

# CFS: Curve Fitting Software

Malavika Srinivasan

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# 1 Revision History

Date	Version	Notes
Sep 28, 2018	1.0	0 <sup>th</sup> draft by Malavika
Oct 2, 2018	1.1	1 <sup>st</sup> draft by Malavika
Oct 6, 2018	1.2	2 <sup>nd</sup> draft submitted by Malavika
Oct 8, 2018	1.2	2 <sup>nd</sup> Feedback from Robert
Oct 10, 2018	1.3	3 <sup>rd</sup> Corrections based on feedback from Robert
Oct 11, 2018	1.4	4 <sup>th</sup> Corrections based on feedback from Robert and Dr. Smith
Oct 12, 2018	1.5	5 <sup>th</sup> Corrections based on feedback from Robert and Dr.Smith
Oct 22, 2018	1.6	6 <sup>th</sup> Corrections based on feedback from Dr.Smith
Oct 29, 2018	1.7	7 <sup>th</sup> Corrections after System VnV plan
Nov 2, 2018	1.8	8 <sup>th</sup> Corrections based on feedback from Dr.Smith
Nov 7, 2018	1.9	9 <sup>th</sup> Corrections based on feedback from Dr.Smith
Nov 22, 2018	2.0	10 <sup>th</sup> Corrections based on feedback from Dr.Smith
Dec 24, 2018	2.1	11 <sup>th</sup> Final draft for submission.

## 2 Reference Material

This section records information for ease of reference. The information includes the units, symbols and abbreviations used in this document.

### 2.1 Table of Units

This library is designed to work for any set of data, irrespective of their units. So, table of units is **not applicable**.

### 2.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The symbols are listed in alphabetical order.

symbol	unit	description
$f$		Function
$P$		Orthogonal matrix
$\Phi$		Basis function
$\Pi$		Basis function
$\sum_{min}^{max}$		Summation
$r$		Residual
$T$		Transpose operation of matrix
$v$		Basis function

## 2.3 Abbreviations and Acronyms

symbol	description
A	Assumption
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
R	Requirement
CA	Commonality Analysis
CFS	Curve Fitting Software
T	Theoretical Model

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### 3 Introduction

Scientific Computation (SC) is the collection of tools, techniques, and theories that are required to solve problems in the field of science and engineering using computer-based mathematical models. The source data for scientific computation problems are often large sets of data from experiments conducted in a laboratory setup. This large set of data (such as time and temperature) is usually complex to analyze and require segmenting and curve-fitting. Curve fitting is the process of constructing a curve, or mathematical function, that has the best fit to a series of data points possibly subject to constraints.

The following section provides an overview of the Commonality Analysis (CA) for a family of softwares developed to fit a set of data points. The developed program will be referred to as Curve Fitting Software(CFS). This section explains the purpose of this document, the scope of the family, the organization of the document and the characteristics of intended reader.

[80 character width for text in tex file, please —SS] [Dr.Smith, I already have it set for 80 character width. —Malavika] [I don't think you understand what I'm requesting. I want a hard wrap at 80 characters. If you look at the tex file your lines are hundreds of characters long. You are probably setting your editor to an 80 character soft wrap. —SS] [Yes Dr.Smith. I set it to 80 character width soft wrap and now changed it to hard wrap. But I don't see places where it is above 80 characters in a line. Maybe we can discuss this during tomorrow's meeting. —Malavika]

[Have a look at your CA.tex file with a web-browser through the GitHub interface (<https://github.com/Malavika-Srinivasan/CAS741/blob/master/docs/SRS/CA.tex>). You'll see the lines that are longer than 80 characters. —SS]

#### 3.1 Purpose of Document

The purpose of this document is to analyze the commonalities and variabilities between the family of softwares produced as part of this library. The commonalities are the elements which are true for each member which is a part of this software family. For instance, curve fitting is common for all the softwares of this family. The variabilities are the elements which may vary between each software member of this family. For instance, the technique used to fit the curve such as interpolation, regression, smoothing are examples of variabilities.

#### 3.2 Scope of the Family

The scope of CFS is restricted to finding the best fit parameters of linear systems using methods of interpolation and regression discussed in chapter 3 and 7 of [Heath \(2002\)](#) . To reduce the complexity of CFS, we use only polynomials and piecewise polynomials as our basis functions for interpolation. In regression, we restrict ourselves to over determined linear systems and least squares methods to minimize the residual. This software will allow only run-time binding for the degree of interpolation and regression. There could be also be

variabilities associated with the dimension of the interpolation which could be fixed at build time but this is out of scope for CFS.

### 3.3 Characteristics of Intended Reader

The reader of this document is expected to know the basic concepts of curve fitting. However to obtain a deeper understanding of this document, the reader is expected to be proficient in elementary linear algebra.

### 3.4 Organization of Document

The organization of this document follows the template for a Commonality analysis (CA) for scientific computing software proposed by Dr.Spencer Smith which is based on the SRS template [Smith et al. \(2007\)](#), the template for general purpose scientific software [Smith \(2006\)](#) and the family of material models example [Smith et al. \(2017\)](#). The sections of this document are grouped into commonalities and variabilities of the CFS. The presentation starts with the analyzing commonalities between the softwares of CFS which will contain goals, theories, and definitions which will be common for the family members of CFS. Then the variabilities of the family members is presented which will contain the assumptions, instance models and the output. The goal statements are refined to the theoretical models, and theoretical models to the instance models.

## 4 General System Description

This section identifies the interfaces between the system and its environment, describes the potential user characteristics and lists the potential system constraints.

