{e}^2_\alpha(P)$ in the Hilbert space $\mathcal{H}_2$. They use the sequence $\left(\frac{n}{N} \oplus \sigma\right)_{n=0}^{N-1}$ where $\oplus$ is a digit-wise addition modulo a base b. They prove that the mean of the error over all $\sigma \in [0,1]$ using this sequences is greater than using the sequences $\Phi\left(\left(\frac{n}{N} \oplus \sigma\right)\right)_{n=0}^{N-1}$ where Φ is the tent function. It should be mentioned that the paper [CDLP] actually deals with the multidimensional case.

In the second section of this paper the sequences $P = \left(\frac{n}{N} + \sigma \mod 1\right)_{n=0}^{N-1}$ are considered and we compute the squared worst-case error $e^2_2(P)$ with the parameter σ which enables us to count the concrete value of σ for which the error is minimal. Section 3 deals with the sequence $\Phi(P)$, where Φ is the tent function and P is the same sequence as above. From our results the same result as in [CDLP] can be deduced: the mean of the squared worst-case error $e_2^2(\Phi(P))$ over all $\sigma \in [0,1]$ is lower than the mean of $\mathrm{e}_2^2(P)$. Moreover the squared worst-case error is lower with the tent function for all σ's except $\frac{k}{2N}$, k odd.

The most important result is the corollary to Theorem 3, where we find a sequence $\widetilde{P}$, for which the squared worst-case error $\mathrm{e}_2^2(\widetilde{P})$ is lower than with the centered regular lattice points set in the Hilbert space of continuous functions with square integrable first and second derivatives. For completeness it is proved in Theorem 4 that in the Hilbert space of absolutely continuous functions with only first square integrable derivative the centered regular lattice point set is better than the sequence $\widetilde{P}$.

Theorem 1 recalls the known formula [DP10: Th. 15.12] for the error $e_\alpha^2(P)$ in the Hilbert spaces $\mathcal{H}_\alpha$ which is used in the following theorems.

Theorem 1. *The squared worst-case error* e_α^2 *in the Hilbert space* $\mathcal{H}_\alpha$ *defined in* (1) *using the sequence* $P = (x_n)_{n=0}^{N-1}$ *is*

$$\mathrm{e}_\alpha^2(P) = \frac{1}{N^2} \sum_{m,n=0}^{N-1} K_\alpha(x_m, x_n) - 1.$$

2. The shifted regular lattice sequence

By the shifted regular lattice sequence we mean the sequence of N points defined as follows:

$$P_\sigma = \left(\frac{n+\sigma}{N}\right)_{n=0}^{N-1}, \qquad \sigma \in [0,1].$$

Notice that this sequence is apart from the order the same as $\left(\frac{n}{N}+\sigma_1 \bmod 1\right)_{n=0}^{N-1}$, where $\sigma_1 \in \mathbb{R}$ because the sets of points

$$\left\{\tfrac{n}{N} + \tfrac{\sigma}{N} :\ n = 0,1,\dots,N-1\right\} \qquad \text{and}$$
$$\left\{\left(\tfrac{n}{N} + \tfrac{\sigma+k}{N}\right) \mod 1 :\ n = 0,1,\dots,N-1,\ \ k \in \mathbb{N}_0\right\}$$

are the same as indicated by Fig. 2. Clearly the order does not affect the value of the error.

Figure 2

The following theorem provides a formula for the squared worst-case error depending on the value of σ, which enables us to compute the "best" σ. This will be done in the following Corollary 1.

Theorem 2. *For any $\sigma \in [0,1]$ we have*

$$\mathrm{e}_2^2(P_\sigma) = \frac{1}{N^2}\left(\sigma - \frac{1}{2}\right)^2 + \frac{1}{720N^4} + \frac{1}{4N^4}\left(\frac{1}{6} - \sigma + \sigma^2\right)^2.$$

P r o o f. By Theorem 1 the squared worst-case error $\mathrm{e}_2^2(P_\sigma)$ is given by

$$\begin{aligned} N^2\mathrm{e}_2^2(P_\sigma) = &-\frac{1}{24}\sum_{m,n=0}^{N-1}\left(|x_m - x_n|^4 - 2|x_m - x_n|^3 + |x_m - x_n|^2 - \frac{1}{30}\right) \\ &+ \left(\sum_{n=0}^{N-1}\left(x_n - \frac{1}{2}\right)\right)^2 + \frac{1}{4}\left(\sum_{n=0}^{N-1}\left(x_n^2 - x_n + \frac{1}{6}\right)\right)^2, \end{aligned} \tag{3}$$

where $P_\sigma = \left(\frac{n}{N} + \frac{\sigma}{N}\right)_{n=0}^{N-1}$.

