Univerzita Karlova v Praze

Matematicko-fyzikální fakulta

BAKALÁŘSKÁ PRÁCE

Zuzana Bílková

Numerické řešení inverzních integrálních rovnic matematického modelování ve výzkumu biopaliv

Katedra numerické matematiky

Vedoucí bakalářské práce: RNDr. Iveta Hnětynková, Ph.D.

Studijní program: Matematika

Studijní obor: Obecná matematika

Praha 2012

Acknowledgement

I would like to thank my supervisor RNDr. Iveta Hnětynková, Ph.D. and my consultant Prof. Dr. Rosemary Anne Renaut for their time dedicated to consultations and reading this bachelor thesis, for many valuable suggestions and comments.

I declare that I carried out this bachelor thesis independently, and only with the cited sources, literature and other professional sources.

I understand that my work relates to the rights and obligations under the Act No. 121/2000 Coll., the Copyright Act, as amended, in particular the fact that the Charles University in Prague has the right to conclude a license agreement on the use of this work as a school work pursuant to Section 60 paragraph 1 of the Copyright Act.

In Prague date 23th May 2012

Zuzana Bílková

Název práce: Numerické řešení inverzních integrálních rovnic matematického modelování ve výzkumu biopaliv

Autor: Zuzana Bílková

Katedra / Ústav: Katedra numerické matematiky

Vedoucí bakalářské práce: RNDr. Iveta Hnětynková, Ph.D., Katedra numerické matematiky MFF UK

Abstrakt: Cílem této bakalářské práce je numerické řešení Fredholmových integrálních rovnic prvního řádu, které se vyskytují ve výzkumu biopaliv. Práce se zaměřuje na studium Lagrangových interpolačních kvadraturních formulí. Uvažujeme lichoběžníkové a Simpsonovo pravidlo s využitím ekvidistantního a logaritmického dělení. Cílem práce je srovnání těchto pravidel a nalezení nejvhodnější metody. Práce se dále zabývá určením minimálního počtu naměřených dat tak, abychom dosáhli dané přesnosti. Poznatky jsou demonstrovány na numerických experimentech se simulovanými daty.

Klíčová slova: inverzní integrální rovnice, kvadratura, konvergence, odhad chyby

Title: Numerical solution of inverse integral equations arising in mathematical modeling for biofuel research

Author: Zuzana Bílková

Department: Department of Numerical Mathematics

Supervisor: RNDr. Iveta Hnětynková, Ph.D., Department of Numerical Mathematics

Abstract: The aim of this bachelor thesis is numerical solution of a Fredholm integral equation of the first kind arising in the biofuel research. The thesis focuses on the Lagrange interpolatory quadrature formulae. The Trapezoidal and the Simpson rules with equidistant and logarithmic spacing are considered. The goal is to compare these formulae and to determine the most applicable. The thesis also concerns the minimum number of required measurement data to achieve given accuracy. Numerical experiments with simulated data are presented.

Keywords: inverse integral equation, quadrature, convergence, error estimates

Contents

Introduction

In many physical and chemical applications we are faced with the problem of calculating the solution of a Fredholm integral equation of the first kind from experimental data. We consider the solution of the Fredholm integral equation which arises in the analysis of polarization processes occurring at the electrode-electrolyte interfaces of solid fuel cells (SOFC) [1, 2, 3]. These processes may be investigated physically using Electrochemical Impedance Spectroscopy (EIS). From measured impedance data it is of practical relevance to determine the relaxation times for the measured distribution functions [1, 4, 5, 6, 7]. The specific mathematical model is derived from an equivalent circuit model. The modeling is often insufficient. Due to the high complexity of the system, the individual impedance-related processes within single cell operation can usually not be separated by the model. In impedance data analysis the Distribution function of Relaxation Times (DRT) is the basic quantity of interest [2]. It has been used to differentiate resistances from different processes from impedance spectra of solid oxide fuel cells [1, 4, 5, 6, 7]. Two different approaches have been suggested in the literature to the problem of unfolding the DRT from the observed impedance data; a convolutional model introduced by [2] and used in [5, 6, 7, 8] or direct quadrature solution of the ill-posed Fredholm integral equation of the first kind, first introduced for this application by [3], see also [9, 10, 1]. From integral transforms it was obtained a convolution equation that connects the distribution function to the impedance spectrum

$$Z(\omega) = R_0 + Z_{pol}(\omega) = R_0 + R_{pol} \int_0^\infty \frac{\gamma(\tau)}{1 + i\omega\tau} d\tau, \tag{1}$$

$$\int_0^\infty \gamma(\tau) d\tau = 1,$$

where $\gamma(\tau)$ is the DRT, $Z(\omega)$ is the impedance data, R_0 is the ohmic (frequency independent) part of the impedance, $Z_{pol}(\omega)$ is the polarization part and R_{pol} is the polarization resistance of the impedance, see [2]. However, in practical measurements, the entire impedance spectrum $Z(\omega)$ cannot be measured. Only a part of the spectrum is sampled at a certain number of discrete points over a finite frequency range and therefore the convolution equation cannot be solved analytically. In the DRT analysis we seek the function $\gamma_k(\tau) = R_k K_k(\tau)$ for each k, corresponding, in this terminology, to the DRT for process k, practically obtaining $\gamma(\tau) = \sum_k \gamma_k(\tau)$, see [1]. The equation can be separated into its real and imaginary parts

$$\begin{aligned} Z(\omega) &= Z_1(\omega) + iZ_2(\omega) \\ &= \left(R_0 + R_{pol} \int_0^\infty \frac{\gamma(\tau)}{1+\omega^2\tau^2} d\tau\right) - i \left(R_{pol} \int_0^\infty \frac{\omega\tau\gamma(\tau)}{1+\omega^2\tau^2} d\tau\right). \end{aligned} \quad (2)$$

Numerically the challenge generally is to find $\gamma(\tau)$ given measurements $Z(\omega_m)$, $m = 1, ..., M$, for some M. For the specific Anode-respiring bacteria application R_{pol} is not known and is absorbed into the unknown $\gamma(\tau)$, see [1]. The integrals in both the real and imaginary parts $(Z_{1,} Z_2)$ are Fredholm integral equations of the first kind.

This thesis studies numerical quadratures for the integrals in (2). We focus on the Lagrange interpolatory quadrature formulae; the Trapezoidal formula and the Simpson formula. It has been observed, see [1], that equidistant spacing of quadrature nodes is for the considered problem inappropriate. Thus after reviewing formulae using equidistant spacing according to literature, we derive formulae for non-equidistant spacing. The quadrature errors for the rules using non-equidistant spacing are also derived. We compare the Trapezoidal and the Simpson formulae with equidistant and logarithmic spacing in numerical experiments for simulated data. We discuss which formula is the most applicable in our case. The thesis also concerns determination of the minimum number of measurement data required for each experiment to achieve given error tolerance.

The structure of the thesis is the following. The first chapter presents quadrature formulae and the corresponding error estimates. The second chapter is dedicated to initial numerical experiments with simulated functions. We show approximations of integrals, error estimations and the minimum number of measurement data required. The third chapter presents numerical experiments with the integrals in (2).

Notation

$\mathbb{N}$	set of natural numbers
$\mathbb{P}_k$	set of polynomials of degree $k \in \mathbb{N}$
$[a, b]$	interval of integration
$C^n([a, b])$	space of functions over interval $[a, b]$ with continuous derivative of order $n \in \mathbb{N}$
l_i	characteristic Lagrange polynomial, $l_i(x) = \prod_{j=0,\, j\neq i}^{n} \frac{x-x_j}{x_i-x_j}$
f_n	Lagrange polynomial of function f of degree n, $f_n(x) = \sum_{i=0}^{n} f(x_i)l_i(x)$
m	number of subintervals for quadrature
h	interval size for regular quadrature spacing
x_i	nodes of the quadrature, $i = 0, 1, \ldots, n$
$I(f)$	exact value of integral, $I(f) \equiv \int_a^b f(x)dx$
$I_n(f)$	numerical approximation, $I_n(f) \equiv I(f_n)= \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)dx$
$\hat{E}_n(x)$	interpolation error, $\hat{E}_n(x) \equiv f(x) - f_n(x)$
$E_n(f)$	quadrature error, $E_n(f) \equiv I(f) - I_n(f) = I(f) - I(f_n) = E(f_n)$
$I_{n,m}(f)$	numerical approximation using m equally spaced subintervals and Lagrange polynomial of function f of degree n, $I_{n,m}(f) = I_m(f_n)$
$E_{n,m}(f)$	quadrature error of composite formula with equidistant spacing, $E_{n,m}(f) \equiv I(f) - I_{n,m}(f) = E_m(f_n)$
$\tilde{I}_{n,m}(f)$	numerical approximation using m non-equally spaced subintervals and Lagrange polynomial of function f of degree n, $\tilde{I}_{n,m}(f) = \tilde{I}_m(f_n)$
$\tilde{E}_{n,m}(f)$	quadrature error of composite formula with non-equidistant spacing, $\tilde{E}_{n,m}(f) \equiv I(f) - \tilde{I}_{n,m}(f) = \tilde{E}_m(f_n)$

1 Quadrature Formulae

This chapter addresses methods of numerical integration. Calculating explicitly a definite integral of a function may be difficult or even impossible. We may not know the function analytically; it may only be given by measured data values. The goal of numerical integration is to approximate the value of an integral. Any explicit formula computing an approximation of a definite integral is said to be a quadrature formula.

