Software Requirements Specification for ROC: Software estimating the radius of convergence of a power series

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Contents

Revision History

Date	Version	Notes
12 October 2020	1.0	First submission
24 December 2020	2.0	Second submission

1 Reference Material

This section records information for easy reference.

1.1 Table of Units

A Table of Units is not applicable to ROC.

1.2 Table of Symbols

The table that follows summarizes the mathematical notation used in this document.

symbol	description
$z \in \mathbb{C}$	A member z of the complex numbers $\mathbb{C}$
$x \in \mathbb{R}$	A member x of the real numbers $\mathbb{R}$
$\left\{c_n\right\} \subset \mathbb{C}$	A sequence of complex numbers whose n^{th} term is $c_n \in \mathbb{C}$
$\left\{c_n\right\}_{n=0}^{N-1} \subset \mathbb{C}$	A finite sequence of N complex numbers whose n^{th} term is $c_n \in \mathbb{C}$
$\sum_{n=0}^{\infty} c_n(z-z_0)^n$	A power series. $c_n \in \mathbb{C}$ is the n^{th} coefficient. z^n is the n^{th} power of $z \in \mathbb{C}$. z_0 is the center point.
$\liminf\limits_{n\to\infty}$	Lower subsequential limit
$\limsup\limits_{n\to\infty}$	Upper subsequential limit
R_c	Radius of the circle of convergence
$\mathbb{R}^d$	A d-dimension real vector space
$\mathcal{D}$	An open subset of $\mathbb{R}^d$
$[a,b] \subset \mathbb{R}$	Interval of real numbers, $t \in [a,b]$ means $a \leq t \leq b$ and $t \in \mathbb{R}$
$(x_n)_n$	n^{th} Taylor coefficient of $t \in \mathbb{R} \mapsto x \in \mathbb{R}^d$ evaluated at $t_n \in \mathbb{R}$

1.3 Abbreviations and Acronyms

symbol	description
A	Assumption
$\mathbb{C}$	Complex numbers
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
IVP	Initial Value Problem
LC	Likely Change
$\mathbb{N}$	The non-negative integers
ODE	Ordinary Differential Equation
$\mathbb{R}$	Real numbers
R	Requirement
ROC	Radius of Convergence software developed for this project
SRS	Software Requirements Specification
T	Theoretical Model
TC	Taylor coefficient
TS	Taylor series
TLA	Top Line Analysis
3TA	Three Term Analysis
6TA	Six Term Analysis

2 Introduction

Given a sequence $\{c_n\}$ of complex numbers, the series

$$\sum_{n=0}^{\infty} c_n (z - z_0)^n \tag{1}$$

is called a *power series*. The number $c_n \in \mathbb{C}$ is the n^{th} coefficient in the power series. The symbol z^n denotes the n^{th} power of the complex number z. This power series is *centered* at $z_0 \in \mathbb{C}$.

In general, a power series will converge or diverge, depending on the magnitude of $z - z_0$. With every power series, there is associated a circle of convergence such that (1) converges if z is in the interior of the circle of convergence or diverges if z is in the exterior of the circle of convergence. The convergence/divergence behavior of (1) on the circle of convergence can not be described so simply. By convention, the entire complex plane is the interior of a circle of infinite radius, and a point is the interior of a circle of zero radius.

This project is concerned with estimating the radius R_c of the circle of convergence.

2.1 Purpose of Document

The purpose of this document is to facilitate communication between the stakeholders and developers during the software development of project ROC by communicating and reflecting its software requirements. The scientific and business problem ROC solves is described in Section 4.1, the "Problem Description".

2.2 Scope of Requirements

In the late 1800's, several authors resolved problems concerning the characterization and analysis of singularities for power series. Chang and Corliss (1982) discuss this history and their approach to computing R_c.

> Our approach to series analysis was motivated by the observation that series for solutions to ODEs follow a few very definite patterns which are characterized by the location of primary singularities. In general, the coefficients of a power series follow no patterns, so few theorems about truncated series can be proved. However, series which are real-valued on the real axis can have poles, logarithmic branch points, and essential singularities only on the real axis or in conjugate pairs. Further, the effects of all secondary singularities disappear if sufficiently long series are used. (Chang and Corliss, 1982, p. 122)

A primary singularity of (1) is the closest singularity to the series expansion point in the complex plane. All other singularities are secondary singularities.

Chang and Corliss (1982) proposed a method of four parts to estimate the radius R_c of the circle of convergence as well as the order and location of primary singularities. The top-hump analysis applies to the power series of entire functions. The 3TA analysis applies to the power series of functions exhibiting a single primary singularity. The 6TA applies to the power series of functions exhibiting a conjugate pair of primary singularities. Whenever these three analysis fail to resolve the R_c, singularity order, and singularity location parameters for the series, the Chang and Corliss (1982) method does a top-line analysis. Each Chang and Corliss (1982) sub-method works by fitting R_c, singularity order, and singularity location parameters of a known model to the given sequence.

Top-line analysis always applies to power series. It resolves situations where secondary singularities are less distinguishable from primary singularities. However it is less accurate, but it does have a convergence analysis (Chang and Corliss, 1982).

The scope of this ROC project includes three term analysis of primary real poles, six term analysis of primary pair of complex conjugate poles, and top line analysis. ROC does not yet include an analysis for essential singularities.

2.3 Characteristics of Intended Reader

This document assumes the intended reader has familiarity with basic real analysis, complex analysis, and Taylor arithmetic. Courses which contribute to background knowledge may be titled Ordinary Differential Equations and Linear Algebra (undergrad), Introduction to Real Analysis (undergrad), Multivariate Calculus (undergrad), Functional Analysis (Graduate), Real Analysis (Graduate), and Complex Analysis (Graduate). Sequences and power series as well as the ratio and root tests will be discussed in this document. However, our exposition will only cover the concepts needed for our purposes. For proofs and for a complete exposition of all background materials, the interested reader should consult a beginning level graduate text such as Rudin (1976). For a brief but sufficient introduction to Taylor arithmetic, consult Bendsten and Stauning (1997).