For the second summand in the above equation we have

$$\left(\frac{1}{N}\sum_{n=0}^{N-1} n + \sigma - \frac{N}{2}\right)^2 = \left(\sigma - \frac{1}{2}\right)^2, \tag{4}$$

the third one is equal to

$$\frac{1}{4}\left(\frac{1}{N^2}\sum_{n=0}^{N-1}(n+\sigma)^2 - \frac{1}{N}\sum_{n=0}^{N-1}(n+\sigma) + \frac{N}{6}\right)^2 = \frac{1}{4N^2}\left(\frac{1}{6} - \sigma + \sigma^2\right)^2. \tag{5}$$

In the first summand in (3) we have the differences $|x_m - x_n|$ which are equal to:

- 0: N times,
- $\frac{k}{N}$: $(2N - 2k)$ times, where $k = 1, 2, \dots, N-1$.

So the first summand is equal to

$$\begin{aligned} &-\frac{1}{24}\left(-\frac{N}{30} + \sum_{k=1}^{N-1}(2N-2k)\left(\left(\frac{k}{N}\right)^4 - 2\left(\frac{k}{N}\right)^3 + \left(\frac{k}{N}\right)^2 - \frac{1}{30}\right)\right) \\ &= -\frac{1}{24}\left(-\frac{N}{30} - \frac{2}{N^4}\sum_{k=1}^{N-1}k^5 + \frac{6}{N^3}\sum_{k=1}^{N-1}k^4 - \frac{6}{N^2}\sum_{k=1}^{N-1}k^3 + \frac{2}{N}\sum_{k=1}^{N-1}k^2\right. \\ &\quad \left. + \frac{2}{30}\sum_{k=1}^{N-1}k - \frac{2N(N-1)}{30}\right) = \frac{1}{720N^2}. \end{aligned} \tag{6}$$

From (4), (5) and (6) the result follows immediately. □

Using Theorem 2 we can compute the mean square worst-case error

$$\int_0^1 e_2^2(P_\sigma)\,\mathrm{d}\sigma = \frac{1}{12N^2} + \frac{1}{360N^4}$$

but the more interesting is the following:

Corollary 1. *The squared worst-case error is minimized for $\sigma = \frac{1}{2}$, i.e. the centered regular lattice point set. This error is*

$$\mathrm{e}_2^2(P_{\frac{1}{2}}) = \frac{1}{320N^4}.$$

This is the only case, where the squared worst-case error is of the order $O\left(\frac{1}{N^4}\right)$.

3. The tent function

The second considered sequence is the shifted regular lattice sequence transformed by the tent function. We assume that the number of points of this sequence is even. Obviously, it is also possible to assume an odd number of points but in this case we would have slightly worse results than with an even number of points.

The tent function $\Phi(x) = 1 - |2x - 1|$ is the uniform distribution preserving function and it can be rewritten as:

$$\Phi(x) = \begin{cases} 2x & \text{if } x \in \left[0, \frac{1}{2}\right], \\ 2 - 2x & \text{if } x \in \left(\frac{1}{2}, 1\right]. \end{cases}$$

The considered sequence in this section is then $\Phi(P_\sigma)$ but here it is sufficient to study only $\Phi\left(\frac{n}{N} + \frac{\sigma}{N}\right)$, $\sigma \in \left[0, \frac{1}{2}\right]$ because $\left\{\Phi\left(\frac{n}{N} + \frac{\sigma}{N}\right) : n = 0, 1, \ldots, N-1\right\} = \left\{\Phi\left(\frac{n}{N} + \frac{1-\sigma}{N}\right) : n = 0, \ldots, N-1\right\}$ as indicated by Fig. 3.