The quadrature formulae considered will be of the form

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i), \tag{3}$$

where f is a given function, $n \in \mathbb{N}$, $[a, b]$ is a finite interval, $\{x_i\}$, $i = 0, \ldots, n$, are distinct *nodes*, and $\{w_i\}$, $i = 0, \ldots, n$ the corresponding *weights*, see [12].

1.1 The Lagrange Quadrature Formulae

In this thesis we will focus on the Lagrange interpolatory quadrature formulae. These formulae are obtained by replacing a function with its Lagrange interpolating polynomial. Let f be a real integrable function over the interval $[a, b]$, and f_n its Lagrange interpolating polynomial of degree n over $\{x_i\}$. Then

$$f_n(x) = \sum_{i=0}^{n} f(x_i) l_i(x), \tag{4}$$

where $l_i(x)$ is the characteristic Lagrange polynomial,

$$l_i(x) = \prod_{j=0,\, j\neq i}^{n} \frac{x - x_j}{x_i - x_j},$$

see [11, 12]. It is immediate that $f_n(x_i) = f(x_i)$. Assume that $f \in C^{n+1}([a, b])$, the interpolation error $\hat{E}_n(x) \equiv f(x) - f_n(x)$ is, according to [11],

$$\hat{E}_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i), \tag{5}$$

where $\xi \in (a, b)$.

Denote

$$I(f) \equiv \int_a^b f(x)dx, \tag{6}$$

and $I_n(f) \equiv I(f_n)$. Then substituting from (4) leads to

$$I_n(f) = \sum_{i=0}^{n} f(x_i) \int_a^b l_i(x)dx, \tag{7}$$

which is the Lagrange interpolatory quadrature formula, see also [11]. Formula (7) is a special instance of the general quadrature formula (3) with weights $w_i = \int_a^b l_i(x)dx$, $i = 0, \ldots, n$. Note that any interpolatory quadrature formula using $n+1$ distinct nodes is exact for polynomials of degree less or equal n. If $f \in \mathbb{P}_n$, then $f = f_n$ and $I_n(f_n) = I(f_n)$.

The two most simple interpolatory quadrature formulae are described in the following sections. These rules are the Trapezoidal and the Simpson formulae. The nodes are usually constrained to be equally spaced. The purpose of this study is to examine the use of nodes which are not equally spaced. We will consider logarithmic spacing. First we derive results for the equal spacing.

1.2 The Trapezoidal Formula

1.2.1 The simple rule

The Trapezoidal formula is obtained by replacing f with its Lagrange interpolating polynomial of degree 1 using the nodes $x_0 = a$ and $x_1 = b$. It is easy to see that

$$I_1(f) = \frac{b-a}{2}[f(a) + f(b)], \tag{8}$$

which is the area of the trapezoid illustrated in Figure 1, see also [11, 12].

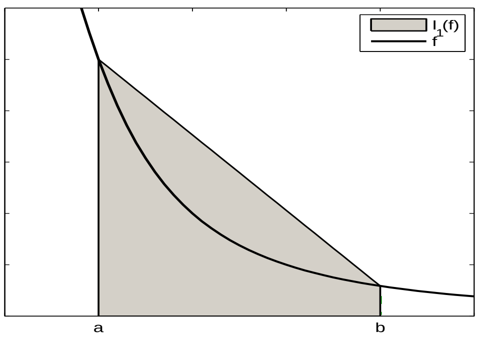


Figure 1: The integral of function f approximated by a linear function.

Error analysis of the simple rule

The quadrature error $E_n(f) \equiv I(f) - I_n(f)$ is the difference between the exact integral and the numerical approximation. To examine $E_1(f)$, when $f \in C^2([a,b])$, we use the expression of the interpolation error (5), according to [11], which leads to

$$E_1(f) = \int_a^b (f(x) - f_1(x))dx = \frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)dx,$$

where $\xi(x) \in (a,b)$. Since the nodal polynomial $\omega_2(x) = (x-a)(x-b) < 0$ in (a,b), we can use the mean-value theorem to obtain

$$E_1(f) = \frac{f''(\xi)}{2}\int_a^b \omega_2(x)dx = -f''(\xi)\frac{(b-a)^3}{12}, \tag{9}$$

for some $\xi \in (a,b)$.

1.2.2 The composite rule with equidistant spacing

To obtain an approximation for the integral over the interval $[a,b]$ using more than just 2 points we introduce the composite rule, in which we approximate the integral over m subintervals, for $m \geq 1$. The function f is replaced with its composite Lagrange polynomial constructed on the subintervals.

If we consider the regular spacing, the width of the subintervals is $h = (b-a)/m$ and the nodes are $x_i = a + ih$, for $i = 0, \ldots, m$. The composite formula is

$$I_{1,m}(f) = \frac{h}{2}\sum_{i=0}^{m-1}(f(x_i) + f(x_{i+1})), \tag{10}$$

which can be also written as

$$I_{1,m}(f) = h\left[\frac{1}{2}f(x_0) + f(x_1) + \ldots + f(x_{m-1}) + \frac{1}{2}f(x_m)\right],$$

see [11].

Error analysis

According to [11] the quadrature error $E_{1,m}(f) \equiv I(f) - I_{1,m}(f)$ is given by

$$E_{1,m}(f) = -\frac{b-a}{12}h^2 f''(\xi),$$

provided that $f \in C^2([a,b])$, where $\xi \in (a,b)$. This can be proved by recalling the error of the simple rule (9) and the additivity of integrals. For $i = 0, \ldots, m-1$

and $\xi_i \in (a+ih, a+(i+1)h)$, we have

$$E_{1,m}(f) = -\sum_{i=0}^{m-1} \frac{h^3}{12} f''(\xi_i) = -\sum_{i=0}^{m-1} f''(\xi_i) \frac{h^2}{12}\frac{(b-a)}{m} = -\frac{b-a}{12} h^2 f''(\xi). \quad (11)$$

The last equality is a consequence of the discrete mean-value theorem, see [11].

1.2.3 The composite rule with non-equidistant spacing

For non-equidistant spacing of the m subintervals the composite formula (10) is replaced by the more general formula

$$\tilde{I}_{1,m}(f) = \frac{1}{2}\sum_{i=0}^{m-1} h_i(f(x_i) + f(x_{i+1})), \quad (12)$$

where h_i is the length of the $(i+1)^{st}$ subinterval, $h_i = x_{i+1} - x_i$, $i = 0, \ldots, m-1$ with $x_0 = a$, $x_m = b$, and the nodes are $x_i = x_{i-1} + h_i$, $i = 1, \ldots, m$.

Then, as in (11),

$$\begin{aligned} \tilde{E}_{1,m}(f) &\equiv I(f) - \tilde{I}_{1,m}(f) \\ &= -\sum_{i=0}^{m-1} \frac{h_i^3}{12} f''(\xi_i). \end{aligned}$$

This gives the following estimation of the quadrature error,

$$\begin{aligned} |\tilde{E}_{1,m}(f)| &= \left| -\sum_{i=0}^{m-1} \frac{h_i^3}{12} f''(\xi_i) \right| \\ &\leq \sum_{i=0}^{m-1} \left| \frac{h_i^3}{12} f''(\xi_i) \right| \\ &\leq \frac{1}{12} |f''(\eta)| \left(\sum_{i=0}^{m-1} h_i^3 \right), \end{aligned} \quad (13)$$

for some $\eta \in (a,b)$, so that $\max_{\zeta_i \in [a,b]} |f''(\zeta)| = |f''(\eta)|$. Note that we introduce the use of the notation $\tilde{F}$ as compared to F to denote operation F applied for the irregular spacing as compared to the equidistant spacing. We notice

$$|E_{1,m}(f)| = \frac{b-a}{12} h^2 |f''(\xi)| \leq \frac{b-a}{12} h^2 |f''(\eta)|$$

while

$$|\tilde{E}_{1,m}(f)| \leq \frac{b-a}{12} h_{max}^2 |f''(\eta)|,$$

where $h_{max} = \max_{i \in (0,m-1)} h_i$. Thus we expect the tilde value to be greater than the non tilde value for a given interval.

1.3 The Simpson Formula

1.3.1 The simple rule

The Simpson formula can be obtained by replacing f over $[a, b]$ with the Lagrange interpolating polynomial of degree 2, interpolated at nodes $x_0 = a$, $x_1 = \frac{a+b}{2}$ and $x_2 = b$, see Figure 2. It is not hard to obtain the Simpson formula, see [11, 13],

$$I_2(f) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right], \tag{14}$$

by integrating f_2 over $[a, b]$.

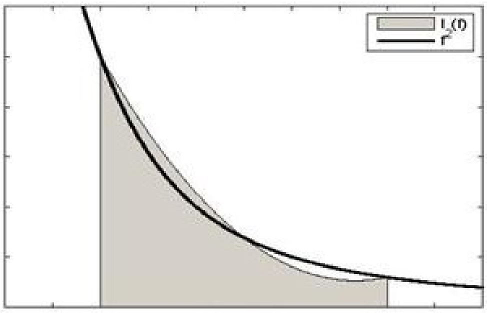


Figure 2: Function f approximated by quadratic polynomial interpolated at a, b and $\frac{a+b}{2}$.