### 4.1 Potential System Contexts

Figure 1 shows the system context. A circle represents an external entity outside the software, the user in this case. A rectangle represents the software system itself (CFS). Arrows are used to show the data flow between the system and its environment.

[Your figure isn't showing the use of your library correctly. Your library is not used by a User, but by a program. You can show the user using the program, if you like. —SS]  
[Change made —Malavika]

- User Responsibilities:
  - Enter input data points to be fit.
  - Understand what each point  $t_i, y_i$  means with respect to CFS.
  - Input whether to use interpolation or regression.



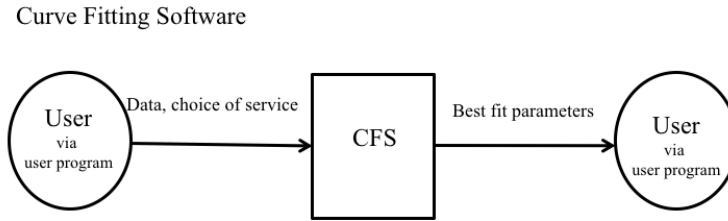


Figure 1: System Context

- Input interpolating method or regression method based on their choice in the previous step.
- CFS Responsibilities:
  - Detect data type mismatch, such as a string of characters instead of a number.
  - Compute best fit parameters.

## 4.2 Potential User Characteristics

The end user of CFS should have an understanding of undergraduate Level regression and interpolation. [You don't need capitals here. —SS][Changes made —Malavika]

## 4.3 Potential System Constraints

Not Applicable.

# 5 Commonalities

This section presents the common concepts or the information which is true for both the methods of curve fitting such as regression and interpolation. The background information is available in section 5.1, followed by important terminologies in section 5.2. The basic equations and laws used by CFS is given in sections 5.3 and 5.4. The data definitions and the goal statements are explained in sections 5.5 and 5.6. [It is good to have text between

section headings. You should put a mini roadmap here explaining the contents of this section.  
—SS][Makes sense, changes made —Malavika]

## 5.1 Background Overview

Curve fitting is the process of constructing a curve, or mathematical function, to a series of data points possibly subject to constraints. For regression, the best possible fit is chosen and for interpolation, The figure below(2) shows the best fit curve through a series of points. [best fit is for regressions. Interpolation is not a best fit. Interpolation is the only fit that passess exactly through all of the data points. —SS]

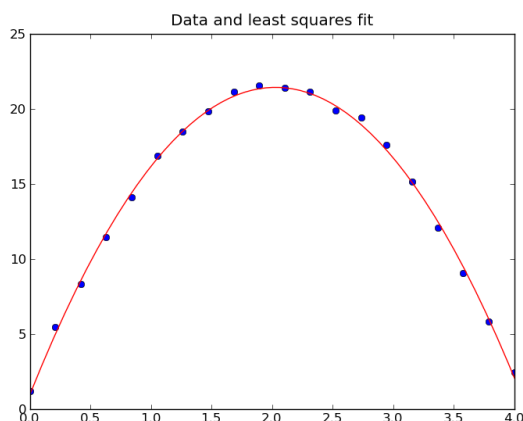


Figure 2: Typical example of a curve fitting process

A fit for the data can be obtained by different methods like interpolation, data smoothing and regression.

### 5.1.1 Interpolation

Interpolation is a process of fitting a function to given data so that the function passes exactly through the data points.

### 5.1.2 Smoothing

Smoothing is a process of creating an approximating function that attempts to capture important patterns in the data, while leaving out noise or other rapid phenomena.

### 5.1.3 Regression

Regression analysis is the process of finding the best fit parameters for a regression model for a given set of data points and thus obtain a curve through a set of data points.

## 5.2 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- Basis functions: A basis function is an element of a particular basis for a function space. Every continuous function can be represented as a linear combination of basis functions.
- Transpose: This is a mathematical operation on a matrix by which the rows of a matrix becomes its columns and vice versa.
- Cholesky Factorization: This is a particular form of this factorization which is commonly used to solve the normal equations that characterize the least squares solution to the overdetermined linear system.
- Orthogonality: Orthogonality is the generalization of the notion of perpendicularity.
- Interpolant: An interpolant is a function  $L = L(t)$  which agrees with a particular function  $f$  at a set of known points  $t_0, t_1, t_2, \dots, t_n$  and which is used to compute values for  $f(t)$  at points  $t \neq t_i$  where  $i = 0, 1, 2, \dots, n$ .

## 5.3 General Definitions

This section collects the equations that will be used in deriving the data definitions, which in turn will be used to build the instance models.

Number	GD1
Label	<b>General form of linear curve fitting</b>
SI Units	Not applicable
Equation	$f(t) = \sum_{j=1}^n x_j \Phi_j(t)$ where $j = 1, 2, 3 \dots m$ [There is no $i$ in this equation. Where is the connection to the data? —SS][changed i to j —Malavika]
Description	<p>The above equation gives the general form of linear curve fitting where,</p> <ul style="list-style-type: none"> <li>• <math>(t_i, y_i)</math> is the given set of data points, where <math>i = 1, 2, 3 \dots m</math>.</li> <li>• The functions <math>\Phi(t), \Phi_1(t), \dots \Phi_n(t)</math> are basis functions whose linear combination yields the curve fitting function <math>f</math>.</li> <li>• <math>x_j</math> is the parameters of the best fit.</li> </ul>
Source	Heath (2002)
Ref. By	T3, T4, IM1, IM2, IM3, IM4, IM5, IM6 and IM7