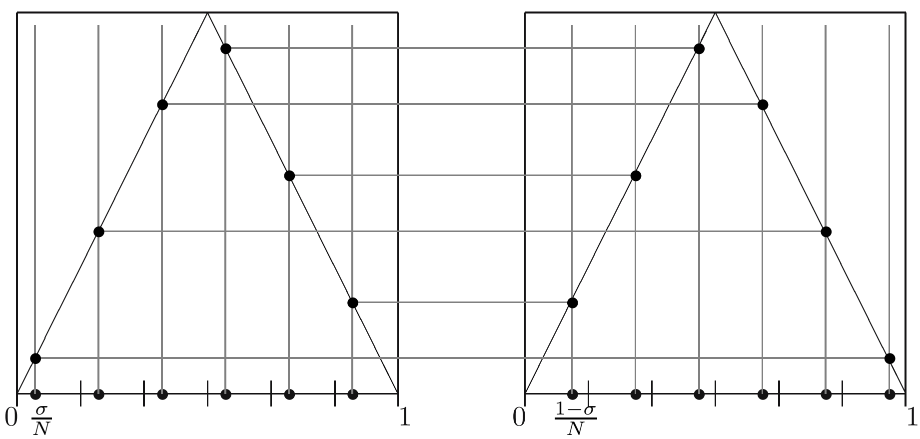

Figure 3

The above expression of the sequence $\Phi(P_\sigma)$ is not appropriate for the calculations, therefore we give another expression where the points are reordered by the size.

Lemma 1. *For any even N and any $\sigma \in [0,1)$ we have*

$$\Phi(P_\sigma) = \left(\frac{2\left\lfloor \frac{n+1}{2} \right\rfloor + (-1)^n 2\sigma}{N} \right)_{n=0}^{N-1},$$

where $\lfloor x \rfloor$ means the integer part of x.

P r o o f. Since N is even we have

$$\Phi(P_\sigma) = \begin{cases} \frac{2k+2\sigma}{N} & \text{for } k = 0,1,\dots,\frac{N}{2}-1, \\ 2 - \frac{2k+2\sigma}{N} & \text{for } k = \frac{N}{2},\dots,N-1, \end{cases}$$

and

$$\left(\frac{2\left\lfloor \frac{n+1}{2} \right\rfloor + (-1)^n 2\sigma}{N} \right)_{n=0}^{N-1} = \begin{cases} \frac{n+2\sigma}{N} & \text{for even } n = 0,2,\dots,N-2, \\ \frac{n+1-2\sigma}{N} & \text{for odd } n = 1,3,\dots,N-1. \end{cases}$$

In the first case substitute $2k$ for n and in the second $2N-(2k+1)$ for n. □

The exact value of the squared worst-case error $e_2^2(\Phi(P_\sigma))$ is given in the following theorem. This is then compared with the squared worst-case error $e_2^2(P_\sigma)$.

Theorem 3. *For any even N and any $\sigma \in \left[0, \frac{1}{2}\right]$ we have*

$$e_2^2(\Phi(P_\sigma)) = \frac{1}{N^4}\left(-\frac{4\sigma^4}{3} - \frac{8\sigma^3}{3} + 4\sigma^2 - \frac{4\sigma}{3} + \frac{2}{15} \right),$$

where Φ is the tent function.

P r o o f. By Lemma 1 the sequence $\Phi(P_\sigma)$ is

$$\frac{2\sigma}{N}, \frac{2}{N} - \frac{2\sigma}{N}, \frac{2}{N} + \frac{2\sigma}{N}, \frac{4}{N} - \frac{2\sigma}{N}, \dots, \frac{N-2}{N} - \frac{2\sigma}{N}, \frac{N-2}{N} + \frac{2\sigma}{N}, 1 - \frac{2\sigma}{N}.$$

Notice that these points are symmetric with respect to the point $\frac{1}{2}$ and so

$$\sum_{n=0}^{N-1} x_n = \frac{N}{2}.$$

For the squared worst-case error based on $\Phi(P_\sigma)$ we have

$$N^2 e_2^2(\Phi(P_\sigma)) = -\frac{1}{24}\sum_{m,n=0}^{N-1}\left(|x_m-x_n|^4-2|x_m-x_n|^3+|x_m-x_n|^2-\frac{1}{30}\right) + \left(\sum_{n=0}^{N-1}\left(x_n-\frac{1}{2}\right)\right)^2+\frac{1}{4}\left(\sum_{n=0}^{N-1}\left(x_n^2-x_n+\frac{1}{6}\right)\right)^2. \tag{7}$$