2.4 Organization of Document

This document is built on the template recommendations in Smith and Lai (2005); Smith et al. (2007) that seeks to standardize communication tools for software development. The suggested order for reading this SRS document is: Goal Statement (Subsection 4.1.3), Instance Models (Subsection 4.2.5), Requirements (Section 5), Introduction (Section 2), and Specific System Description (Section 4).

3 General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics, and lists the system constraints.

3.1 System Context

The following figure depicts a system context view of ROC. This context appears, for example, in the numerical solution of ordinary differential and differential algebraic equations.

Figure 1: System Context

After generating a real-valued Taylor series (TS) approximate solution of order p to the ordinary differential equation (ODE) initial-value problem (IVP)

$$y'(t) = f\Big(t, y(t)\Big), \quad y(t_0) = y_0 \in \mathcal{D} \subset \mathbb{R}^d, \quad t \in [t_0, t_{\text{end}}] \subset \mathbb{R}, \tag{2}$$

the TS methods defined in Jorba and Zou (2005), Bergsma and Mooij (2016), and Chang and Corliss (1982) explicitly require an estimate for the TS radius of convergence.

At each (t_n, x_n), $n \geq 0$, the TS method for the numerical solution of (2) computes Taylor coefficients (TCs) $(x_n)_i$ at t_n to construct the TS approximate solution

$$T(t) = x_n + \sum_{i=1}^{p} (x_n)_i (t - t_n)^i \quad \text{on} \quad [t_n, t_{n+1}]. \tag{3}$$

Analysis of Equation (3) for its radius of convergence provides a practical system context for ROC as depicted in Figure 1. In this system context, developers like Bergsma and Mooij (2016), Jorba and Zou (2005), or Chang and Corliss (1982) of a TS method seek the accuracy assurance from knowing the domain $[t_n, t_{n+1}]$ is in the circle of convergence.

3.2 User Characteristics

One intended user of ROC is a user of MAPLE or MATLAB. While neither MATLAB nor MAPLE currently implements an estimate for R_c, presumably the companies that develop MATLAB and MAPLE will want to provide such a facility when robust, reliable, and accurate computational tools are available. Users of ROC would be a calculus student, a user of MAPLE or MATLAB, and a developer of a Taylor series method as in Subsection 3.1.

3.3 System Constraints

The method developed in this project is expected to be independent of system constraints. However most TS methods are developed in C++ or FORTRAN 77, the goto languages of scientific computing. Certainly a scripting language would not be sufficient for large systems.

4 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models.

4.1 Problem Description

ROC is intended to estimate the radius of the circle of convergence of a power series.

4.1.1 Terminology and Definitions

A *sequence* is a function f whose domain is the non-negative integers $\mathbb{N}$ and range is in E, that is, a sequence is the mapping $n \in \mathbb{N} \mapsto f(n) = c_n \in E$. It is customary to denote the sequence f by the symbol $\left\{c_n\right\}$ or by $c_0, c_1, c_2, \ldots$. The values of f, that is, the elements c_n are called the *terms* of the sequence. If A is a subset of E and if $c_n \in A$ for all $n \in \mathbb{N}$, the $\left\{c_n\right\}$ is said to be a *sequence in* A. The terms of a sequence need not be distinct. Typically, E is the complex numbers $\mathbb{C}$ or the real numbers $\mathbb{R}$.

Given a sequence $\left\{c_n\right\}$, we use the notation

$$\sum_{n=p}^{q} c_n \qquad \text{with} \qquad p \leq q \tag{4}$$

to denote the sum $c_p + c_{p+1} + \cdots + c_q$. With the sequence $\left\{c_n\right\}$, we associate a sequence $\left\{s_n\right\}$, where

$$s_n \stackrel{\text{def}}{=} \sum_{k=0}^{n} c_k. \tag{5}$$

For the sequence $\left\{s_n\right\}$, we may use the symbolic expression $c_0 + c_1 + c_2 + \ldots$ or

$$\sum_{n=0}^{\infty} c_n. \tag{6}$$

The symbol (6) is called an *infinite series* or just *series*. The terms s_n are called *partial sums* of the series, they are just numbers. If $\left\{s_n\right\} \to s$ as $n \to \infty$, then we say $\left\{s_n\right\}$ converges to s, the series converges, and write

$$\sum_{n=0}^{\infty} c_n = s. \tag{7}$$

The number s is the limit of a sequence of sums called the *sum of the series*. If $\left\{s_n\right\}$ diverges, then the series is said to diverge.

Given a sequence $\{e_n\}$, consider a sequence $\{n_k\}$ of non-negative integers such that $n_0 < n_1 < n_2 < \cdots$. Then the sequence $\{e_{n_k}\}$ is called a *subsequence* of $\{e_n\}$. If $\{e_{n_k}\}$ converges, its limit is called a *subsequential limit* of $\{e_n\}$.

Let $\{s_n\}$ be a sequence of real numbers. Let E be the set of numbers x in the extended real number system such that $s_{n_k} \to x$ for some subsequence $\{s_{n_k}\}$. This set E contains all subsequential limits plus possibly $+\infty$ and $-\infty$. Define $s^* \stackrel{\text{def}}{=} \sup E$ and $s_* \stackrel{\text{def}}{=} \inf E$. The numbers s^* and s_* are called the *upper limit* and *lower limit* of $\{s_n\}$. We use the notation

$$\liminf_{n\to\infty} s_n = s_* \qquad \text{and} \qquad \limsup_{n\to\infty} s_n = s^*. \tag{8}$$

4.1.2 Physical System Description

This subsection doesn't apply to ROC.