Note

$$f_2(x) = f(a)\frac{(x-x_1)(x-b)}{(a-x_1)(a-b)} + f(x_1)\frac{(x-a)(x-b)}{(x_1-a)(x_1-b)} + f(b)\frac{(x-a)(x-x_1)}{(b-a)(b-x_1)},$$

and thus

$$\begin{aligned}
\int_a^b f_2(x)dx &= \frac{f(a)}{(a-x_1)(a-b)}\int_a^b (x-x_1)(x-b)dx \\
&\quad + \frac{f(x_1)}{(x_1-a)(x_1-b)}\int_a^b (x-a)(x-b)dx \\
&\quad + \frac{f(b)}{(b-a)(b-x_1)}\int_a^b (x-a)(x-x_1)dx \\
&= f(a)\frac{-(a-b)^2(2a+b-3x_1)}{6(a-x_1)(a-b)} + f(x_1)\frac{(a-b)^3}{6(x_1-a)(x_1-b)} \\
&\quad + f(b)\frac{(a-b)^2(a+2b-3x_1)}{6(b-a)(b-x_1)}.
\end{aligned} \tag{15}$$

Since $x_1 = (a+b)/2$ we obtain

$$\int_a^b f_2(x)dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

which is the Simpson formula (14).

Error analysis of the simple rule

To obtain the error $E_2(f) \equiv I(f) - I_2(f)$ we will use the Peano kernel theorem, see [15].

Theorem. *(Peano kernel theorem) Suppose $f \in C^{k+1}[a,b]$ and let $I(f) = \sum_{i=0}^{n} w_i f(x_i)$ be a quadrature rule that exactly integrates all polynomials of degree k or less on $[a,b]$. Then*

$$E(f) = \frac{1}{k!}\int_a^b f^{(k+1)}(t)K(t)dt, \tag{16}$$

where $K(t) \equiv E((x-t)_+^k)$ and

$$(x-t)_+^k \equiv \begin{cases} (x-t)^k, & t \le x; \\ 0, & t > x. \end{cases}$$

According to Section 1.1 the formula (14) is exact for quadratic polynomials. Noting that

$$I_2(x^3) = \frac{b-a}{6}(a^3 + \frac{1}{2}(a+b)^3 + b^3) = \frac{1}{4}(b^4 - a^4) = I(x^3),$$

it is immediate that $I_2(Ax^3+Bx^2+Cx+D) = I(Ax^3+Bx^2+Cx+D)$. Thus the rule is exact for all cubics $p(x) \in \mathbb{P}_3(x)$. For $p_4(x) \in \mathbb{P}_4(x)$ we consider $p(x) = x^4$ and observe. Let $a = 0$, $b = 1$. Then

$$\begin{aligned} I_2(x^4) &= \frac{b-a}{6}\left(a^4 + \frac{1}{2}(a+b)^4 + b^4\right) \\ &= \frac{1}{6}\left(\frac{1}{2}+1\right) \\ &= \frac{1}{4} \\ &\neq \frac{1}{5} \\ &= \frac{1}{5}(b^5 - a^5) = I(x^4). \end{aligned}$$

Therefore we can apply the Peano kernel theorem to calculate (16) for $k = 3$.

The Peano kernel theorem gives that

$$E_2(f) = \frac{1}{3!}\int_a^b f^{(4)}(t)K(t)dt, \tag{17}$$

where $K(t) = E((x-t)_+^3)$. By definition

$$\begin{aligned} K(t) &= \left(\int_a^b (x-t)_+^3 dx\right) - I_2((x-t)_+^3) \\ &= \left[\frac{(x-t)^4}{4}\right]_t^b - \frac{b-a}{6}\left((a-t)_+^3 + 4(\frac{1}{2}(a+b)-t)_+^3 + (b-t)_+^3\right) \\ &= \frac{(b-t)^4}{4} - \frac{b-a}{6}\left(4(\frac{1}{2}(a+b)-t)_+^3 + (b-t)_+^3\right), \end{aligned} \tag{18}$$

where we used the fact that $(a-t)_+ = 0$ for $t \in [a,b]$. Because $K(t)$ does not change sign for $t \in [a,b]$, see [12], we can use the mean value theorem, which guarantees the existence of some $\xi \in [a,b]$ such that

$$E_2(f) = \frac{1}{3!}\int_a^b f^{(4)}(t)K(t)dt = \frac{1}{3!}f^{(4)}(\xi)\int_a^b K(t)dt. \tag{19}$$

We can than integrate the simplified formula for $K(t)$,

$$\begin{aligned} \int_a^b K(t)dt &= \int_a^b \frac{(b-t)^4}{4}dt - \frac{b-a}{6}\int_a^b \left(4(\frac{1}{2}(a+b)-t)_+^3 + (b-t)_+^3\right) dt \\ &= -\left[\frac{(b-t)^5}{20}\right]_a^b \\ &\quad -\frac{b-a}{6}\left[4\int_a^{(a+b)/2} (\frac{1}{2}(a+b)-t)dt + \int_a^b (b-t)^3 dt\right] \\ &= -\left[\frac{(b-t)^5}{20}\right]_a^b - \frac{b-a}{6}\left[\left(\frac{a-b}{2}\right)^4 - \left(\frac{a-b}{4}\right)^4\right] \\ &= -\frac{(b-a)^5}{480}. \end{aligned} \tag{20}$$

Inserting (20) into (19), the expression for $E_2(f)$, we obtain the error of the Simpson rule:

$$E_2(f) = -\frac{(b-a)^5}{2880}f^{(4)}(\xi), \tag{21}$$

where $\xi \in (a,b)$, provided that $f \in C^4([a,b])$, see [11].

1.3.2 The composite rule with equidistant spacing

To obtain the composite Simpson formula we proceed similarly to the composite Trapezoidal formula by replacing f over $[a,b]$ with its composite quadratic polynomial on m subintervals, with $m \geq 1$.

Considering equidistant spacing, let $h = (b-a)/m$ and introduce the quadrature nodes $x_i = a + ih/2$, for $i = 0, \dots, 2m$, so that in this case for the formula on m intervals there are $2m+1$ nodes, we obtain the composite formula, see [11],

$$I_{2,m}(f) = \frac{h}{6}\left[f(x_0) + 2\sum_{i=1}^{m-1} f(x_{2i}) + 4\sum_{i=0}^{m-1} f(x_{2i+1}) + f(x_{2m})\right]. \tag{22}$$

Following the derivation of (11) for the Trapezoidal rule we obtain, as in [11],

$$E_{2,m}(f) = -\frac{b-a}{180}\left(\frac{h}{2}\right)^4 f^{(4)}(\xi) = -\frac{b-a}{2880}h^4 f^{(4)}(\xi), \tag{23}$$

where $\xi \in (a,b)$, provided that $f \in C^4([a,b])$.

1.3.3 The simple rule with non-equidistant spacing

We can derive $\tilde{I}_2$, the simple Simpson rule with non-equidistant spacing, similarly as in (15). For the nodes x_0, x_1, x_2, where $x_1 \in (x_0, x_2)$ we obtain

$$\begin{aligned}\tilde{I}_2(f) &= f(x_0)\frac{(x_2-x_0)(2x_0+x_2-3x_1)}{6(x_0-x_1)} + f(x_1)\frac{(x_0-x_2)^3}{6(x_1-x_0)(x_1-x_2)} \\ &\quad + f(x_2)\frac{(x_2-x_0)(x_0+2x_2-3x_1)}{6(x_2-x_1)}.\end{aligned}$$

According to Section 1.1 the formula for $\tilde{I}_2(f)$ is exact for quadratic polynomials. For $p_3(x) \in \mathbb{P}_3(x)$ we consider $p(x) = x^3$ and observe. Let $x_0 = 0$, $x_1 = h$, $x_2 = 1$, where $h \in (0,1)$.

$$\begin{aligned}\tilde{I}_2(x^3) &= \frac{1}{6}(x_0-x_2)(-2x_0^3 + x_0^2x_1 - x_0^2x_2 - 2x_0x_1x_2 - x_0x_2^2 + x_1x_2^2 - 2x_2^3) \\ &= \frac{1}{6}(-1)(h-2) \\ &\neq \frac{1}{4} \\ &= \frac{1}{4}(x_2^4 - x_0^4) = I(x^3).\end{aligned}$$

We can see that the equality only holds when $h = 1/2$.

Thus we may apply the Peano kernel theorem (16) with $k = 2$ to give the quadrature error

$$\tilde{E}_2(f) \equiv I(f) - \tilde{I}_2(f) = \frac{1}{2}\int_{x_0}^{x_2} f^{(3)}(t)K(t)dt,$$

where $K(t) = E((x-t)_+^2)$. Using the definition of $K(t)$ we obtain

$$\begin{aligned}
K(t) &= \left(\int_{x_0}^{x_2} (x-t)_+^2 dx\right) - \tilde{I}_2((x-t)_+^2) \\
&= \frac{(x_2-t)^3}{3} - (x_1-t)_+^2 \frac{(x_0-x_2)^3}{6(x_1-x_0)(x_1-x_2)} \\
&\quad -(x_2-t)_+^2 \frac{(x_2-x_0)(x_0+2x_2-3x_1)}{6(x_2-x_1)},
\end{aligned}$$

where we used the fact that $(x_0-t)_+ = 0$ for $t \in [x_0, x_2]$. We can show that $K(t)$ changes sign for $t \in [x_0, x_2]$. Let $x_0 = 0$, $x_1 = h$, $x_2 = 1$, then

$$\begin{aligned}
K(t) &= \frac{(1-t)^3}{3} - (h-t)_+^2 \frac{1}{6h(1-h)} \\
&\quad -(1-t)_+^2 \frac{(2-3h)}{6(1-h)}.
\end{aligned}$$

Considering $h=\frac{1}{2}$, we obtain

$$\begin{aligned}
K(t) &= \frac{(1-t)^3}{3} - (\frac{1}{2}-t)_+^2 \frac{2}{3} \\
&\quad -(1-t)_+^2 \frac{(2-3/2)}{3}.
\end{aligned}$$