Number	GD2
SI Units	Not applicable
Label	<b>Overdetermined Linear Systems</b>
Equation	<p>For a given set of <math>n</math> data points, <math>(t_i, y_i)</math> <math>i = 1, 2, \dots n</math> represented in matrix form <math>Ax = y</math> as in T1, where <math>A</math> is an <math>m \times n</math> matrix with <math>m &gt; n</math> which means there are more equations than unknowns.</p> <p>A solution to the system <math>x</math> can be computed such that the residual vector,</p> $r = y - Ax$ <p>is small. where <math>i = 1, 2, 3 \dots n</math>.</p>
Description	<p>The symbols used in this equation are .</p> <p><math>(t_i, y_i)</math> is the given input data.</p> <p>To find a solution to this problem we use least squares method.(T2)</p>
Sources	Some related information is available at: <a href="https://s-mat-pcs.oulu.fi/~mpa/matreng/ematr5_5.htm">https://s-mat-pcs.oulu.fi/~mpa/matreng/ematr5_5.htm</a>
Ref. By	T1, IM8, IM9, IM10

## 5.4 Theoretical Models

This section focuses on the general equations that CFS is based on.

Number	T1
Label	<b>Matrix-Vector notation for a system of linear equations.</b>
Equation	$Ax = y$
Description	<p>The above equation gives the general form of system of linear equations in matrix vector notation where,</p> <p><math>A</math> is a <math>m \times n</math> matrix</p> <p><math>y</math> is an <math>m</math>-vector</p> <p><math>x</math> is an <math>n</math>-vector</p>
Source	<a href="#">Heath (2002)</a>
Ref. By	IM3, IM4, IM5, IM6, IM8, IM9 and IM10

Number	T2
Label	<b>Least Squares method.</b>
Equation	<p>For a given overdetermined system of equations represented in matrix form as in T1, a best fit solution <math>x</math> is found such that, the square of the difference between the actual and expected output is minimum. This is mathematically represented as shown below.</p> $\min_x \sum_{i=1}^m (y_i - f(t_i, x))^2$
Description	<p>The above mathematical expression gives the definition of best fit solution in least squares method.</p> <p>A is a <math>m \times n</math> matrix</p> <p>y is a m-vector</p> <p>x is an n-vector</p>
Source	Heath (2002)
Ref. By	IM8, IM9 and IM10

[What is the connection between the equation and the description? Is this a copy and paste error? —SS][Yes, I guess it should say mathematical expression instead of equation. Changed —Malavika]

Number	T3
Label	<b>General form of Interpolation</b>
Equation	$f(t_i) = \sum_{j=1}^n x_j \Phi_j(t) = y_i$ where $i = 1, 2, 3 \dots m$
Description	<p>The above equation gives the general form of interpolating function where,</p> <ul style="list-style-type: none"> <li>• <math>(t_i, y_i)</math> is the given set of data points, where <math>i = 1, 2, 3 \dots m</math>.</li> <li>• The functions <math>\Phi(t), \Phi_1(t), \dots \Phi_n(t)</math> are basis functions whose linear combination yields the interpolating function <math>f</math> whose value at a given <math>t_i</math> is <math>y_i</math>.</li> <li>• <math>x_j</math> is the parameters of the curve fit. [The terminology best fit doesn't make sense here. Curve fit would be fine. —SS][changed the terminology —Malavika]</li> <li>• <math>y_i</math> is the given data point at <math>t_i</math>.</li> </ul>
Source	Heath (2002)
Ref. By	GD1, IM1, IM2, IM3, IM4, IM5, IM6, IM8, IM9 and IM10

Number	T4
Label	<b>General form of Linear Regression using Least squares method and best fit in least squares.</b>
Equation	<p>For <math>i = 1, 2, 3...m</math>, general form of regression is given by</p> $f(t_i) = \sum_{j=1}^n x_j \Phi_j(t)$ <p>Since we deal with only linear problems(3.2), <math>\Phi_j</math> depend only on <math>t</math>. Hence <math>f(t_i, x)</math> can be expressed as,</p> $f(t_i) = x_1 + x_2 t + x_3 t^2 + \dots + x_n t^{n-1}.$ <p>where <math>x_i</math> is the parameters of the curve fit, such that the Least squares as defined T2 is minimum. [I don't see the connection to T2 as T2 is currently written. —SS][I can see the disconnection. I changed it now. Can you please review this? —Malavika] [You are on the right track now. There are still some issues with attention to detail, like <math>f</math> is sometimes a function of one variable and sometimes a function of two variables, but this is now on the right track. —SS][Corrected. —Malavika]</p>
Description	<p>The above equation gives the general form of linear regression function and the definition of best fit in least squares method.</p> <p><math>(t_i, y_i)</math> is the given set of data points, where <math>i = 1, 2, 3...m</math>.</p> <p>The functions <math>\Phi(t), \Phi_1(t), \dots \Phi_n(t)</math> are basis functions whose linear combination yields the function <math>f</math> whose value at any <math>t</math> is the best fit to the given data.</p> <p><math>x_j</math> is the parameters of the best fit.</p>
Source	Heath (2002)
Ref. By	GD1, IM8, IM9 and IM10