4.1.3 Goal Statements

Given a tolerance TOL, a truncated finite sequence $\{c_n\}$, and the applied scale to the coefficients c_n, the goals of this project are:

GS1: Implement Chang and Corliss (1982) three term analysis to estimate R_c, the order of singularity, the modelling error, and the truncation error committed by truncating the sequence at N for a primary real pole. This appears to be four goals. However, the same setup and computation leads to each quantity. Separating these quantities into four goals would lead to a verbose, redundant document.

GS2: Implement Chang and Corliss (1982) six term analysis to estimate R_c, the order of singularity, the modelling error, and the truncation error committed by truncating the sequence at N for a pair of primary complex conjugate poles. This appears to be four goals. However, the same setup and computation leads to each quantity. Separating these quantities into four goals would lead to a verbose, redundant document.

GS3: Implement Chang and Corliss (1982) top line analysis to estimate R_c and the modelling error for a mix of primary and secondary poles, logarithmic branch points, and essential singularities.

4.2 Solution Characteristics Specification

This section characterizes the attributes of an acceptable solution. Both analysts and stakeholders should agree on these attributes so that the solution can be accepted when the project is complete.

4.2.1 Assumptions

Given a tolerance TOL, consider the sequence $\left\{c_n\right\}$ and its power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$ under the following assumptions:

A1: We know an integer N such that, for all $m \geq n \geq N$, $|\sum_{k=n}^{m} c_k| <$ TOL.

A2: The software ROC will estimate the radius of convergence from a finite number of terms in the power series. It will not compute R_c exactly.

A3: The sequence $\left\{c_n\right\}$ is a subset of $\mathbb{R}$.

A4: The scope of three term analysis is to compute the radius of convergence of a real power series at a point $z_0 \in \mathbb{R}$ that has a primary singularity.

A5: The scope of six term analysis is to compute the radius of convergence of a real power series at a point $z_0 \in \mathbb{R}$ that has a complex conjugate pair of primary singularity.

A6: The scope of top line analysis is to compute the radius of convergence of a real power series at a point $z_0 \in \mathbb{R}$ that has a secondary singularity.

4.2.2 Theoretical Models

Applying the terminology and definitions from Subsection 4.1.1, this section records theorems required to identify a convergent/divergent series.

Consider the sequence $\left\{c_n\right\}$ and its power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$. The following TM is used to show that the coefficients in the terms of a series tend to zero as the index of the term tends to infinity.

Number	T1
Label	**Cauchy convergence condition**
Theorem	A series $\sum_{n=0}^{\infty} c_n$ converges if an only if, for every $\epsilon > 0$, there is an integer N such that $\lvert\sum_{k=n}^{m} c_k\rvert < \epsilon$ whenever $m \geq n \geq N$.
Description	Tools to identify when a series converges.
Source	Theorem 3.22 (Rudin, 1976, p. 59)
Ref. By	IM5

Number	T2
Label	**Convergence of sequence**
Theorem	If series $\sum_{n=0}^{\infty} c_n$ converges, then $\lim_{n\to\infty} c_n = 0$.
Description	If a series converges, then its terms converge to zero.
Source	Theorem 3.28 (Rudin, 1976, p. 60)
Ref. By	IM5

Number	T3
Label	**Root test**
Theorem	Given a series $\sum_{n=0}^{\infty} c_n$. Set $\alpha \stackrel{\text{def}}{=} \limsup\limits_{n\to\infty} \sqrt[n]{\lvert c_n\rvert}$. Then (a) if $\alpha < 1$, then $\sum_{n=0}^{\infty} c_n$ converges; (b) if $\alpha > 1$, then $\sum_{n=0}^{\infty} c_n$ diverges; (c) if $\alpha = 1$, then this test gives no information.
Description	Tools to identify when a series converges/diverges.
Source	Theorem 3.33 (Rudin, 1976, p. 65)
Ref. By	GD1 and IM5

Number	T4
Label	**Ratio test**
Theorem	The series $\sum_{n=0}^{\infty} c_n$ (a) converges if $\limsup\limits_{n\to\infty} \lvert\frac{c_{n+1}}{c_n}\rvert < 1$, (b) diverges if $\lvert\frac{c_{n+1}}{c_n}\rvert \geq 1$ for $n \geq N$, where N is some fixed integer.
Description	Tools to identify when a series converges/diverges.
Source	Theorem 3.34 (Rudin, 1976, p. 66)
Ref. By	IM5

The ratio test is often easier to apply than the root test. However, the root test resolves more application than the ratio test. Both the ratio test and the root test deduce divergence from the statement in Theoretical Model 2, if a series converges, then its terms converge to zero.

Number	T5
Label	**Comparing the Ratio test and the Root test**
Theorem	For any sequence $\{c_n\}$ of positive (real) numbers, (a) $\liminf_{n\to\infty} \frac{c_{n+1}}{c_n} \le \liminf_{n\to\infty} \sqrt[n]{c_n}$, (b) $\limsup_{n\to\infty} \sqrt[n]{c_n} \le \limsup_{n\to\infty} \frac{c_{n+1}}{c_n}$
Description	If the ratio test converges, then the root test converges and if the root test is inconclusive, then the ratio test is inconclusive. Whenever the limit exists and it is unique, then there is equality in (a) and (b) and $\lim_{n\to\infty} \frac{c_{n+1}}{c_n} = \lim_{n\to\infty} \sqrt[n]{c_n}$.
Source	Theorem 3.37 (Rudin, 1976, p. 68)
Ref. By	IM5

The characterization and analysis of singularities of analytic functions by its Laurent series was known by the 1870s (Chang and Corliss, 1982, p. 122). The following theoretical model characterizes singularities that a power series with real coefficients can exhibit.