When $t = \frac{1}{4}$, then

$$\begin{aligned}
K(1/4) &= \frac{(1-1/4)^3}{3} - (\frac{1}{2}-\frac{1}{4})_+^2 \frac{2}{3} \\
&\quad -(1-1/4)_+^2 \frac{(2-3/2)}{3} \\
&= \frac{1}{192},
\end{aligned}$$

when $t = \frac{3}{4}$, then

$$\begin{aligned}
K(3/4) &= \frac{(1-3/4)^3}{3} - (\frac{1}{2}-\frac{3}{4})_+^2 \frac{2}{3} \\
&\quad -(1-3/4)_+^2 \frac{(2-3/2)}{3} \\
&= -\frac{3}{64}.
\end{aligned}$$

Because $K(t)$ changes sign for $t \in [x_0, x_2]$, we can not use the mean value theorem, so we use an error estimation in the worst case scenario,

$$\tilde{E}_2(f) \equiv I(f) - \tilde{I}_2(f) = \frac{1}{2}\int_{x_0}^{x_2} f^{(3)}(t)K(t)dt \leq \frac{1}{2}\max_{\xi\in(x_0,x_2)} f^{(3)}(\xi)\int_{x_0}^{x_2} K(t)dt. \tag{24}$$

Integration of the simplified formula for $K(t)$ leads to

$$\begin{aligned}
\int_{x_0}^{x_2} K(t)dt &= \int_{x_0}^{x_2}\frac{(x_2-t)^3}{3}dt - \frac{(x_0-x_2)^3}{6(x_1-x_0)(x_1-x_2)}\int_{x_0}^{x_1}(x_1-t)_+^2 dt \\
&\quad -\frac{(x_2-x_0)(x_0+2x_2-3x_1)}{6(x_2-x_1)}\int_{x_0}^{x_2}(x_2-t)_+^2 dt \\
&= -\frac{(x_2-x_0)^4}{12} - \frac{(x_0-x_1)^2(x_0-x_2)^3}{18(x_1-x_2)} \\
&\quad -\frac{(x_2-x_0)^4(x_0+2x_2-3x_1)}{18(x_2-x_1)} \\
&= \frac{1}{36}(x_0-x_2)^3(x_0-2x_1+x_2).
\end{aligned} \tag{25}$$

Inserting (25) into (24) we obtain the formula for the estimation of the error of the Simpson rule with non-equidistant spacing:

$$\tilde{E}_2(f) \leq \frac{1}{72}\max_{\xi\in(x_0,x_2)} f^{(3)}(\xi)(x_0-x_2)^3(x_0-2x_1+x_2).$$

1.3.4 The composite rule with non-equidistant spacing

The composite rule with non-equidistant spacing on m subintervals is then

$$\begin{aligned}
\tilde{I}_{2,m}(f) &= f(x_0)\frac{(x_2-x_0)(2x_0+x_2-3x_1)}{6(x_0-x_1)} \\
&\quad +\sum_{i=1}^{m} f(x_{2i-1})\frac{(x_{2i-2}-x_{2i})^3}{6(x_{2i-1}-x_{2i-2})(x_{2i-1}-x_{2i})} \\
&\quad +\sum_{i=1}^{m-1} f(x_{2i})\frac{(x_{2i}-x_{2i-2})(x_{2i-2}+2x_{2i}-3x_{2i-1})}{6(x_{2i}-x_{2i-2})} \\
&\quad +\sum_{i=1}^{m-1} f(x_{2i})\frac{(x_{2i+2}-x_{2i})(2x_{2i}+x_{2i+2}-3x_{2i+1})}{6(x_{2i}-x_{2i+1})} \\
&\quad +f(x_{2m})\frac{(x_{2m}-x_{2m-2})(x_{2m-2}+2x_{2m}-3x_{2m-1})}{6(x_{2m}-x_{2m-1})},
\end{aligned} \tag{26}$$

where x_i, $i = 0, \ldots, 2m$, are the quadrature nodes.

The estimation of the quadrature error, $\tilde{E}_{2,m}(f) \equiv I(f) - \tilde{I}_{2,m}(f)$, obtained by summing over all intervals is then

$$|\tilde{E}_{2,m}(f)| \leq \sum_{i=0}^{m-1} \max_{\xi_i \in (x_{2i}, x_{2i+2})} \left(|f^{(3)}(\xi_i)| \frac{1}{72} (x_{2i+2} - x_{2i})^3 |x_{2i} - 2x_{2i+1} + x_{2i+2}| \right) \tag{27}$$

which is derived similarly as the estimation of error of the composite Trapezoidal rule (13).

1.4 The formulae

The formulae which are validated are given by equations (10), (12), (22), (26), the estimations of errors are the errors in the worst case scenario, see also (11), (21), and (27). The formulae are tabulated in Table 1. Derivatives of f used in error formulae are following: $f''(x) = \frac{6x^2-2}{(x^2+1)^3}$, $f^{(3)}(x) = \frac{6(x^4-6x^2+1)}{(x^2+1)^4}$, $f^{(4)}(x) = \frac{24x(x^4-10x^2+5)}{(x^2+1)^5}$, derivatives ar plotted in Figure 3.

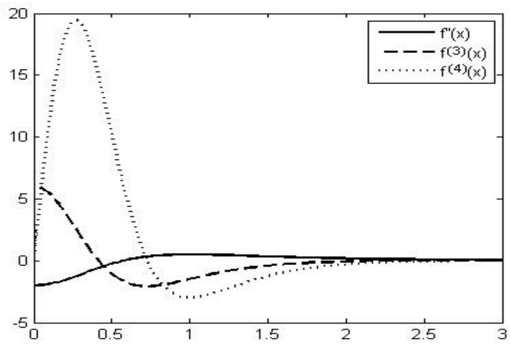


Figure 3: Derivatives of function $f = \frac{1}{1+x^2}$

	Quadrature formula
Trapezoidal	$\frac{h}{2}\sum_{i=0}^{m-1}(f(x_i)+f(x_{i+1}))$
Log. Trapezoidal	$\frac{1}{2}\sum_{i=0}^{m-1} h_i(f(x_i)+f(x_{i+1}))$
Simpson	$\frac{h}{6}\left[f(x_0)+2\sum_{i=1}^{m-1} f(x_{2i})+4\sum_{i=0}^{m-1} f(x_{2i+1})+f(x_{2m})\right]$
Log. Simpson	$f(x_0)\frac{(x_2-x_0)(2x_0+x_2-3x_1)}{6(x_0-x_1)}+\sum_{i=1}^{m} f(x_{2i-1})\frac{(x_{2i-2}-x_{2i})^3}{6(x_{2i-1}-x_{2i-2})(x_{2i-1}-x_{2i})}+\sum_{i=1}^{m-1} f(x_{2i})\frac{(x_{2i}-x_{2i-2})(x_{2i-2}+2x_{2i}-3x_{2i-1})}{6(x_{2i}-x_{2i-2})}$ $+\sum_{i=1}^{m-1} f(x_{2i})\frac{(x_{2i+2}-x_{2i})(2x_{2i}+x_{2i+2}-3x_{2i+1})}{6(x_{2i}-x_{2i+1})}+f(x_{2m})\frac{(x_{2m}-x_{2m-2})(x_{2m-2}+2x_{2m}-3x_{2m-1})}{6(x_{2m}-x_{2m-1})}$
	Error formula
Trapezoidal	$\sum_{i=0}^{n-1}\max_{\xi_i\in(x_i,x_{i+1})}\left(\lvert f''(\xi_i)\rvert\frac{h^3}{12}\right)$
Log. Trapezoidal	$\sum_{i=0}^{n-1}\max_{\xi_i\in(x_i,x_{i+1})}\left(\lvert f''(\xi_i)\rvert\frac{h_{i+1}^3}{12}\right)$
Simpson	$\sum_{i=0}^{(n/2)-1}\max_{\xi_i\in(x_{2i},x_{2i+2})}\left(\lvert f^{(4)}(\xi_i)\rvert\frac{h^5}{2880}\right)$
Log. Simpson	$\sum_{i=0}^{(n/2)-1}\max_{\xi_i\in(x_{2i},x_{2i+2})}\left(\lvert f^{(3)}(\xi_i)\rvert\frac{h_{i+1}^3}{72}\lvert x_{2i}-2x_{2i+1}+x_{2i+2}\rvert\right)$

Table 1: Formulae for quadrature and errors for composite Trapezoidal and Simpson rule with equidistant and non-equidistant spacing

2 Initial experiments

This chapter is dedicated to analysis of numerical experiments for definite integrals of chosen functions. The definite integrals of the functions are aproximated using the Trapezoidal and Simpson composite rules with equidistant or logarithmic spacing. The distances between nodes in logarithmic spacing are determined as a function of a base 10 logarithm. Let $x_0 = a$, $x_n = b$, the formula for x_i, $i = 1, ..., n-1$, when chosen logarithmically on the interval $(0, 1)$ is $x_i = 10^{(\log b - \log a)i/n}$. The numerical experiments and visualizations of the results are performed using Matlab. The chapter is divided into 3 parts. Approximations of integrals are presented in the first part, estimations of errors in the second part. The third part of the initial experiments deals with the minimum number of measurement data in order to decrease the level of the quadrature error under 0.01.

For the initial experiments we use

$$f(x) = \frac{1}{1 + x^2}, \tag{28}$$

which is illustrated in Figure 4.

2.1 Approximations of integrals

The following tables show the numerical approximation for $\int_a^b f(x)dx$, with f defined in (28), for the considered quadrature formulae based on the Trapezoidal and Simpson rules. Each table presents the results rounded to six decimals on different intervals. In these tables the best results are given in boldface. We notice first that the error decreases as n increases, and on the interval $[0, 1]$ the results are exact to 6 significant figures when calculated using the spacing with Simpson's rule already for $n = 12$.