## 5.5 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.



Number	DD1
Label	<b>Data definitions of monomial interpolation method.</b>
Symbol	$\Phi$ , $A$ and $y$ .
SI Units	Not applicable
Equation	<p>For the given set of data <math>(t_i, y_i)</math> where <math>j = 1, 2, \dots, n</math>, the below equation gives the basis functions.</p> $\Phi_j(t) = t^{j-1}$ <p>The matrix <math>A</math> and <math>y</math> is given by,</p> $A = \begin{bmatrix} 1 & t_1 & t_1^2 & \dots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \dots & t_2^{n-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & \dots & t_n^{n-1} \end{bmatrix}$ $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$
Description	<p>To provide the basis functions and matrices necessary for monomial interpolation IM3.</p> <p>The symbols used in the above equation are <math>\Phi_j(t)</math> which represents the basis function at any <math>t</math> in the data <math>(t_i, y_i)</math>.</p> <p><math>A</math> and <math>y</math> are matrices representing the system of equations through the given set of data points.</p>
Sources	Heath (2002)
Ref. By	IM3

Number	DD2
Label	<b>Data definitions of Lagrange's interpolation method.</b>
Symbol	$l$ , $A$ and $y$ .
SI Units	Not applicable
Equation	<p>For the given set of data <math>(t_i, y_i)</math> where <math>j = 1, 2, \dots, n</math>, the below equation gives the basis functions.</p> $l_j(t) = \frac{\prod_{k=1, k \neq j}^n (t - t_k)}{\prod_{k=1, k \neq j}^n (t_j - t_k)} = \frac{(t - t_1)}{(t_j - t_1)} \cdots \frac{(t - t_{j-1})}{(t_j - t_{j-1})} \frac{(t - t_{j+1})}{(t_j - t_{j+1})} \cdots \frac{(t - t_n)}{(t_j - t_n)}$ <p>The matrix <math>A</math> (Identity matrix) and <math>y</math> is given by,</p> $A = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$ $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$
Description	<p>To provide the basis functions and matrices necessary for lagrange's interpolation IM4.</p> <p>The symbols used in the above equation are <math>l_j(t)</math> which represents the basis function at any <math>t</math> in the data <math>(t_i, y_i)</math>.</p> <p><math>A</math> and <math>y</math> are matrices representing the system of equations through the given set of data points.</p>
Sources	Heath (2002)
Ref. By	IM4

Number	DD3
Label	<b>Data definitions of Newton interpolation method.</b>
Symbol	$\pi$ , $A$ and $y$ .
SI Units	Not applicable
Equation	<p>For the given set of data <math>(t_i, y_i)</math> where <math>j = 1, 2, \dots, n</math>, the below equation gives the basis functions.</p> $\pi(t) = \prod_{k=1}^{j-1} (t - t_k)$ <p>When the limits make it vacuous, the product is taken to be 1.</p> <p>Also, <math>\pi_j(t) = 0</math> for <math>i &lt; j</math>.</p> <p>The matrix <math>A</math> and <math>y</math> is given by,  <math>A</math> is a lower triangular as <math>\pi_j(t) = 0</math> for <math>i &lt; j</math> with its entries defined by <math>a_{ij} = \pi_j(t_i)</math></p> $A = \begin{bmatrix} \pi_0(t_0) & 0 & 0 & \dots & 0 \\ \pi_0(t_1) & \pi_1(t_1) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \pi_0(t_n) & \pi_1(t_n) & \pi_2(t_n) & \dots & \pi_n(t_n) \end{bmatrix}$ $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$
Description	<p>To provide the basis functions and matrices necessary for Newton's interpolation IM5.</p> <p>The symbols used in the above equation are <math>\pi_j(t)</math> which represents the basis function at any <math>t</math> in the data <math>(t_i, y_i)</math>.</p> <p><math>A</math> and <math>y</math> are matrices representing the system of equations through the given set of data points.</p>
Sources	Heath (2002)
Ref. By	IM5

Number	DD4
Label	<b>Data definitions of Hermite Cubic interpolation method.</b>
Symbol	$A$ and $y$ .
SI Units	Not applicable
Equation	<p>The matrix <math>A</math> and <math>y</math> is given by,</p> $A = \begin{bmatrix} 1 & t_0 & t_0^2 & t_0^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & t_n^3 \\ 0 & 1 & 2t_0 & 3t_0^2 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2t_n & 3t_n^2 \\ 0 & 0 & 2 & 6t_0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 2 & 6t_n \\ 0 & 0 & 0 & 6 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 6 \end{bmatrix} \quad \text{and } y = \begin{bmatrix} y_0 \\ \vdots \\ y_0^{(1)} \\ y_1^{(1)} \\ \vdots \\ y_n^{(1)} \\ y_1^{(2)} \\ \vdots \\ y_n^{(2)} \\ y_1^{(3)} \\ \vdots \\ y_n^{(3)} \end{bmatrix}$
Description	<p>To provide the matrices necessary for Hermite cubic interpolation IM6.</p> <p><math>A</math> and <math>y</math> are matrices representing the system of equations through the given set of data points.</p>
Sources	Some related information can be obtained at: <a href="https://coast.nd.edu/jjwteach/www/www/30125/pdfnotes/lecture5_9v14.pdf">https://coast.nd.edu/jjwteach/www/www/30125/pdfnotes/lecture5_9v14.pdf</a>
Ref. By	IM6

Number	DD5
Label	<b>Data definitions of B-Spline interpolation.</b>
Symbol	$v_i^k(t)$
SI Units	Not applicable
Equation	<p>The basis function for B-Spline is given by:</p> $v_i^k = \frac{t - t_i}{t_{i+k} - t_i}$
Description	To provide the basis function for BSpline interpolation IM7.
Sources	Heath (2002)
Ref. By	IM7