Number	T6
Label	**Series with primary poles**
Theorem	For any sequence $\{c_n\}$ of real numbers, its power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$ when $z_0 \in \mathbb{R}$ can have poles, logarithmic branch points, and essential singularities only on the real axis or in conjugate pairs. Further, the effects of all secondary singularities disappear if sufficiently long series are used.
Description	Characterization of singularities of power series with real coefficients.
Source	(Chang and Corliss, 1982, p. 122)
Ref. By	IM1, IM2, IM3, IM4, and IM5

4.2.3 General Definitions

The proofs of the theorem in this section apply the terminology and definitions from Subsection 4.1.1 as well as the Theoretical models from Subsection 4.2.2.

The radius of the circle of convergence is defined in the next General Definition, a theorem that enables us to justify and construct the IM for TLA so that ROC will estimate R_c.

Number	GD1
Label	**Define the radius of the circle of convergence**
Theorem	Given any sequence $\{c_n\}$, construct the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$. Set $\alpha \stackrel{\text{def}}{=} \limsup_{n\to\infty} \sqrt[n]{\lvert c_n\rvert}$ and $R_c \stackrel{\text{def}}{=} 1/\alpha$. Then $\sum_{n=0}^{\infty} c_n(z-z_0)^n$ converges whenever $\lvert z-z_0\rvert < R_c$.
Description	This General Definition defines R_c, the radius of convergence of the power series. By our convention stated Subsection 4.1.1, $\alpha = 0$ implies $R_c = +\infty$ and $\alpha = +\infty$ implies $R_c = 0$.
Source	Theorem 3.39 (Rudin, 1976, p. 69)
Ref. By	IM5

We need to relate the root test to the ratio test to obtain our IM. It is instructive to understand the role of the root test in the proof of GD1.

Inside GD1

Given any sequence $\{c_n\}$, construct the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$. Set $a_n = c_n(z-z_0)^n$, and apply the root test TM3 to the series $\sum_{n=0}^{\infty} a_n$.

$$\limsup_{n\to\infty} \sqrt[n]{\lvert a_n\rvert} = \lvert z-z_0\rvert \limsup_{n\to\infty} \sqrt[n]{\lvert c_n\rvert} \stackrel{\text{def}}{=} \frac{\lvert z-z_0\rvert}{R_c}. \tag{9}$$

Obtain from the root test that

(a) if $\lvert z-z_0\rvert < R_c$, then the power series converges;

(b) if $\lvert z-z_0\rvert > R_c$, then the power series diverges;

(c) if $\lvert z-z_0\rvert = R_c$, then this test gives no information.

The next section presents a Data Definition on order of singularity.

4.2.4 Data Definitions

We quoted from Chang and Corliss (1982) in Section 2.2, the scope section, that, in general, the coefficients of a power series follow no patterns, so few theorems about truncated series can be proved. However, TM6 asserts that series which are real-valued on the real axis can have poles, logarithmic branch points, and essential singularities only on the real axis or in conjugate pairs. The sequence $\left\{c_n\right\}$ is a subset of $\mathbb{R}$ under Assumption 3. The following DD concerns a procedure to approximate the order of singularity in TLA for series which are real-valued on the real axis.

Number	DD1
Label	**Order of singularity**
Symbol	μ
Conditions	Assume Assumption 3. Further assume the real coefficients $\left\{c_n\right\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$ are obtained as a TS solution of an ODE and consider finding the order μ of the singularity from the graph of $\log_{10}\lvert c_n\rvert$ versus n.
Observations	The order μ is increased or decreased by term-by-term differentiation or integration, respectively. The upper envelope of the graph of $\log_{10}\lvert c_n\rvert$ versus n will follow the following patterns: • If the order of the primary singularity, the closest singularity to z_0, is $\mu = 1$, then the slope is $\log_{10}\lvert z-z_0\rvert/R_c$. • If the order of the primary singularity $\mu \neq 1$, then the slope converges to $\log_{10}\lvert z-z_0\rvert/R_c$ at a rate proportional to $1/n$. • If the order of the primary singularity $\mu \neq 1$, then the upper envelope is not linear. For orders $\mu > 1$, the graph opens downward. The concavity approaches zero as $1/n^2$ as $n \to \infty$. For orders $\mu < 1$, the graph is concave up which means the slope underestimates $\log_{10}\lvert z-z_0\rvert/R_c$, and R_c is overestimated.
Description	
Sources	Chang and Corliss (1982)
Ref. By	IM6

Our analysis requires the following DD, a basic formula of Taylor arithmetic.

Number	DD2
Label	**Taylor arithmetic formula: analytic function to a constant power**
Symbol	$(u^a)_k$
Conditions	Let $z \in \mathcal{D} \subset \mathbb{R} \mapsto u(z) \in \mathbb{R}$ be an analytic function. Denote by $(u)_k$ the k^{th} TC of u evaluated at some real $z_0 \in \mathcal{D}$. Assume $u(z_0) \neq 0$. Let a be a real constant.
Observations	Then the k^{th} TC of $(u^a)_k$ is given by the Taylor arithmetic formula $$(u^a)_k = \frac{1}{k(u)_0} \sum_{j=0}^{k-1} (a(k-j)-j)(u^a)_j(u)_{k-j}, \qquad \text{for} k \geq 1. \qquad (10)$$
Description	TCs of an analytic function to a constant power
Sources	Bendsten and Stauning (1997)
Ref. By	IM1 and IM3

The next section derives an IM to approximate R_c.