Description of the table headings

The first column of each table, $n + 1$, represents the number of nodes used in the composite quadrature formulae, so that the results in each row are approximations

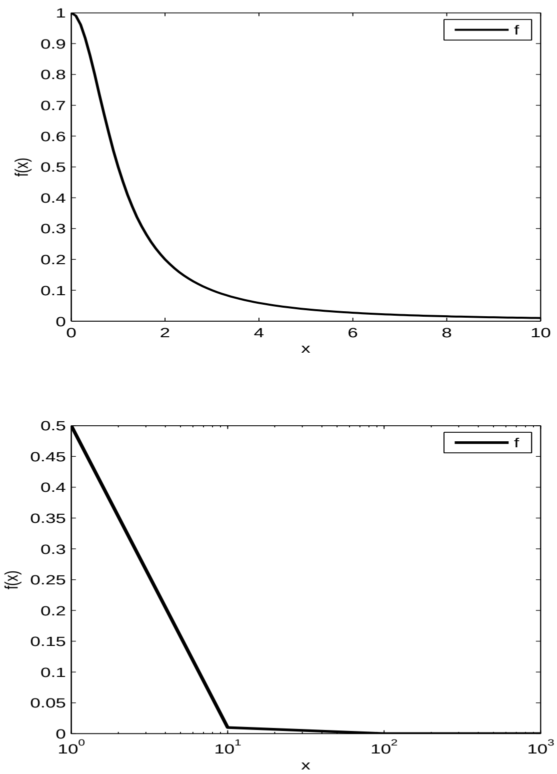


Figure 4: Function $f(x) = \frac{1}{1+x^2}$ on linear and logarithmic scale

of the integral of f using the same number of nodes but different methods. The Trapezoidal formulae use $n + 1$ nodes over n subintervals, see Section 1.2, and the Simpson formulae use $n/2$ subintervals, n even, see Section 1.3.

The second column, Trapezoidal, shows the results calculated by the composite Trapezoidal formula with equidistant spacing using (10). The third column represents approximations using the composite Trapezoidal formula with logarithmic spacing described in (12). Likewise columns four and five show results using the composite Simpson formula with equidistant, respectively logarithmic spacing described in (22), respectively in (26).

Description of the numerical results

From the Table 2 we see that the differences among the results on intervals $[0, 1]$ and $[0, 10]$ are not that substantive. Nevertheless, the Simpson rule produces more accurate approximations than the Trapezoidal rule and the logarithmic spacing is more accurate than equidistant spacing.

There are significant differences between the numerical results on intervals $[0, 100]$ and $[0, 1000]$. The equidistant formula is practically unusable in this case, while the Simpson rule is more accurate than the Trapezoidal rule.

The results in Table 2 suggest that logarithmic Simpson rule is the most accurate. From Figure 4 this can be explained by observing that logarithmic spacing is needed to capture both rapid change for small x and the decay for large x.

Interval $[0, 1]$, $I = \int_0^1 f \doteq 0.785398$				
n+1	Trapezoidal	Log. Trapezoidal	Simpson	Log. Simpson
13	0.785109	0.785278	**0.785398**	0.785400
25	0.785326	0.785368	0.785398	**0.785398**
49	0.785380	0.785391	0.785398	0.785398
97	0.785394	0.785396	0.785398	0.785398
193	0.785397	**0.785398**	0.785398	0.785398

Interval $[0, 10]$, $I = \int_0^{10} f \doteq 1.471128$				
n+1	Trapezoidal	Log. Trapezoidal	Simpson	Log. Simpson
13	1.472685	1.486059	1.448643	1.470530
25	1.471100	1.474860	1.470657	1.471090
49	1.471121	1.472060	1.471127	1.471125
97	1.471126	1.471361	**1.471128**	**1.471128**
193	1.471127	1.471186	1.471128	1.471128

Interval $[0, 100]$, $I = \int_0^{100} f \doteq 1.560797$				
n+1	Trapezoidal	Log. Trapezoidal	Simpson	Log. Simpson
13	4.352202	1.623511	2.995686	1.555193
25	2.453919	1.576459	1.821159	1.560194
49	1.722667	1.564711	1.478916	1.560759
97	1.568358	1.561775	1.516921	1.560794
193	1.560814	1.561041	1.558300	**1.560797**

Interval $[0, 1000]$, $I = \int_0^{1000} f \doteq 1.569796$				
n+1	Trapezoidal	Log.Trapezoidal	Simpson	Log.Simpson
13	41.685403	1.711002	27.799804	1.530420
25	20.871797	1.605288	13.933928	1.567110
49	10.494504	1.578664	7.035406	1.569605
97	5.364298	1.572013	3.654229	1.569784
193	2.911590	1.570350	2.094020	**1.569796**

Table 2: Numerical results on different intervals

2.2 Error estimates

In this part we study the validity of the error formulae derived in Sections 1.2 and 1.3 for estimating the errors in calculating $\int_a^b f(x)dx$ with $a = 0$, b increasing and $f = \frac{1}{1+x^2}$. See Table 1 for the formulae.

The following tables each correspond to a particular formula for a particular interval. The tables show errors and error estimates of the formulae. The Figures

5 - 8 show furthermore order of errors h^p, $E_{n,m}(f) = Ch^p$, $p = 3$ for the Trapezoidal rule, $p = 5$ for the Simpson rule. The error estimates are plotted only for interval $[0, 1]$ because the estimates on the other intervals do not correspond with the real error.

Trapezoidal rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	2.893516e-004	5.206308e-004	1.199123e-004	4.569276e-004
25	7.233796e-005	1.229859e-004	2.986999e-005	1.072599e-004
49	1.808449e-005	2.982534e-005	7.460737e-006	2.592231e-005
97	4.521122e-006	7.340682e-006	1.864762e-006	6.370722e-006
193	1.130280e-006	1.820760e-006	4.661641e-007	1.578492e-006

Simpson rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	5.191125e-011	3.308813e-006	1.127827e-007	4.870740e-002
25	8.111290e-013	1.832601e-007	7.043887e-009	2.653828e-002
49	1.254552e-014	1.063610e-008	4.401649e-010	1.384162e-002
97	2.287234e-015	6.378677e-010	2.750921e-011	7.068716e-003
193	2.220446e-016	3.903279e-011	1.719402e-012	3.572010e-003

Table 3: Actual and estimated errors for the Trapezoidal and the Simpson rules with equidistant and logarithmic spacing, on interval [0,1]. Errors are least for the logarithmic spacing.

The errors are relatively small for the interval $[0, 1]$ according to the Table 3. Results are also plotted on graphs, see Figure 5. There are noticeable differences between the Trapezoidal formula and the Simpson formula. The Simpson rule is in general more accurate. Application of equidistant or logarithmic spacing is not a key factor in this case, however, equidistant spacing leads to the more accurate results. We can see that the real error of the Simpson formula is much lower then its estimate. The error estimates of the Trapezoidal formula correspond with the real error.

The estimates on the interval $[0, 10]$ in the Table 4 correspond with the numerical results in the Table 2 in the sense that the Simpson rule or the equidistant spacing leads to more accurate results than the Trapezoidal rule or the logarithmic spacing, see also Figure 6. The error estimates of the Simpson formula do not correspond with the real error, unlike the Trapezoidal formula.

The difference between real error and its estimate on intervals $[0, 100]$ and $[0, 1000]$ is marked, see Tables 5, 6, and Figures 7 and 8. According to the estimations of errors the Trapezoiodal formula is more applicable than the Simpson formula because of the higher powers in the formula for computing the errors, see Table 1. However, the real error is smaller for the Simpson rule. Equidis-

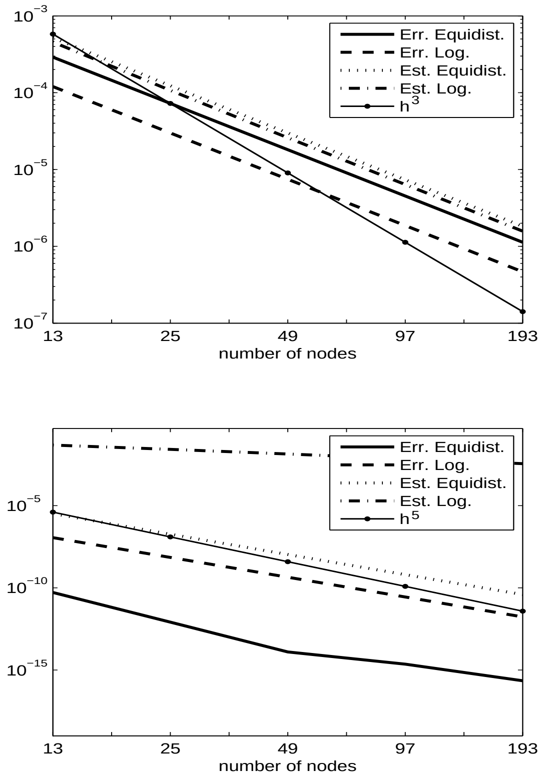


Figure 5: Errors and estimations of errors of the Trapezoidal an the Simpson rules with equidistant, respectively with logarithmic spacing, on interval [0,1], $E_{n,m}(f) = Ch^p$, errors are order h^p, $p = 3$ for the Trapezoidal rule, $p = 5$ for the Simpson rule

tant spacing can yield enormous quadrature errors for this example. Logarithmic spacing is prefered, which is not surprising, see Figure 4.

