Algorithms and software for fitting polynomial functions constrained to pass through the origin

Ian M Smith and Alistair B Forbes
National Physical Laboratory, Hampton Road, Teddington TW11 0LW, UK
E-mail: ian.smith@npl.co.uk

Abstract. Fitting a polynomial function to data, accounting for uncertainty information associated with that data, is a problem that is commonly encountered in metrology and for which algorithms and software are widely available. For reasons of numerical stability, Chebyshev polynomials are often employed rather than monomials. The problem of fitting a polynomial function that is constrained to pass through the origin, again taking uncertainty information into account, which arises in a number of metrology areas, has not been addressed to the same extent. This paper describes algorithms to determine the best fit polynomial function passing through the origin to data, accounting for uncertainty, and using Chebyshev polynomials. Software that implements the algorithms, and is available free to download, is also described.

1. Introduction
Problems involving fitting polynomial functions to data, taking uncertainty information associated with the data into account, are frequently encountered within metrology. A commonly implemented approach to solving such problems involves the use of Chebyshev polynomials as a means of ensuring numerical stability.

Related problems that occur in metrology involve determining the best-fit polynomial function, constrained to pass through the origin, again taking uncertainty information into account. As in the case of fitting an unconstrained polynomial function to data, it is important that solution algorithms are developed that are numerically stable when implemented in software.

This paper describes algorithms for fitting polynomial functions, both unconstrained and constrained (to pass through the origin), to data. The algorithms have been implemented in software that is freely available to download from the website of the National Physical Laboratory (NPL).

The paper is organised as follows. Section 2 describes the main uncertainty structures considered and the subsequent fitting problems (termed ‘weighted least squares’ and ‘generalised distance regression’) that have to be solved. Section 3 provides a reminder of the representation of an unconstrained polynomial function using Chebyshev polynomials. Section 4 then discusses how a polynomial function constrained to pass through the origin may be represented. In section 5, software that solves the fitting problems, for both unconstrained and constrained polynomial functions, is described.
2. Problem formulation

2.1. Functional model

The behaviour of a response variable $Y$ is modelled as a function $Y = f(X, B)$ of a stimulus variable $X$ and a vector $B = (B_1, \ldots, B_n)^\top$ of coefficients that parametrise the range of possible response behaviour. In many cases, the functional model is linear and $f$ can be expressed in the form

$$f(X) = \sum_{j=1}^{n} B_j f_j(X),$$

where $f_j(X)$ represents a basis function.

2.2. Measured data

Let $x_i, i = 1, \ldots, m$, and $y_i, i = 1, \ldots, m$, represent measurements made, respectively, of the stimulus and response variables.

2.3. Weighted least squares

In weighted least squares (WLS) problems [1], the measured $y$-values are subject to uncertainty while the $x$-values are considered to be accurate or to have associated uncertainties that may be considered negligible. There is no correlation associated with any pair of measured values.

Let $u(y_i)$ represent the standard uncertainty associated with the $i$th measured $y$-value. The optimisation problem is to determine estimates $\tilde{b} = (b_1, \ldots, b_n)^\top$ of the coefficients $B$ that minimise

$$\sum_{i=1}^{m} \left( \frac{y_i - f(x_i, B)}{u(y_i)} \right)^2.$$

For reasons of numerical stability and efficiency, WLS problems are typically solved using orthogonal factorisation such as QR factorisation [2].

2.4. Generalised distance regression

In generalised distance regression (GDR) problems [1], both the $x$- and $y$-values are subject to appreciable uncertainty. Again, there is no correlation associated with any pair of measured values.

Let $u(x_i)$ and $u(y_i)$ represent the standard uncertainty associated with, respectively, the $i$th measured $x$-value and the $i$th measured $y$-value. The optimisation problem is to determine estimates $\tilde{x_i}$ of the $x$-values $X_i, i = 1, \ldots, m$, and $\tilde{b} = (b_1, \ldots, b_n)^\top$ of the coefficients $B$ that minimise the sum of squares

$$\sum_{i=1}^{m} \left\{ \left( \frac{x_i - X_i}{u(x_i)} \right)^2 + \left( \frac{y_i - f(X_i, B)}{u(y_i)} \right)^2 \right\}.$$

GDR problems may be solved using an iterative approach such as the Gauss-Newton algorithm [2].

3. Unconstrained polynomial functions

3.1. Representation using Chebyshev polynomials

The Chebyshev polynomials [3] are defined by the recurrence relation

$$T_0(Z) = 1, \quad T_1(Z) = Z, \quad T_j(Z) = 2ZT_{j-1}(Z) - T_{j-2}(Z), \quad j \geq 2, \quad (1)$$

for $Z$ lying in the interval $[-1, 1]$. 

When fitting a polynomial of order \( n \) (degree \( n - 1 \)) in \( X \) to data \((x_i, y_i), i = 1, \ldots, m\), where \( m \geq n \), the normalised variable
\[
\hat{X} = \frac{X - x_{\text{min}} - (x_{\text{max}} - X)}{x_{\text{max}} - x_{\text{min}}} = \frac{2X - (x_{\text{max}} + x_{\text{min}})}{x_{\text{max}} - x_{\text{min}}} = \frac{2X - \Sigma}{\Delta},
\]
where \( x_{\text{min}} \leq \min\{x_i\}, x_{\text{max}} \geq \max\{x_i\}, x_{\text{max}} > x_{\text{min}}, \Sigma = x_{\text{max}} + x_{\text{min}}, \Delta = x_{\text{max}} - x_{\text{min}}, \) is used.