4.2.5 Instance Models

This section transforms the problem defined in Section 4.1 into one which can be translated into software. We will define finite sequences and series to replace the infinite counterparts identified in Sections 4.2.2 and 4.2.3.

Given real constants a and $s > 0$, real expansion point $z_0 = 0$, and scaling h, Chang and Corliss (1982) choose the real valued function

$$v(z) \stackrel{\text{def}}{=} (a - z)^{-s} \tag{11}$$

to model one primary pole or logarithmic branch point. The model is relevant because, for any fixed but arbitrary z_0, any analytic function f at z_0 with only one primary pole or logarithmic branch point has the form $f(z) = C(v(z))$, where C is an analytic function near z_0 (Chang and Corliss, 1982).

Number	IM1
Label	TCs for one primary real pole or logarithmic branch point
Theorem	Given real constants a and $s > 0$, real expansion point $z_0 = 0$, and scaling h, the TCs of Equation (11) at $z_0 = 0$ are $$k(v)_k = (v)_{k-1}(k + s - 1)\frac{h}{z_0}, \qquad \text{for} \quad k \geq 1. \tag{12}$$
Description	TCs of Equation (11)
Sources	Chang and Corliss (1982)
Ref. By	IM2

We now justify IM1.

Inside IM1

Given real constants a and $s > 0$, real expansion point z_0, and scaling h, Equation (11) is a pole or a logarithmic branch point, which are two possibilities of the four total enumerated in TM6.

Compute the TS for Equation (11) at $z_0 = 0$. R_c is the distance to primary singularity. We employ the Taylor arithmetic formula for analytic function to a constant power provided in DD2. Set $u = a - z$. Then $(u)_0 = z_0$, $(u)_1 = -1$, and $(u)_k = 0$ for $k > 1$. Compute $j = k \Rightarrow k - j = 0$ and $j = k - 1 \Rightarrow k - j = 1$. A scaled R_c is related to the unscaled $\widetilde{R}_c$ by $h\widetilde{R}_c = R_c$. As a matter of notation, $\widetilde{R}_c = z_0$. Apply DD2 to this problem and simplify to observe the statement of IM1.

Number	IM2
Label	3TA: Model one primary real pole or logarithmic branch point
Theorem	Given tolerance TOL, real constants a and $s > 0$, a real expansion point z_0, scaling h, $N >$ nUses $>$ MINTERMS > 0, and real coefficients $\{c_n\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$, set $W(i,1) = (k(i)-1)c_{k(i)}$, $W(i,2) = c_{k(i)}$, and $b(i) = k(i)c_{k(i)+1}$ for $k(i) = N-\text{nUses}, \ldots, N$ and $i = 1, \ldots, \text{nUses}$ to obtain the linear system $W\beta = b$ where $\beta(1) = h/R_c \stackrel{\text{def}}{=} h/z_0$ and $\beta(2) = s\beta(1)$. Let β solve $\min_{\beta \in \mathbb{R}^2} \|\beta\|_2^2$ such that $W\beta = b$. Then the least squares best fit of the data $\{c_n\}$ to the model problem (11) is $R_c = h/\beta(1)$ and $\mu = \beta(2)/\beta(1)$.
Description	Use 3TA to compute R_c and μ and approximate truncation error
Sources	The full details are my own contribution. However the ideas are inspired by conversations with G. Corliss and N. Nedialkov.
Ref. By	Final product

We now justify IM2.

Inside IM2

Given tolerance TOL, let Assumption 1 and Assumption 3 hold. Assumption 1 provides the parameter N such that, for all $m \geq n \geq N$, $|\sum_{k=n}^{m} c_k| <$ TOL. Given real constants a and $s > 0$, a real expansion point z_0, scaling h, $N >$ nUses $>$ MINTERMS > 0, and real coefficients $\{c_n\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$, we formulate the optimization problem.

We use optimal least squares fitting to fit the real coefficients $\{c_{\text{nUses}}, \ldots, c_N\}$ from any given real sequence $\{c_n\}$ to the sequence $\{v_n\}$ of IM1.

We rearrange the IM1 system

$$k(v)_k = (v)_{k-1}(k+s-1)\frac{h}{z_0}, \qquad \text{for} \quad k \geq 1. \tag{13}$$

to

$$k(v)_k = (v)_{k-1}(k-1)\frac{h}{z_0} + (v)_{k-1}s\frac{h}{z_0}, \qquad \text{for} \quad k \geq 1. \tag{14}$$

Set $W(i,1) = (k(i)-1)c_{k(i)}$, $W(i,2) = c_{k(i)}$, and $b(i) = k(i)c_{k(i)+1}$ for $k(i) = N-\text{nUses}, \ldots, N$ and $i = 1, \ldots, \text{nUses}$ to obtain the linear system $W\beta = b$ where $\beta(1) = h/R_c \stackrel{\text{def}}{=} h/z_0$ and $\beta(2) = s\beta(1)$.

At the optimal solution, $R_c = h/\beta(1)$ and $\mu = \beta(2)/\beta(1)$.

Suppose R_c and μ computed as in IM2 have a small fitting error. The quality for small is not yet defined. Then R_c and μ satisfy Assumption 2 and Assumption 4. Moreover using $(v)_k$ as c_k in Assumption 1, we have an estimate for the truncation error.

Given real constants a, b, and $s > 0$, real expansion point $z_0 = 0$, and scaling h, Chang and Corliss (1982) choose the real valued function

$$w(z) \stackrel{\text{def}}{=} (1/2z^2 - 2bz + a^2)^{-s} \tag{15}$$

to model one complex conjugate pair of primary pole. Let $\cos\theta \stackrel{\text{def}}{=} b/a$.