Error estimares of other functions

In this section we will show some results for new function $f_{x_0} = \frac{1}{1+(x-x_0)^2}$, where $x_0 \in \{10, 100, 1000\}$. Since we have shown logarithmic spacing is preferable we will not consider equidistant spacing for the function f_{x_0}. From Table 7 we can see that the difference between the Trapezoidal formula and the Simpson formula is not substantive on interval $[0, 100]$. However, the Trapezoidal formula leads to more accurate results.

Table 8 shows error estimates for function f_{x_0} for $x_0 \in \{0.1, 1, 10, 100, 1000\}$ on interval $[0, 10000]$. We use the Trapezoidal and the Simpson formula with logarithmic spacing with 49 and 97 nodes. The Simpson formula leads to much more accurate results than the Trapezoidal formula. However, we can see that the error estimate of the Simpson formula is overestimated. As x_0 increases the errors grow, which is not surprising because of the shape of the function. The peak of the function shifts as x_0 increases, so the logarithmic spacing might not

Trapezoidal rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	1.557311e-003	0.141676	0.014930	0.030155
25	2.746805e-005	0.024639	3.732794e-003	0.006365
49	7.090664e-006	0.005735	9.331961e-004	0.001456
97	1.777278e-006	0.001304	2.332988e-004	3.470239e-004
193	4.432015e-007	3.105135e-004	5.832468e-005	8.467286e-005

Simpson rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	0.022485	0.047127	5.969683e-004	1.495950
25	5.557279e-004	0.002345	3.722240e-005	0.857343
49	2.982021e-007	1.813403e-004	2.333956e-006	0.462073
97	1.493774e-010	9.050227e-006	1.458896e-007	0.240138
193	9.332758e-012	5.044943e-007	9.119637e-009	0.122450

Table 4: Actual and estimated errors for the Trapezoidal Simpson rules with equidistant and logarithmic spacing, on interval [0,10]. Errors are least for the equidistant spacing.

capture it.

2.3 Number of nodes required to decrease the quadrature error

In this section we are looking for the minimum number of nodes required to decrease the quadrature error under 0.01. We will not contemplate interval $[0, 1]$ because all of the mentioned formulae are accurate enough for the considered number of nodes.

We consider the function $f = \frac{1}{1+x_2}$. The Simpson formula with logarithmic stepsizes is the most suitable formula, it needs less then 20 nodes on each interval to achieve given accuracy, see Table 9. The logarithmic spacing is generally more convenient in our case. The formulae with equidistant division have almost no meaning in our situation.

In Table 10 we present the numbers of nodes for function $f_{x_0} = \frac{1}{1+(x-x_0)^2}$, where $x_0 \in \{0.1, 1, 10, 100, 1000\}$, on interval $[0, 10000]$. Because we showed that the formulae with equidistant spacing are not useful in our case, we consider only the Trapezoidal and Simpson rules with logarithmic spacing. The required number of nodes increases as x_0 increases because of shifting of peak of f_{x_0}. When $x_0 \in \{100, 1000\}$ the number of nodes is more than 1000 for both formulae, which is not applicable in our case. Both formulae require less than 115 nodes for $x_0 \in \{0.1, 1, 10\}$ which is positive, because in the real problem we can get about 100 measurement data for each experiment. The Simpson formula achieves the

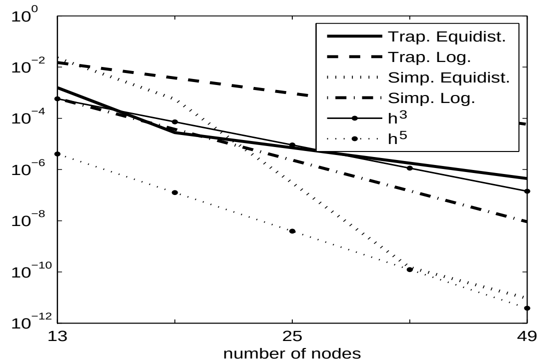


Figure 6: Errors of the Trapezoidal and the Simpson rules with equidistant, respectively with logarithmic spacing, on interval [0,10], $E_{n,m}(f) = Ch^p$, errors are order h^p, $p = 3$ for the Trapezoidal rule, $p = 5$ for the Simpson rule

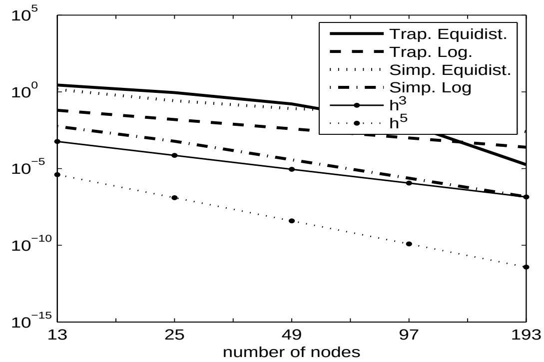


Figure 7: Errors of the Trapezoidal and the Simpson rules with equidistant, respectively with logarithmic spacing, on interval [0,100], $E_{n,m}(f) = Ch^p$, errors are order h^p, $p = 3$ for the Trapezoidal rule, $p = 5$ for the Simpson rule

best results with minimum number of measurement data.

Trapezoidal rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	2.791406	24.174735	0.062714	0.164663
25	0.893123	3.123057	0.015663	0.030117
49	0.161870	0.512594	0.003915	0.006429
97	0.007561	0.257513	9.785918e-004	0.001468
193	1.806600e-005	0.043282	2.446436e-004	3.508924e-004

Simpson rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	1.434890	4.521125e+003	0.005634	2.191761e+001
25	0.260362	1.412897e+002	6.030108e-004	1.444506e+001
49	0.081880	4.422008	3.758309e-005	8.324329
97	0.043876	0.331187	2.352902e-006	4.472056
193	0.002496	0.004630	1.471188e-007	2.318219

Table 5: Actual and estimated errors for the Trapezoidal and the Simpson rules with equidistant and logarithmic spacing, on interval [0,100]. Errors are least for the logarithmic spacing.

Trapezoidal formula				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	40.115607	2.411266e+004	0.141206	0.513932
25	19.302000	3.014094e+003	0.035498	0.080991
49	8.924708	3.767860e+002	0.008868	0.015809
97	3.794501	47.145506	0.002217	0.0034683
193	1.341793	5.979640	5.541306e-004	8.108447e-004

Simpson rule				
n+1	Err. Equidist.	Estim. Equidist.	Err. Log.	Estim. Log.
13	26.230008	1.674490e+007	0.039376	4.476908e+002
25	12.364131	1.412850e+007	0.002686	1.876580e+002
49	5.465610	1.635244e+004	1.908978e-004	1.160830e+002
97	2.084432	1.379737e+004	1.197078e-005	6.461387e+001
193	0.524224	4.311717e+002	7.488580e-007	3.409340e+001

Table 6: Actual and estimated errors for the Trapezoidal and the Simpson rules with equidistant and logarithmic spacing, on interval [0,1000]. Errors are least for the logarithmic spacing.

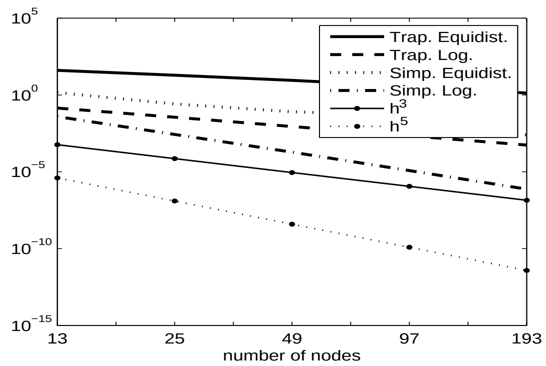


Figure 8: Errors of the Trapezoidal and the Simpson rules with equidistant, respectively with logarithmic spacing, on interval [0,1000], $E_{n,m}(f) = Ch^p$, errors are order h^p, $p = 3$ for the Trapezoidal rule, $p = 5$ for the Simpson rule

$f_{10} = \frac{1}{1+(x-10)^2}$				
n+1	Err.Trap.	Estim.Trap.	Err. Simp.	Estim. Simp.
49	0.021407	0.384475	0.321261	26.396657
97	0.001205	0.091974	0.126766	9.691087
193	2.901779e-004	0.019463	0.005545	4.807445

$f_{100} = \frac{1}{1+(x-100)^2}$				
n+1	Err.Trap.	Estim.Trap.	Err. Simp.	Estim. Simp.
49	3.231907	33.112627	4.848258	14.369474
97	1.133818	4.524826	1.845297	8.328863
193	0.244314	0.701728	0.432838	4.548905

$f_{1000} = \frac{1}{1+(x-1000)^2}$				
n+1	Err.Trap.	Estim.Trap.	Err. Simp.	Estim. Simp.
49	2.169181e-009	2.204492e-009	1.055802e-009	14.365771
97	5.434546e-010	5.478682e-010	9.917991e-010	8.309066
193	1.359363e-010	1.364874e-010	9.874902e-010	4.468869

Table 7: Actual and estimated errors for the Trapezoidal and the Simpson rule with logarithmic spacing on interval [0,100]

49 nodes				
x_0	Err.Trap.	Estim.Trap.	Err. Simp.	Estim. Simp.
0.1	0.015735	0.0339	6.003002e-004	1.441150e+003
1	0.016006	0.0741	0.001655	1.441286e+003
10	0.288480	2.5817	0.281566	1.452840e+003
100	6.731965	1.7996e+003	3.283812	1.200295e+004
1000	1.009258e+002	1.7997e+006	63.636170	1.056410e+007

97 nodes				
x_0	Err.Trap.	Estim.Trap.	Err. Simp.	Estim. Simp.
0.1	0.003936	0.007115	3.202296e-005	8.311410e+002
1	0.004004	0.015247	4.143097e-005	8.311726e+002
10	0.020909	0.551529	0.124979	8.324809e+002
100	2.032018	74.587210	0.450937	1.936424e+003
1000	48.679300	2.021147e+005	31.10335	1.106135e+006

Table 8: Actual and estimated errors for the Trapezoidal and the Simpson rule with logarithmic spacing on interval [0,10000] for the function $f_{x_0} = \frac{1}{1+(x-x_0)^2}$ using 49 and 97 nodes

Interval	Trap. Equidist.	Trap. Log.	Simp. Equidist.	Simp. Log.
[0,10]	11	15	37	9
[0,100]	100	30	300	13
[0,1000]	950	47	3000	17

Table 9: Approximate number of nodes required to achieve accuracy of 0.01 for $f = \frac{1}{1+x^2}$ on different intervals

x_0	0.1	1	10	100	1000
Trap.	65	65	115	1000	8000
Simp.	17	30	95	1260	6000

Table 10: Approximate number of nodes required to achieve accuracy of 0.01 for $f_{x_0} = \frac{1}{1+(x-x_0)^2}$ on the interval $[0, 10000]$ using logarithmic spacing

3 Numerical experiments with functions arising in the mathematical modeling

3.1 Functions in the imaginary part of the convolutional equation

According to the initial experiments we choose the most acurate method and we present some results using the method in the chapter.