The second summand of (7) is zero for every σ, the third one is

$$\frac{1}{4}\left(\frac{1}{N^2}(4\sigma^2+2\cdot 2^2+2\cdot 4\sigma^2+2\cdot 4^2+2\cdot 4\sigma^2+\cdots+2(N-2)^2+2\cdot 4\sigma^2 + N^2-4N\sigma+4\sigma^2)-\frac{N}{2}+\frac{N}{6}\right)^2$$
$$=\frac{1}{4}\left(\frac{1}{N^2}\left(2\cdot 4\sigma^2\frac{N}{2}+8\sum_{k=1}^{\frac{N}{2}-1}k^2+N^2-4N\sigma\right)-\frac{N}{2}+\frac{N}{6}\right)^2$$
$$=\frac{1}{4N^2}\left(4\sigma^2-4\sigma+\frac{2}{3}\right)^2. \tag{8}$$

In the first summand in (7) we have the differences $|x_m-x_n|$ which are equal to:

- 0: N times,
- $\frac{4\sigma}{N}$: $(N-2)$ times,
- $\frac{2k}{N}$: $(2N-4k)$ times, where $k=1,2,\ldots,\frac{N}{2}-1$,
- $\frac{2k}{N}-\frac{4\sigma}{N}$: $(N-2k+2)$ times, where $k=1,2,\ldots,\frac{N}{2}$,
- $\frac{2k}{N}+\frac{4\sigma}{N}$: $(N-2k-2)$ times, where $k=1,2,\ldots,\frac{N}{2}-2$.

Now compute the sum

$$\sum_{m,n=0}^{N-1}\left(|x_m-x_n|^4-2|x_m-x_n|^3+|x_m-x_n|^2-\frac{1}{30}\right). \tag{9}$$

First consider the differences $0, \frac{4\sigma}{N}, 1-\frac{4\sigma}{N}$:
The difference 0 appears $-\frac{N}{30}$ times,
the difference $\frac{4\sigma}{N}$ appears $(N-2)\left(\frac{256\sigma^4}{N^4}-\frac{128\sigma^3}{N^3}+\frac{16\sigma^4}{N^2}-\frac{1}{30}\right)$ times and
the difference $1-\frac{4\sigma}{N}$ appears in the forth case for $k=\frac{N}{2}$:
$2\Big(\left(1-\frac{4\sigma}{N}\right)^4-2\left(1-\frac{4\sigma}{N}\right)^3+\left(1-\frac{4\sigma}{N}\right)^2-\frac{1}{30}\Big)$ times.

These three expressions together sum up to

$$\frac{4^4\sigma^4}{N^3}-2\frac{4^3\sigma^3}{N^2}+\frac{16\sigma^2}{N}-\frac{N}{15}. \tag{10}$$

To the fifth case we can add also $k = \frac{N}{2} - 1$ since the difference $\frac{2k}{N} + \frac{4\sigma}{N}$ appears $(N - 2k - 2) = 0$ times. Therefore all the remaining cases in (9) sum up to

$$\sum_{k=1}^{\frac{N}{2}-1} \Bigg[(2N-2k)\left(\left(\frac{2k}{N}\right)^4 - 2\left(\frac{2k}{N}\right)^3 + \left(\frac{2k}{N}\right)^2 - \frac{1}{30}\right) + (N-2k+2)\left(\left(\frac{2k}{N} - \frac{4\sigma}{N}\right)^4 - 2\left(\frac{2k}{N} - \frac{4\sigma}{N}\right)^3 + \left(\frac{2k}{N} - \frac{4\sigma}{N}\right)^2 - \frac{1}{30}\right) + (N-2k-2)\left(\left(\frac{2k}{N} + \frac{4\sigma}{N}\right)^4 - 2\left(\frac{2k}{N} + \frac{4\sigma}{N}\right)^3 + \left(\frac{2k}{N} + \frac{4\sigma}{N}\right)^2 - \frac{1}{30}\right)\Bigg].$$