Number	IM3
Label	TCs for one complex conjugate pair of primary pole
Theorem	Given real constants a, b, and $s > 0$, real expansion point $z_0 = 0$, and scaling h, the TCs of Equation (15) at $z_0 = 0$ are $$k(w)_k = 2(w)_{k-1}(k+s-1)\frac{h}{z_0}\cos\theta - (w)_{k-2}(k+2s-2)\left(\frac{h}{z_0}\right)^2, \quad \text{for} \quad k \geq 1. \tag{16}$$
Description	TCs of Equation (15)
Sources	Chang and Corliss (1982)
Ref. By	IM4

We now justify IM3.

Inside IM3

Given real constants a, b, and $s > 0$, real expansion point $z_0 = 0$, and scaling h, Equation (15) is a complex conjugate pair of pole, which is one more additional possibility of the four total enumerated in TM6, distinct from the two covered possibilities discussed in IM1.

Compute the TS for Equation (15) at $z_0 = 0$, R_c is the distance to primary singularity, using the Taylor arithmetic formula for analytic function to a constant power provided in DD2. Set $u = 1/2z^2 - 2bz + a^2$. Then $(u)_0 = z_0$, $(u)_1 = -2b$, $(u)_2 = 1$, and $(u)_k = 0$ for $k > 2$. Compute $j = k \Rightarrow k - j = 0$, $j = k - 1 \Rightarrow k - j = 1$, and $j = k - 2 \Rightarrow k - j = 2$. A scaled R_c is related to the unscaled $\widetilde{R}_c$ by $h\widetilde{R}_c = R_c$. As a matter of notation, $\widetilde{R}_c = z_0$. Apply DD2 to this problem and simplify to observe the statement of IM3.

Number	IM4
Label	6TA: Model one primary real pole or logarithmic branch point
Theorem	Given real constants a, b, and $s > 0$, real expansion point $z_0 = 0$, and scaling h, $N >$ nUses $>$ MINTERMS > 0, and real coefficients $\left\{c_n\right\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z - z_0)^n$, set $W(i, 1) = 2c_{k(i)-1}$, $W(i, 2) = 2(k(i) - 1)c_{k(i)-1}$, $W(i, 3) = -2c_{k(i)-2}$, $W(i, 4) = -(k(i) - 2)c_{k(i)-2}$, and $b(i) = k(i)c_{k(i)}$ for $k(i) = N - \text{nUses}, \dots, N$ and $i = 1, \dots, \text{nUses}$ to obtain the linear system $W\beta = b$. Let β solve $\min_{\beta\in\mathbb{R}^4} \|\beta\|_2^2$ such that $W\beta = b$. Then the least squares best fit of the data $\left\{c_n\right\}$ to the model problem (15) is interpreted as $\sqrt{\beta(4)} = h/R_c \stackrel{\text{def}}{=} h/z_0$, $\cos\theta = \beta(2)R_c/h$, $s_1 = \beta(1)/\beta(2)$, and $s_2 = \beta(3)/\beta(4)$. For a viable computation, we maintain that $\beta(4) \geq 0$, $-1 \leq \cos\theta \leq 1$, and $s_1 \approx s_2$.
Description	Use 6TA to compute R_c and μ and approximate truncation error
Sources	The full details are my own contribution. However the ideas are inspired by conversations with G. Corliss and N. Nedialkov.
Ref. By	Final product

We now justify IM4.

Inside IM4

Given tolerance TOL, let Assumption 1 and Assumption 3 hold. Assumption 1 provides the parameter N such that, for all $m \geq n \geq N$, $|\sum_{k=n}^{m} c_k| <$ TOL. Given real constants a, b, and $s > 0$, real expansion point $z_0 = 0$, and scaling h, $N >$ nUses $>$ MINTERMS > 0, and real coefficients $\left\{c_n\right\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z - z_0)^n$, we formulate the optimization problem.

We use optimal least squares fitting to fit the real coefficients $\left\{c_{\text{nUses}}, \dots, c_N\right\}$ from any given real sequence $\left\{c_n\right\}$ to the sequence $\left\{w_n\right\}$ of IM3.

We rearrange the IM3 system

$$k(w)_k = 2(w)_{k-1}(k + s - 1)\frac{h}{z_0}\cos\theta - (w)_{k-2}(k + 2s - 2)\left(\frac{h}{z_0}\right)^2, \quad \text{for} \quad k \geq 1. \tag{17}$$

to

$$\begin{aligned} k(w)_k \quad = \quad & 2(w)_{k-1}s\tfrac{h}{z_0}\cos\theta + 2(w)_{k-1}(k-1)\tfrac{h}{z_0}\cos\theta \\ & -2(w)_{k-2}s\left(\tfrac{h}{z_0}\right)^2 - (w)_{k-2}(k-2)\left(\tfrac{h}{z_0}\right)^2, \quad \text{for} \quad k \geq 1. \end{aligned} \tag{18}$$

Set $W(i, 1) = 2c_{k(i)-1}$, $W(i, 2) = 2(k(i) - 1)c_{k(i)-1}$, $W(i, 3) = -2c_{k(i)-2}$, $W(i, 4) = -(k(i) - 2)c_{k(i)-2}$, and $b(i) = k(i)c_{k(i)}$ for $k(i) = N - \text{nUses}, \dots, N$ and $i = 1, \dots, \text{nUses}$ to obtain the linear system $W\beta = b$.

At the optimal solution, $\beta(1) = sh/R_c \cos\theta$, $\beta(2) = h/R_c \cos\theta$, $\beta(3) = s(h/R_c)^2$, and $\beta(4) = (h/R_c)^2$. If follows that $\sqrt{\beta(4)} = h/R_c \stackrel{\text{def}}{=} h/z_0$, $\cos\theta = \beta(2)R_c/h$, $s_1 = \beta(1)/\beta(2)$, and $s_2 = \beta(3)/\beta(4)$. For a viable computation, we maintain that $\beta(4) \geq 0$, $-1 \leq \cos\theta \leq 1$, and $s_1 \approx s_2$.