Number	DD6
Label	<b>Matrix Transpose</b>
Symbol	$A^T$
SI Units	Not applicable
Equation	$[A^T]_{ij} = [A]_{ji}$
Description	<p>The symbols used in the equations are,</p> <p><math>i, j</math> represents the rows and columns of a matrix.</p> <p>T represents the transpose operation of a matrix.</p>
Sources	Heath (2002)
Ref. By	IM8, IM9

Number	DD7
Label	<b>Data definitions of Regression using Normal Equations.</b>
Symbol	$A^T A$
SI Units	Not applicable
Equation	$A^T A = L L^T$ $[A^T]_{ij} = [A]_{ji}$
Description	<p>The symbols used in the equations are,</p> <p><math>L</math> represents the lower triangular matrix for Cholesky Factorization.</p> <p><math>i, j</math> represents the rows and columns of a matrix.</p> <p>T represents the transpose operation of a matrix.</p>
Sources	<a href="#">Heath (2002)</a>
Ref. By	IM8

Number	DD8
Label	<b>Orthogonality Matrix</b>
Symbol	$P$
SI Units	Not applicable
Equation	$P = \left( \frac{A A^T}{A^T A} \right) y$
Description	<p>The symbols used in the equations are,</p> <p><math>P</math> represents the orthogonal matrix of A.</p> <p>T represents the transpose operation of a matrix.</p>
Sources	Some related information is given at: <a href="http://uspas.fnal.gov/materials/05UCB/4_LSQ.pdf">http://uspas.fnal.gov/materials/05UCB/4_LSQ.pdf</a>
Ref. By	IM10

## 5.6 Goal Statements

Given the set of data points, the choice of software from CFS and the variabilities of the software the CFS should:

GS1: compute the parameters of the curve which is the best possible fit through the set of data points.

## 6 Variabilities

### 6.1 Assumptions

A1: For the given 'n' number of data points  $(t_i, y_i)$  where  $i = 0, 1, 2, \dots, n$ ,  $n \geq 2$ .(R1)

A2: For the given 'n' number of data points  $(t_i, y_i)$  where  $i = 0, 1, 2, \dots, n$ ,  $t_i < t_{i+1}$ .(IM6,IM7)

A3: For the given set of data points  $(t_i, y_i)$  where  $i = 0, 1, 2, \dots, n$ , there exists an interpolant.(IM1, IM2, IM3, IM4, IM5, IM6 and IM7).

A4: For the given set of data points  $(t_i, y_i)$ , there exists a least squares solution.(IM8, IM9 and IM10)

A5: We assume only linear basis functions for B-Splines. (IM7)

### 6.2 Calculation

#### 6.2.1 Instance Model

This section transforms the goal of CFS defined in the Section 5.6 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 5.5 to replace the abstract symbols in the models identified in the Sections 5.4 and 5.3. All the instance models presented below are based on system of equations which is solved using matrices.

Number	IM1
Label	<b>Polynomial Interpolation</b>
Input	A set of $n$ data points, $(t_i, y_i)$ $i = 1, 2, \dots, n$
Output	$P_{n-1}(t)$ is a polynomial of degree at most $n - 1$ such that $P_{n-1}(t_i) = y_i$ where $i = 1, 2, 3, \dots, n$
Description	<p>The symbols used in this equation are <math>P_{n-1}</math> which represents the polynomial of degree at the most <math>n - 1</math>.</p> <p><math>(t_i, y_i)</math> is the given input data where no two <math>t_i</math> are the same.</p> <p>Polynomial interpolation has different variabilities which are discussed in separate instance models IM3, IM4 and IM5. <a href="#">[You should make an explicit connection. —SS][Changes made —Malavika]</a></p>
Sources	Some related information is available at <a href="#">Heath (2002)</a>
Ref. By	T3, IM3, IM4, IM5, and R5



Number	IM2
Label	<b>Piecewise Interpolation</b>
Input	A set of n data points, $(t_i, y_i)$ $i = 1, 2, \dots, n$ where $t_{i+1} > t_i$ .
Output	<p><math>P(t) = L_i(t)</math> is a piecewise linear function where <math>L_i</math> is given <a href="#">[spell check —SS][changed —Malavika]</a> by the following equation.</p> $L_{i,i+1}(t) = p(x)$ <p>for each interval <math>[t_i, t_{i+1})</math>, where <math>i = 1, 2, 3, \dots, n</math>. The degree of the polynomial can be varied as per requirement in each interval.</p>
Description	<p>The symbols used in this equation are <math>P(t)</math> which represents the piecewise polynomial of degree 1.</p> <p><math>(t_i, y_i)</math> is the given input data where no two <math>t_i</math> are the same.</p> <p>Piecewise interpolation has different variabilities which are discussed as separate instance models.</p> <p>By default, the interval is same as <math>t</math> array. So, the interval in an array <math>t = [t_0, t_1, t_2, t_3]</math> is <math>[t_0, t_1)</math>, <math>[t_1, t_2)</math> and <math>[t_2, t_3]</math>.</p>
Sources	Some related information is available at: <a href="http://www.math.umd.edu/~petersd/460/spline.pdf">http://www.math.umd.edu/~petersd/460/spline.pdf</a>
Ref. By	T3, IM6, IM7 and R5