The polynomial is then expressed as the linear sum
\[
p_n(X, A) = \frac{1}{2} A_0 T_0(\hat{X}) + A_1 T_1(\hat{X}) + \ldots + A_{n-1} T_{n-1}(\hat{X}),
\]
where \( A = (A_0, \ldots, A_{n-1})^\top \) represents the vector of Chebyshev polynomial coefficients, the factor \( \frac{1}{2} \) allows for a simpler recursion formula when evaluating the partial derivative of \( p_n(X, A) \) with respect to \( X \), and the polynomial representation is valid only on the interval \([x_{\text{min}}, x_{\text{max}}]\).

Equation (3) can be expressed as
\[
p_n(X, A) = c^\top(X) A,
\]
where \( c(X) = \left( \frac{1}{2} T_0(\hat{X}), T_1(\hat{X}), \ldots, T_{n-1}(\hat{X}) \right)^\top \).

4. Constrained polynomial functions

4.1. Representation using Chebyshev polynomials

A polynomial of order \( n \) (degree \( n - 1 \)) in \( X \) passing through the origin can be expressed as the product of \( X \) and a polynomial of order \( n - 1 \) (degree \( n - 2 \)) in \( X \), i.e.,
\[
p_{0,n}(X, A_0) = X p_{n-1}(X, A_0),
\]
where \( A_0 = (A_{0,0}, \ldots, A_{0,n-2})^\top \).

Equation (4) can be expressed in terms of the normalised variable \( \hat{X} \), defined in expression (2), as
\[
p_{0,n}(X, A_0) = \frac{1}{2} \left( \Sigma + \Delta \hat{X} \right) \left( \frac{1}{2} A_{0,0} T_0(\hat{X}) + A_{0,1} T_1(\hat{X}) + \ldots + A_{0,n-2} T_{n-2}(\hat{X}) \right).
\]

The first term of the right-hand side of expression (5),
\[
\frac{1}{2} \Sigma \left( \frac{1}{2} A_{0,0} T_0(\hat{X}) + A_{0,1} T_1(\hat{X}) + \ldots + A_{0,n-2} T_{n-2}(\hat{X}) \right),
\]
can be written as
\[
c_{0,1}(X) A_0,
\]
where \( c_{0,1}(X) = \frac{1}{2} \Sigma \left( \frac{1}{2} T_0(\hat{X}), T_1(\hat{X}), \ldots, T_{n-2}(\hat{X}) \right)^\top \).

The second term of the right-hand side of expression (5),
\[
\frac{1}{2} \Delta \hat{X} \left( \frac{1}{2} A_{0,0} T_0(\hat{X}) + A_{0,1} T_1(\hat{X}) + \ldots + A_{0,n-2} T_{n-2}(\hat{X}) \right),
\]
may be written similarly as follows. Using the fact that
\[
\hat{X} T_0(\hat{X}) = T_1(\hat{X}),
\]
and rearranging recurrence relation (1) to give
\[
\hat{X} T_{j-1}(\hat{X}) = \frac{1}{2} \left( T_{j-2}(\hat{X}) + T_j(\hat{X}) \right), \quad j \geq 2,
\]
allows the term to be written as
\[ c_{0,2}(X)A_0, \]
where
\[ c_{0,2}(X) = \frac{1}{7} \Delta \left( \frac{1}{2} T_1(\hat{X}), \frac{1}{2} T_0(\hat{X}) + \frac{1}{2} T_2(\hat{X}), \ldots, \frac{1}{2} T_{n-3}(\hat{X}) + \frac{1}{2} T_{n-1}(\hat{X}) \right)^T. \]

Combining the expressions for the first and second terms gives
\[ p_{0,n}(X, A_0) = c_0^T(X)A_0, \]
where
\[ c_0(X) = c_{0,1}(X) + c_{0,2}(X). \]

5. **Software implementations**

Two implementations of software for (low degree) polynomial function fitting have been developed and made available free to download from the NPL website [4]:

- **XLGENLINE** – Software developed in Microsoft Excel (calling a FORTRAN DLL). Data and uncertainties are entered in the columns of an Excel worksheet, options (fitting method [WLS or GDR], polynomial degree [1, 2, 3 or 4], type of fit [unconstrained or constrained]) are selected from drop-down menus, and fitting is then implemented by pressing a button. Additionally, ‘inverse evaluation’ can be implemented – given a number of measured \( y \)-values and their associated standard uncertainties entered in columns of the Excel worksheet, estimates of the corresponding \( x \)-values and their associated standard uncertainties can be determined. Results are written to Excel worksheets.

- **XGENLINE** – Software developed in MATLAB and compiled into a standalone Windows executable. Data and uncertainties are provided in the lines of a user-selected ASCII file, options (fitting method [WLS or GDR], polynomial degree [1, 2, 3 or 4], type of fit [unconstrained or constrained]) are selected from graphical user interfaces, and fitting is then implemented. Additionally, ‘inverse evaluation’ can be implemented – given a number of measured \( y \)-values and their associated standard uncertainties provided in the lines of the ASCII file, estimates of the corresponding \( x \)-values and their associated standard uncertainties can be determined. Results are written to ASCII files.

**Acknowledgments**

The work described here was supported by the UK’s National Measurement System programme for Data Science. The authors also thank Maurice Cox and Peter Harris (NPL) for useful discussions about this work.

**References**

[1] Cox M G, Forbes A B, Harris P M and Smith I M 2004 The classification and solution of regression problems for calibration NPL Report CMSC 24/03

[2] Golub G H and Van Loan C F 1996 *Matrix computations* (John Hopkins University Press, Baltimore, third edition)

[3] Fox L and Parker I B 1968 *Chebyshev polynomials in numerical analysis* (Oxford University Press)

[4] NPL Mathematics and Modelling Software Downloads webpage http://www.npl.co.uk/mathematics-scientific-computing/mathematics-and-modelling-for-metrology/software-downloads-ssfm