Suppose R_c, s_1, s_2, $\cos\theta$, and μ computed as in IM4 have a small fitting error. The quality for small is not yet defined. Then R_c and μ satisfy Assumption 2 and Assumption 5. Moreover using $(w)_k$ as c_k in Assumption 1, we have an estimate for the truncation error.

A heuristically motivated top-line analysis produces a conservative estimate for the radius of convergence R_c from the slope of a linear upper envelope of a graph of $\log_{10}|c_n|$ versus n (Chang and Corliss, 1982). While no proof is given in this paper, the following argument justifies their claim that the slope approaches $\log_{10}|z - z_0|/R_c$ as $n \to \infty$.

Number	IM5
Label	**Approximating the radius of convergence**
Inputs	N and approximation points (19)
Output	R_c or confirmation of divergence.
Description	Approximate the radius of the circle of convergence, $R_c \approx 1/10^m$.
Sources	The full details are my own contribution. However the ideas are inspired by conversations with G. Corliss and N. Nedialkov.
Ref. By	IM6

Given $\text{TOL} > 0$ and any sequence $\{c_n\}$, construct the power series $\sum_{n=0}^{\infty} c_n(z - z_0)^n$. Use Assumption 1 to obtain an integer N such that, for all $m \geq n \geq N$, $|\sum_{k=n}^{m} c_k| < \text{TOL}$. It is no loss in generality to assume $N > 30$, else replace N with 30. TM1 says that $\sum_{n=0}^{\infty} c_n$ converges.

We now invoke Assumption 2 and extract 15 elements $\{c_{N-14}, c_{N-13}, \ldots, c_N\}$ from the sequence. With $k = i + N - 14$, obtain the best linear fit $y(k) = mk + b$ in the 2-norm to the points

$$\Big\{(N - 14, \log_{10}|c_{N-14}|), (N - 13, \log_{10}|c_{N-13}|), \ldots, (N, \log_{10}|c_N|)\Big\}, \tag{19}$$

that is, find m and b such that $\sum_{i=0}^{14} |\log_{10}|c_{i+N-14}| - y(i + N - 14)|^2$ is minimized. Because $\sum_{n=0}^{\infty} c_n$ converges, TM2 says that $c_n \to 0$ as $n \to \infty$. The model parameter m will be negative.

Compute the ratio in the ratio test TM4 with our model. Then

$$\log_{10}\left|\tfrac{y(k+1)}{y(k)}\right| = \log_{10}|y(k + 1)| - \log_{10}|y(k)| = m, \tag{20}$$

which is independent of k. By continuity of $\log_{10}$ and the best linear fit function y as well as $\log_{10}\left|\tfrac{y(k+1)}{y(k)}\right|$ approximates $\log_{10}\left|\tfrac{c_{k+1}}{c_k}\right|$, we observe that $\log_{10}\left|\tfrac{y(k+1)}{y(k)}\right| \to m$ is approximately

$\log_{10}\left|\frac{c_{k+1}}{c_k}\right| \to m$. By TM5, the ratio test TM4 converging implies the root test TM3 converges, because they converge to a single limit and the same limit. See description section of TM5. It follows from GD1 that the power series converges whenever $m < 0$ and diverges whenever $m > 0$. Moreover GD1 says $R_c = 1/10^m$.

Number	IM6
Label	**Compute μ the order of singularity and underestimate R_c**
Inputs	Tolerance TOL, N, and approximation points (19)
Output	R_c and μ
Description	Start with the series resulting from integration of the given series three times and fit the coefficients with IM5. If that graph is linear, meaning the minimizer has norm less than TOL, then the slope is accepted and the order of the singularity is 3. If the graph opens upward, then the series is differentiated term-wise to reduce the second derivative of the graph, and a new top-line fit is computed. This process is repeated, reducing μ by 1 each time, until the graph opens downward or until seven term-wise differentiations have been tested. If seven term-wise differentiations have been tested and each result in turn proves unsatisfactory, then the final estimate for R_c is reduced by 10 percent for a conservative estimate for R_c and $\mu = -4$ is returned.
Sources	Chang and Corliss (1982)
Ref. By	Final product.

Let the conditions of Data Definition DD1 hold. Then the real coefficients $\left\{c_n\right\} \subset \mathbb{R}$ of the power series $\sum_{n=0}^{\infty} c_n(z-z_0)^n$ are obtained as a TS solution of an ODE and consider finding the order μ of the singularity from the graph of $\log_{10}|c_n|$ versus n.

The order μ is increased or decreased by term-by-term differentiation or integration, respectively. The upper envelope of the graph of $\log_{10}|c_n|$ versus n is concave up for orders $\mu < 1$ which means the slope underestimates $\log_{10}|z-z_0|/R_c$, and R_c is overestimated.

To estimate R_c and the order μ form the graph of $\log_{10}|c_n|$ versus n, shift the order of the series by repeated term-wise differentiation or integration. After each shift, a linear upper envelope is fit with IM5. The singularity may occur with any order. However, it is unusual for a solution to a differential equation to have singularities whose order lies beyond $|\mu - 1| \leq 3$ (Chang and Corliss, 1982).

4.2.6 Input Data Constraints

Given tolerance TOL, the number of terms of the sequence should be sufficient so that Assumption 1 holds. We must know an integer N such that, for all $m \geq n \geq N$, $|\sum_{k=n}^{m} c_k| <$ TOL. Moreover if this $N < 30$, then set $N = 30$ for a sufficient number of terms to do analysis.