Number	IM3
Label	<b>Monomial Interpolation</b>
Input	<p><math>(t_i, y_i)</math> <math>i = 1, 2, \dots, n</math></p> <p>see DD1, from which the basis function of the monomial interpolation is obtained.</p> <p>see DD1, from which the definition of matrix A and b are obtained.</p>
Output	<p>Find <math>P_{n-1}(t)</math> such that for the given input <math>(t_i, y_i)</math>,</p> $P_{n-1}(t_i) = x_1 + x_2 t_i + x_3 t_i^2 + x_4 t_i^3 + \dots x_n t_i^{n-1} = y_i$ <p>Where <math>x_1, x_2, x_3, \dots, x_n</math> can be obtained by representing the above system of linear equations in matrix form <math>Ax = b</math> as in T1 and solving for x using the equation below.</p> $Ax = \begin{bmatrix} 1 & t_1 & t_1^2 & \dots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \dots & t_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_n & t_n^2 & \dots & t_n^{n-1} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = y$
Description	<p>To determine the interpolating polynomial <math>p_{n-1}</math> for a given set of input points.</p> <p>The symbols used in this equation are <math>P_{n-1}</math> which represents the polynomial of degree at the most <math>n - 1</math>.</p> <p><math>x_1, x_2, \dots, x_n</math> are best fit parameters.</p>
Sources	Some related information is available at: <a href="#">Heath (2002)</a>
Ref. By	T3, GD1, R6

Number	IM4
Label	<b>Lagrange's Interpolation</b>
Input	<p><math>(t_i, y_i)</math> <math>i = 1, 2, \dots, n</math></p> <p>see DD2, from which the basis function of the lagrange's interpolation is obtained.</p> <p>see DD2, from which the definition of matrix A and b are obtained.</p>
Output	<p>Find <math>P_{n-1}(t)</math> such that for the given input <math>(t_i, y_i)</math>,</p> $P_{n-1}(t) = y_1 l_1(t) + y_2 l_2(t) + \dots y_n l_n(t).$ <p>Where <math>x_1, x_2, x_3 \dots x_n</math> can be obtained by representing the above system of linear equations in matrix form <math>Ax = b</math> as in T1 and solving for x using the equation below.</p> $Ax = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = y$
Description	<p>To determine the interpolating polynomial <math>p_{n-1}</math> for a given set of input points.</p> <p>The symbols used in this equation are <math>P_{n-1}</math> which represents the polynomial of degree at the most <math>n - 1</math>.</p> <p><math>x_1, x_2 \dots x_n</math> are best fit parameters.</p>
Sources	Some related information is available at: <a href="#">Heath (2002)</a>
Ref. By	T3, GD1, R6

Number	IM5
Label	<b>Newton's Interpolation</b>
Input	<p><math>(t_i, y_i)</math> <math>i = 1, 2, \dots, n</math></p> <p>see DD3, from which the basis function of the Newton's interpolation is obtained.</p> <p>see DD3, from which the definition of matrix A and b are obtained.</p>
Output	<p>Find <math>P_{n-1}(t)</math> such that for the given input <math>(t_i, y_i)</math>,</p> $P_{n-1}(t) = x_1 + x_2(t - t_1) + x_3(t - t_1)(t - t_2) + \dots x_n(t - t_1)(t - t_2)\dots(t - t_{n-1})$ <p>Where <math>x_1, x_2, x_3 \dots x_n</math> can be obtained by representing the above system of linear equations in matrix form <math>Ax = y</math> as in T1 and solving for x using the equation below.</p> $Ax = \begin{bmatrix} \pi_0(t_0) & 0 & 0 & \dots & 0 \\ \pi_0(t_1) & \pi_1(t_1) & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \pi_0(t_n) & \pi_1(t_n) & \pi_2(t_n) & \dots & \pi_n(t_n) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = y$
Description	<p>To determine the interpolating polynomial <math>p_{n-1}</math> for a given set of input points.</p> <p>The symbols used in this equation are <math>P_{n-1}</math> which represents the polynomial of degree at the most <math>n - 1</math>.</p> <p><math>x_1, x_2 \dots x_n</math> are best fit parameters.</p>
Sources	Some related information is available at: <a href="#">Heath (2002)</a>
Ref. By	T3, GD1, R6

Number	IM6
Label	<b>Hermite Cubic Interpolation</b>
Input	<p><math>(t_i, y_i)</math> where <math>i = 1, 2, \dots, n</math></p> <p><math>m</math> derivatives for the <math>n</math> data points above (where <math>m = 3</math> as a cubic polynomial can have only 3 derivatives) represented by <math>(t_i^{(m)}, y_i^{(m)})</math> where <math>i = 1, 2, \dots, n</math>.</p> <p>see DD4, from which the definition of matrix A and b are obtained.</p>
Output	<p>Find <math>P(t)</math> such that for the given input <math>(t_i, y_i)</math>,</p> $P(t) = x_0 + x_1 t + x_2 t^2 + x_3 t^3$ <p>Where <math>x_0, x_1, x_2, x_3</math> can be obtained by representing the above system of linear equations in matrix form <math>Ax = y</math> as in T1 and solving for x using the equation below.</p> $Ax = \begin{bmatrix} 1 & t_0 & t_0^2 & t_0^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & t_n^3 \\ 0 & 1 & 2t_0 & 3t_0^2 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2t_n & 3t_n^2 \\ 0 & 0 & 2 & 6t_0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 2 & 6t_n \\ 0 & 0 & 0 & 6 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ x_{n(m+1)} \end{bmatrix} = \begin{bmatrix} y_0 \\ \vdots \\ y_0^{(1)} \\ y_1^{(1)} \\ \vdots \\ y_n^{(1)} \\ y_1^{(2)} \\ \vdots \\ y_n^{(2)} \\ y_1^{(3)} \\ \vdots \\ y_n^{(3)} \end{bmatrix} = y$
Description	<p>To determine the interpolating polynomial <math>p</math> for a given set of input points.</p> <p>The symbols used in this equation are <math>P</math> which represents the polynomial of degree at the most <math>n(m+1) - 1</math>.</p> <p><math>x_1, x_2, \dots, x_{n(m+1)}</math> are best fit parameters.</p>
Sources	Some related information can be obtained at: <a href="https://coast.nd.edu/jjwteach/www/www/30125/pdfnotes/lecture5_9v14.pdf">https://coast.nd.edu/jjwteach/www/www/30125/pdfnotes/lecture5_9v14.pdf</a>
Ref. By	T3, GD1, R7