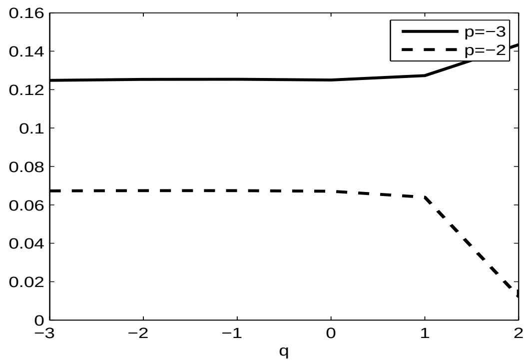
In this chapter we use functions in integrals in (2). In Z_2 there are functions:

$$f_{p,q} = \frac{a(x - x_0)}{1 + (a(x - x_0))^2},$$

where $a = 10^p$, $p = -3, \ldots, 6$, $x_0 = 10^q$, $q = -3, \ldots, 2$. We present accuracy achieved using 100 nodes for pair (p, q) when the interval for x is 0 to 1000. According to the initial tests the best spacing for computing is the logarithmic one, so we will not consider equidistant spacing in this section. We present both the Trapezoidal rule and the Simpson rule. The Simpson rule lead generally to more accurate results, but the Trapezoidal rule was in some cases better.

We can see from Figures 11 and 10 that there is a significant difference between the two formulae for $p = -3, ..., -1$, the Trapezoidal formula is more accurate. The error of the Simpson formula achieves almost 35, the error of the Trapezoidal formula is less than 0.15. The biggest difference of the formulae considering particular p is for $p = -3$.

The formulae lead to similar values of errors for $p = 0, ..., 6$ according to Figures 11-9 and 10-11, the Simpson formula is more accurate. The error of both formulae is less than 4 for $p = 0$, less then 0.9 for $p = 1$ and $p = 2$ for the Trapezoidal formula. The accuracy of Simpson formula for $p = 2$ is 0.045. The error descends as p grows.



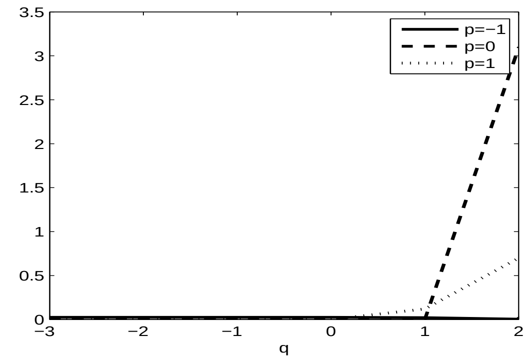


Table 11: Accuracy achieved using the Trapezoidal formula with 100 nodes for functions $f_{p,q} = \frac{10^p(x-10^q)}{1+(10^p(x-10^q))^2}$ on interval $[0, 1000]$

3.2 Functions in the real part of the convolutional equation

The functions arising in Z_1, see (2), are following:

$$g_{p,q} = \frac{1}{1 + (a(x - x_0))^2},$$

where $a = 10^p$, $p = -3, \ldots, 6$, $x_0 = 10^q$, $q = -3, \ldots, 3$. We present accuracy achieved using 100 nodes for pair (p, q) when the interval for x is 0 to 10000 using the Trapezoidal and the Simpson rule with logarithmic spacing. We can see that differences between the rules on this interval are not significant. However, the Simpson formula leads to more accurate results. The worst accuracy, 18, for the both formulae is for $p = -3$, see Figures 12 and 13. The error is less than 1 for $p = 1, 2$ for the Simpson formula and less than 3 for the Trapezoidal formula. The error is less than 0.1 for $p = 3, 4, 5, 6$ for both formulae.

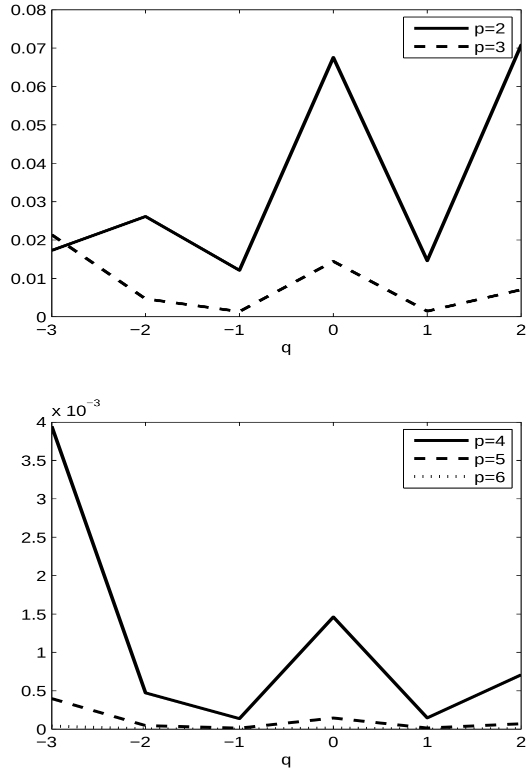


Figure 9: Accuracy achieved using the Trapezoidal formula with 100 nodes for functions $f_{p,q} = \frac{10^p(x-10^q)}{1+(10^p(x-10^q))^2}$ on interval $[0, 1000]$

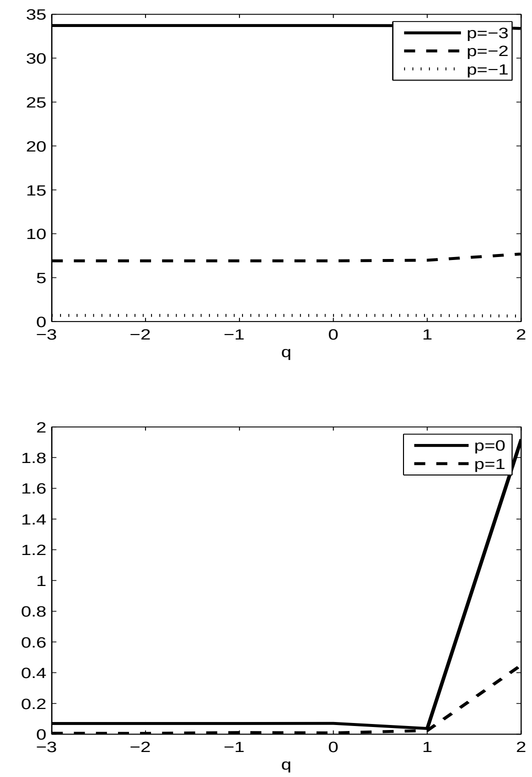
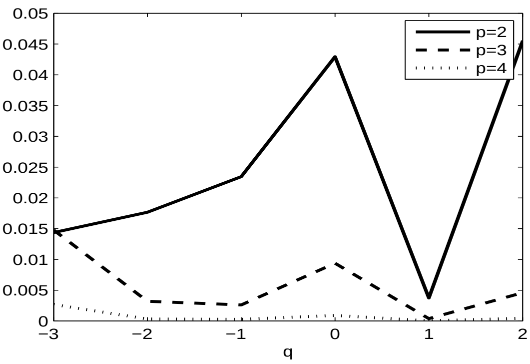


Figure 10: Accuracy achieved using the Simpson formula with 100 nodes, $p = -3, \ldots, 1$, for functions $f_{p,q} = \frac{10^p(x-10^q)}{1+(10^p(x-10^q))^2}$ on interval $[0, 1000]$



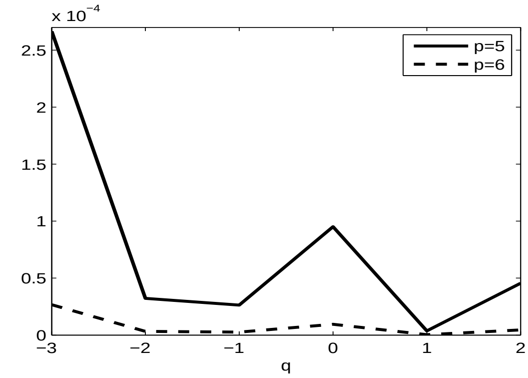


Figure 11: Accuracy achieved using the Simpson formula with 100 nodes, $p = 2, ..., 6$, for functions $f_{p,q} = \frac{10^p(x-10^q)}{1+(10^p(x-10^q))^2}$ on interval $[0, 1000]$