As a second point, the terms in the sequence should not be near overflow/underflow. If this is the case, then the algorithm will properly scaled the sequence.

4.2.7 Properties of a Correct Solution

ROC properties of a correct solution are: R_c, truncation error, and modelling error must be positive.

5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

5.1 Functional Requirements

ROC is the implementation of IM5 in the complex case or IM6 in the real case for TS solutions of ODE.

R1: Input acquisition via software.

R2: Validate input format.

R3: Validate input type.

R4: Inputs should satisfy the assumptions.

R5: Inputs should be scaled to prevent overflow/underflow.

R6: Output via software.

R7: Output format.

R8: Output type.

R9: Parameter acquisition.

R10: Parameter format.

R11: Parameter type.

R12: Parameter distribution.

R13: Parameter constraints.

R14: Algorithm to find the distance to the nearest real pole.

R15: Algorithm to find the distance to the nearest complex conjugate pair of poles.

R16: Algorithm to find the distance to the nearest pole in hard to resolve case.

R17: Find the distance to the nearest real pole.

R18: Find the distance to the nearest complex conjugate pair of poles.

R19: Find the distance to the nearest pole in hard to resolve case.

R20: Pole identification, distinguish a real pole from a complex conjugate pair of poles from a complicated situation.

R21: ROC should be developed in C++.

5.2 Nonfunctional Requirements

NFR1: **Timing:** ROC should execute as fast as the Chang and Corliss (1982) software DRDCV.

The method developed in this project is expected to be independent of system constraints. However most TS methods are developed in C++ or FORTRAN 77, the goto languages of scientific computing. Certainly a scripting language would not be sufficient for large systems.

NFR2: **Accuracy:** ROC must not overestimate R_c.

If R_c is overestimated, then the power-series is a divergence sum on the overestimation.

In ODE solving by TS methods, underestimating R_c is acceptable as an underestimation results in a slight increase in computational effort for solving an ODEIVP.

6 Likely Changes

The likely changes for ROC are enumerated in the design documents.

7 Unlikely Changes

The unlikely changes for ROC are enumerated in the design documents.

8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" may have to be modified as well. Table 2 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 3 shows the dependencies of instance models, requirements, and data constraints on each other. Table 1 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

	A1	A2	A3	A4	A5	A6
TM1				x	x	x
TM2				x	x	x
TM3				x	x	x
TM4				x	x	x
TM5				x	x	x
TM6				x	x	x
GD1				x	x	x
DD1						x
DD2				x	x	
IM1	x	x	x	x		
IM2	x	x	x	x		
IM3	x	x	x		x	
IM4	x	x	x		x	
IM5	x	x	x	x	x	x
IM6	x	x	x			x

Table 1: Traceability Matrix Showing the Connections Between Assumptions and Other Items

	TM1	TM2	TM3	TM4	TM5	TM6	GD1	DD1	DD2	IM1	IM2	IM3	IM4	IM5	IM6
TM1	x													x	
TM2		x												x	
TM3			x				x							x	
TM4				x										x	
TM5					x									x	
TM6						x				x	x	x	x	x	
GD1							x							x	
DD1								x							x
DD2									x	x		x			
IM1										x	x				
IM2											x				
IM3												x	x		
IM4													x		
IM5														x	x
IM6															x

Table 2: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM1	IM2	IM3	IM4	IM5	IM6
R1	x	x	x	x	x	x
R2	x	x	x	x	x	x
R3	x	x	x	x	x	x
R4	x	x	x	x	x	x
R5	x	x	x	x	x	x
R6	x	x	x	x	x	x
R7	x	x	x	x	x	x
R8	x	x	x	x	x	x
R9	x	x	x	x	x	x
R10	x	x	x	x	x	x
R11	x	x	x	x	x	x
R12	x	x	x	x	x	x
R13	x	x	x	x	x	x
R14	x	x				
R15			x	x		
R16			x	x		
R17	x	x				
R18			x	x		
R19					x	x
R20	x	x	x	x	x	x
R21	x	x	x	x	x	x
NFR1	x	x	x	x	x	x
NFR2	x	x	x	x	x	x

Table 3: Traceability Matrix Showing the Connections Between Requirements and Instance Models

9 Values of Auxiliary Constants

ROC does not have symbolic parameters at this time.

References

Claus Bendsten and Ole Stauning. TADIFF, a flexible C++ package for automatic differentiation using Taylor series. Technical Report 1997-x5-94, Department of Mathematical Modelling, Technical University of Denmark, DK-2800, Lyngby, Denmark, April 1997.

Michiel Bergsma and Erwin Mooij. Application of taylor series integration to reentry problems. In *AIAA Atmospheric Flight Mechanics Conference*, page 0024, 2016.

YF Chang and G Corliss. Solving ordinary differential equations using Taylor series. *ACM TOMS*, 8(2):114–144, 1982.

Àngel Jorba and Maorong Zou. A software package for the numerical integration of ODEs by means of high-order Taylor methods. *Experimental Mathematics*, 14(1):99–117, 2005.

Walter Rudin. *Principles of mathematical analysis*. McGraw-Hill, Inc., 1976.

W. Spencer Smith and Lei Lai. A new requirements template for scientific computing. In J. Ralyté, P. Ȧgerfalk, and N. Kraiem, editors, *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP'05*, pages 107–121, Paris, France, 2005. In conjunction with 13th IEEE International Requirements Engineering Conference.

W. Spencer Smith, Lei Lai, and Ridha Khedri. Requirements analysis for engineering computation: A systematic approach for improving software reliability. *Reliable Computing, Special Issue on Reliable Engineering Computation*, 13(1):83–107, February 2007.