Number	IM7
Label	<b>B-Spline Interpolation</b>
Input	<p><math>(t_i, y_i)</math> <math>i = 1, 2, \dots, n</math> such that <math>t_0 &lt; t_1 &lt; \dots &lt; t_n</math></p> <p>see DD5, from which the basis function for B-Splines is obtained.</p>
Output	<p>Find <math>B_i^k(t)</math> such that for the given input <math>(t_i, y_i)</math>,</p> $B_i^k(t) = v_i^k(t)B_i^{k-1}(t) + (1 - v_{i+1}^k(t))B_{i+1}^{k-1}(t)$ <p>for <math>k &gt; 0</math>.</p>
Description	<p>To determine B-Spline <math>B_i^k</math> for a given set of input points.</p> <p>The symbols used in this equation are <math>B_i^k</math> which represents a piecewise polynomial of degree <math>k</math>.</p> <p>Important properties of B-Splines includes:</p> <ul style="list-style-type: none"> <li>• For <math>t &lt; T_i</math> or <math>t &gt; t_{i+k+1}</math>, <math>B_i^k(t) = 0</math></li> <li>• For <math>t_i &lt; t &lt; t_{i+k+1}</math>, <math>B_i^k(t) &gt; 0</math></li> <li>• For all <math>t</math>, <math>\sum_{i=-\infty}^{\infty} B_i^k(t) = 1</math></li> <li>• For <math>k \geq 1</math> <math>B_i^k</math> is <math>k - 1</math> times continuously differentiable.</li> </ul>
Sources	Some related information is available at: <a href="#">Heath (2002)</a>
Ref. By	T3, GD1, R7

Number	IM8
Label	<b>Normal Equations</b>
Input	A set of data points $(t_i, y_i)$ for $i = 1, 2, \dots, n$ represented as a overdetermined [spell check —SS][Changed —Malavika] system of equations as in T1. The matrices $A^T A$ and $A^T$ from DD7 and DD6
Output	$x_j$ for $j = 1, 2, \dots, m$ by solving the equations below, $A^T A x = A^T y$
Description	The symbols used in the above equations are: $T$ which represents the transpose function of a given matrix.
Sources	Heath (2002)
Ref. By	GD1, GD2, T2, T4 and R8

Number	IM9
Label	<b>Augmented System</b>
Input	A set of data points $(t_i, y_i)$ for $i = 1, 2, \dots, n$ represented as a overdetrmined system of equations as in T1. The matrix $A^T$ from DD6
Output	$x_j$ for $j = 1, 2, \dots, m$ by solving the equations below, $r + Ax = y$ $A^T r = 0$
Description	The equations above give the system to be solved for finding $x$ . The symbols used in the equation are, $r$ - The residual vector.
Sources	Heath (2002)
Ref. By	GD1, GD2, T2, T4 and R8

Number	IM10
Label	<b>Orthogonal Transformation</b>
Input	A set of data points $(t_i, y_i)$ for $i = 1, 2, \dots, n$ represented as a overdetrmined system of equations as in T1. The matrix $P$ from DD8
Output	$x_j$ for $j = 1, 2..m$ by solving the equations below, $Ax = Py$
Description	The equation above give the system to be solved for finding $x$ . The symbols used in the equation are, $P$ - The orthogonality matrix.
Sources	Heath (2002)
Ref. By	GD1, GD2, T2, T4 and R8

[The idea of binding time is never mentioned. Although your implementation will only allow run-time binding, the concept of a program family allows for build time binding. There could be variabilities associated with the dimension of the interpolation. It could be fixed at build time. —SS] [I understand. I added a note about this in the scope section —Malavika]

## 6.3 Output

### 6.3.1 Plot and coefficients to screen

The output can just be the plot and the coefficients of the curve fit displayed in the screen. Residual of the fit may be part of the output.

### 6.3.2 Plot and coefficients as files

The output can be written to a file which will include the coefficients of the curve fit and the curve fit plot saved to a specific location. Residual of the fit may be part of the output.

### 6.3.3 coefficients to screen

The output could be the coefficients displayed in the screen. Residual of the fit may be part of the output.

[While editing, I unintentionally removed your comment. You asked for variabilities in output. Can you please review if the above changes are ok? —Malavika] [The current ideas



are an improvement. —SS]

## 7 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.

### 7.1 Functional Requirements

[You are writing these requirements like you are writing a program, not a library. You should list the services you will provide. The user isn't going to provide choices for you to read. Another program is going to call your services. —SS]

[I can see your point. This needs to be discussed. —Malavika]