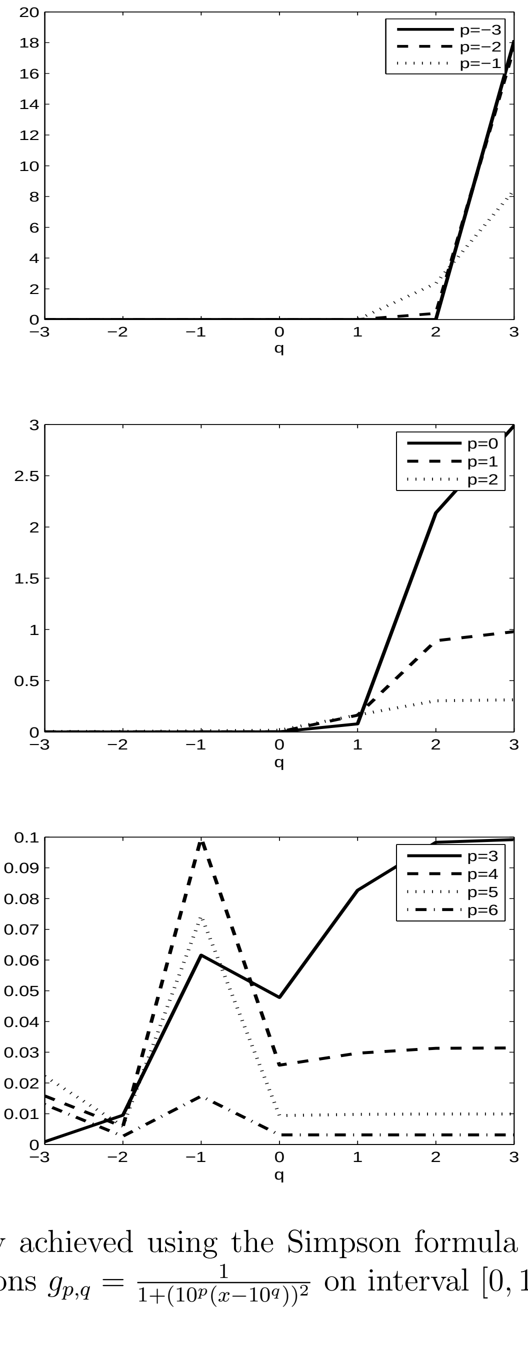


Figure 12: Accuracy achieved using the Simpson formula with 100 nodes, $p = -3, \ldots, 6$, for functions $g_{p,q} = \frac{1}{1+(10^p(x-10^q))^2}$ on interval $[0, 10000]$

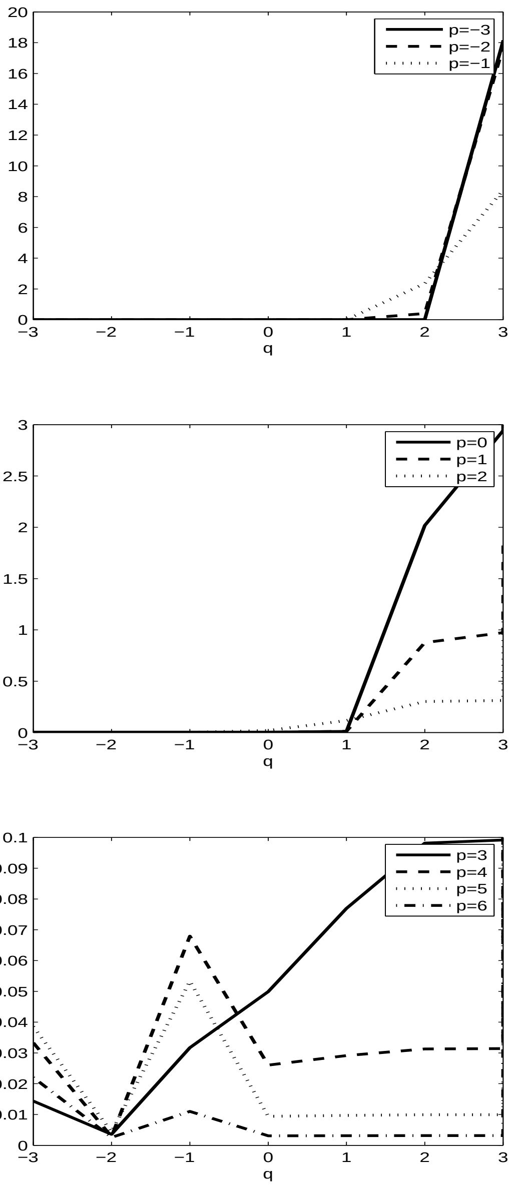


Figure 13: Accuracy achieved using the Trapezoidal formula with 100 nodes, $p = -3, ..., 6$, for functions $g_{p,q} = \frac{1}{1+(10^p(x-10^q))^2}$ on interval $[0, 10000]$

Conclusion

This thesis investigated numerical solution of Fredholm integral equations of the first kind arising in biofuel research. We presented results for numerical integration based on the Lagrange interpolatory quadrature, including simple and composite rules. We showed formulae and error estimates for the Trapezoidal and the Simpson rules. The formulae for errors of quadrature rules using non-equdistant spacing of nodes were derived similarly as the known formulae using equidistant spacing. The theoretical results were then applied in the numerical experiments with simulated data. We studied the validity of error formulae derived in the first chapter for only the composite rules. We disscussed the minimum number of measurement data required for each experiment in order to achieve given accuracy.

From initial experiments we concluded that the logarithmic spacing leads to more accurate results. This can be explained by observing that this spacing captures better both rapid change of functional values for small x and the decay for large x. The equidistant spacing can lead to enormous errors. The Trapezoidal formula leads in some cases to more accurate results, however the Simpson formula is generally better. Numerical experiments further show that the error estimates of the Trapezoidal formula are more accurate. The error estimates for the Simpson rule are often far from the real error because of the higher powers in the formula.

The study of the minimum number of nodes required to achieve given accuracy showed that both the Trapezoidal and the Simpson formulae require less than 115 nodes for functions with the peak near 0 (in our case functions with peak in $[0, 10]$). This result is positive, because in the real problem we can get about 100 measurement data for each experiment. The Simpson formula needs significantly smaller number of nodes. Both considered formulae need hundreds of nodes for functions with the peak in the interval $[100, 1000]$ which is not applicable in our case. We can conclude that generally the Simpson rule with logarithmic spacing achieves the best results with the minimum number of measurement data.

References

[1] Renaut R.A., 2011, *Notes on the Fuel Cell Problem,* paper in preparation

[2] Schichlein H., Muller A.C., Voigts M., Krugel A., Ivers-Tiffée E., 2002, *Deconvolution of electrochemical impedance spectra for the identification of electrode reaction mechanism in solid oxide fuels*, Journal of Applied Electrochemistry, 32, 875-882

[3] Weese J., 1992, *A reliable and fast method for the solution of Fredholm integral equations of the first kind based on Tikhonov regularization*, Computer Physics Communications, 69, 99-111

[4] Endler C., Leonide A., Weber A., Tietz F., Ivers-Tifée E., 2010, *Time-dependent electrode performance changes in intermediate temperature solid oxide fuel cells*, Journal of the Electrochemical Society, 157, B292/B298

[5] Leonide A., Ruger B., Weber A., Meulenberg W.A., Ivers-Tifée E., 2010, *Impedance study of alternative (La,Sr)FeO(3-delta) and (La,Sr)(Co,Fe)O(3-delta) MIEC cathode compositions, Journal of the Electrochemical Society*, 57, B234-B239

[6] Liu B., Muroyama H., Matsui T., Tomida K., Kabata T., Eguchi K., 2010, *Analysis of impedance spectra for segmented-in-series tubular solid oside fuel cells*, Journal of the Electrochemical Society, 157, B1858-B1864

[7] Liu B., Muroyama H., Matsui T., Tomida K., Kabata T., Eguchi K., 2011, *Gas transport impedance in segment-in-series tubular solid oxide fuel cells,* Journal of the Electrochemical Society, 157, B215-B224

[8] Leonide A., Sonn V., Weber A., Ivers-Tiffée E., 2008, *Evaluation and Modeling of the Cell Resistance in Anode-Supported Solid Oxide Fuel Cells*, Journal of the Electrochemical Society, 155, (1), B36-B41

[9] Sonn V., Leonide A., Ivers-Tiffée E., 2008, *Combined Deconvolution and CNLS Fitting Approach Applied on the Impedance Response of Technical Ni/8YSZ Cermet Electrodes,* Journal of the Electrochemical Society, 155, (7), B675-B679

[10] Macutkevic J., Banys J., Matulis A., 2004, *Determination of the Distribution of the Relaxation Times from Dielectric Spectra,* Nonlinear Analysis: Modellling and Control, 9, (1), 7588

[11] Quarteroni A., Sacco R., Saleri F., 2000, *Numerical Mathematics*, Springer, ISBN 0-387-98959-5

[12] Dalquist G., Björck Å., 2008, *Numerical Methods in Scientific Computing: Volume 1*, SIAM, ISBN-10: 0898716446

[13] Davis P.J., Rabinowitz P., 2007, *Methods of Numerical Integration: Second Edition*, Academic Press, ISBN-10: 0486453391

[14] *Simpson's Rule* [online], http://pages.pacificcoast.net/~cazelais/187/simpson.pdf

[15] Embree M, *Lecture 23b: Peano Kernel Analysis* [online], 2009, http://www.caam.rice.edu/~caam453/lecture23b.pdf