From this we get

$$\sum_{k=1}^{\frac{N}{2}-1} k^5 \frac{-128}{N^4} + \sum_{k=1}^{\frac{N}{2}-1} k^4 \frac{192}{N^3} + \sum_{k=1}^{\frac{N}{2}-1} k^3 \left(-\frac{96}{N^2} - \frac{512\sigma}{N^4} - \frac{1536\sigma^2}{N^4}\right) + \sum_{k=1}^{\frac{N}{2}-1} k^2 \left(\frac{16}{N} + \frac{384\sigma}{N^3} + \frac{1536\sigma^2}{N^3}\right) + \sum_{k=1}^{\frac{N}{2}-1} k \left(\frac{8}{30} - \frac{2048\sigma^3}{N^4} - \frac{64\sigma}{N^2} - \frac{448\sigma^2}{N^2} - \frac{1024\sigma^4}{N^4}\right) + \left(\frac{N}{2} - 1\right)\left(-\frac{4N}{30} + \frac{512\sigma^3}{N^3} + \frac{512\sigma^4}{N^3} + \frac{32\sigma^2}{N}\right).$$

After summation and simplification the preceding expression is equal to:

$$\frac{N}{15} - \frac{16\sigma^2}{N} + \frac{1}{N^2}\left(\frac{8}{3} + 32\sigma^2 + 128\sigma^3 - \frac{16}{5}\right) - \frac{256\sigma^4}{N^3}. \tag{11}$$

The expressions (10) and (11) together give the value of (9):

$$\frac{1}{N^2}\left(\frac{8}{3} + 32\sigma^2 - 128\sigma^3 + 128\sigma^4 - \frac{16}{5}\right).$$

So the error is $-\frac{1}{24}$ of the above expression plus the summand (8), which gives the desired result. □

Remark 1. For $\sigma = \frac{1}{4}$ we obtain the centered regular lattice points set, which leads again to the squared worst-case error $\frac{1}{320N^4}$.

As in the previous section, we may compute the mean of the squared worst-case error which is

$$\int_0^1 e_2^2(\Phi(P_\sigma))\,\mathrm{d}\sigma = 2\int_0^{\frac{1}{2}} e_2^2(\Phi(P_\sigma))\,\mathrm{d}\sigma = \frac{1}{30N^4}$$

and thus we get the well-known result, that with the tent function the mean square worst-case error is of the order $O(N^{-4})$ in contrast to the sequence P_σ which gives only the order $O(N^{-2})$. But the more interesting is the minimum of the squared worst-case error.

Corollary 2. *The minimum of the squared worst-case error $e_2^2(\Phi(P_\sigma))$, where Φ is the tent transformation and N is even, is attained for $\sigma = -1 + \frac{\sqrt{6}}{2}$. The squared worst-case error equals $\frac{1}{N^4}\left(\frac{49}{5} - 4\sqrt{6}\right)$.*

So the "best" sequence of the shifted regular lattice sequences transformed with the tent function in the Sobolev space $\mathcal{H}_2$ is

$$\left(\frac{2\left\lfloor\frac{n+1}{2}\right\rfloor + (-1)^n(\sqrt{6}-2)}{N}\right)_{n=0}^{N-1}, \tag{12}$$

where $\lfloor x\rfloor$ is the integer part of x.

From the above corollary it follows, that we can obtain approximately the same squared worst-case error using the sequence of N centered regular lattice points as using only $N_1 = N\sqrt[4]{320\left(\frac{49}{5} - 4\sqrt{6}\right)} \approx 0,89898N$ points of the sequence (12).

For example for $N = 6$ the following Fig. 4 shows on the left the centered regular lattice with the squared worst-case error $2.4113 \cdot 10^{-6}$ and on the right the sequence (12) with the squared worst-case error $1.5749 \cdot 10^{-6}$.

Figure 4

Finally we provide also the value of the squared worst-case error $e_1^2(\Phi(P_\sigma))$ in the space $\mathcal{H}_1$. It is easily seen that the above result does not hold in the space $\mathcal{H}_1$.

Theorem 4. *For any even N and any $\sigma \in \left[0, \frac{1}{2}\right]$ we have*

$$e_1^2(\Phi(P_\sigma)) = \frac{1}{2N^2}\left(\frac{2}{3} + 8\sigma^2 - 4\sigma\right).$$

Moreover, the minimum is attained by the centered regular lattice point set.

The proof is similar to the proof of Theorem 3.

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Mathematical Institute
Slovak Academy of Sciences
Štefánikova 49
SK–814 73 Bratislava
SLOVAKIA
E-mail: jana.fialova@mat.savba.sk