- R1: Read the input data  $(t_i, y_i)$  and the degree of the polynomial  $deg$  (Only for regression).
- R2: Verify the input data to see if only numbers are entered and if regression, verify that the  $deg \geq 1$ .
- R3: Verify the input data to see if A1 and A2 are satisfied.
- R4: The following services are provided by CFS - Interpolation(T3) and Regression(T4).
- R5: In interpolation, two types of services are provided - Polynomial(IM1) and Piecewise(IM2). (A3)
- R6: In Polynomial interpolation, three types of services are provided - Monomial(IM3), Lagrange(IM4) and Newton(IM5). (A3).
- R7: In Piecewise Polynomial, the following services are provided - Hermite cubic(IM6) and B-Splines(IM7). (A3)
- R8: In regression, the following services are provided - Normal equations(IM8), Augmented system(IM9) and Orthogonal transformations(IM10).
- R9: Compute best fit parameters. (IM3, IM4, IM5, IM6, IM7, IM8, IM9 and IM10). [How? You should reference the IMs that tell you how to do this. —SS] [Referenced IMs —Malavika]
- R10: Display the plot with data(R1) or the best fit result from R9 if requested by user program. [These are actually part of output variabilities. The calling program might not always need these services. —SS] [I added the clause 'if requested by user program —Malavika]

[I know you wanted to turn the solution of all problems into solving a system of equations, but this doesn't come through very well in your documentation. You have the matrices, but it wasn't clear that this was a unifying framework. —SS][I understand. I did not want to convert everything to system of equations. Thats how it was discussed in Health1997. But I see that it is the unifying framework. Should I mention this somewhere? —Malavika] [Yes —SS] [This information is mentioned in the introductory blurb of instance models. —Malavika]

## 7.2 Nonfunctional Requirements

### 7.2.1 Portability Requirements

- CFS shall be able to run on Windows 7/10, Linux, and Mac OSX operating systems.

### 7.2.2 Verifiability Requirements

- CFS should be verifiable. The document System verification and validation plan lists the plan for verifying CFS. The document can be found at <https://github.com/Malavika-Srinivasan/CAS741/blob/master/docs/VnVPlan/SystVnVPlan/SystVnVPlan.pdf>. [ambiguous. What results will be compared? You could point to your verification plan here. —SS][Referenced SystemVnVPlan —Malavika]

### 7.2.3 Maintainability and Support Requirements

- CFS should be able to accommodate new fitting methods such as LU optimization, Gram schmidt optimization etc. This addition will involve the creation of new methods in Interpolation module.
- The creation of new methods should be accomplished in less than 10% of the original development time, which is 40 hours of work by one developer.

[What new fitting methods are possible? How long will it take to add them? —SS][Please review —Malavika] [This is still ambiguous. How do I measure this? How do I know if you are successful? The changes come from your list of likely changes and the time to make the changes should be some fraction (specified by you) of the original development time. —SS][Added necessary details —Malavika]

## 8 Likely Changes

NA

## 9 Traceability Matrices and Graphs

The traceability matrix between different sections of this document is presented below. A '✓' entry in the table represents that they are referenced to each other. The way they are referenced is explained in the description of each table.

### 9.1 Traceability Matrix - General definitions and Data definitions

The traceability matrix between data definitions and general definitions is represented below. A '✓' entry in the table means that the Data definition of the corresponding column is based on the General definition in the corresponding row.

	DD1	DD2	DD3	DD4	DD5	DD6	DD7	DD8
GD1	✓	✓	✓	✓	✓	✓	✓	✓
GD2						✓	✓	✓

### 9.2 Traceability Matrix - Theoretical models and Data definitions

The traceability matrix between Theoretical models and Data definitions is represented below. A '✓' entry in the table means that the Data definition in the corresponding column is based on the the Theoretical models in the corresponding row.

	DD1	DD2	DD3	DD4	DD5	DD6	DD7	DD8
T1	✓	✓	✓	✓		✓	✓	✓
T2						✓	✓	✓
T3	✓	✓	✓	✓	✓			
T4						✓	✓	✓

### 9.3 Traceability Matrix - Data definitions and Instance models

The traceability matrix between Data definitions and Instance models is represented below. A '✓' entry in the table means that the Instance model in the corresponding column uses the Data definition in the corresponding row.

	IM1	IM2	IM3	IM4	IM5	IM6	IM7	IM8	IM9	IM10
DD1			✓							
DD2				✓						
DD3					✓					
DD4						✓				
DD5							✓			
DD6								✓	✓	
DD7									✓	
DD8										✓

## 9.4 Traceability Matrix - Theoretical models and Instance models

The traceability matrix between Data definitions and Instance models is represented below. A '✓' entry in the table means that the Instance model in the corresponding column is based on the Theoretical model in the corresponding row.

	IM1	IM2	IM3	IM4	IM5	IM6	IM7	IM8	IM9	IM10
T1			✓	✓	✓	✓		✓	✓	✓
T2								✓	✓	✓
T3	✓	✓	✓	✓	✓	✓	✓			
T4								✓	✓	✓

## References

- Michael T. Heath. *Scientific computing an introductory survey*. Boston McGraw-Hill, 2nd ed edition, 2002. ISBN 0072399104. URL <http://openlibrary.org/books/OL3946055M>. Includes bibliographical references (p. 523-548) and index.
- W. Spencer Smith. Systematic development of requirements documentation for general purpose scientific computing software. In *Proceedings of the 14th IEEE International Requirements Engineering Conference, RE 2006*, pages 209–218, Minneapolis / St. Paul, Minnesota, 2006. URL <http://www.ifi.unizh.ch/req/events/RE06/>.
- 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.
- W. Spencer Smith, John McCutchan, and Jacques Carette. Commonality analysis for a family of material models. Technical Report CAS-17-01-SS, McMaster University, Department of Computing and Software, 2017.

## 10 Appendix

### 10.1 Symbolic Parameters

Not Applicable [Either say “not applicable” or remove this sections. —SS][Changes made —Malavika]