

Nonlinear Regression Analysis by Global Optimization: A Case Study in Space Engineering

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Abstract The search for a better understanding of complex systems calls for quantitative model development. Within this development process, model fitting to observational data (calibration) often plays an important role. Traditionally, local optimization techniques have been applied to solve nonlinear (as well as linear) model calibration problems numerically: the limitations of such approaches in the nonlinear context – due to their local search scope – are well known. In order to properly address this issue, global optimization strategies can be used to find (in practice, to approximate) the best possible model parameterization. This work discusses an application of nonlinear regression model development and calibration in the context of space engineering. We study a scientific instrument, installed on-board of the International Space Station and aimed at studying the Sun’s effect on the Earth’s atmosphere. A complex sensor temperature monitoring objective has motivated the adoption of an *ad hoc* calibration methodology. Due to the apparent non-convexity of the underlying regression model, a global optimization approach has been implemented: the LGO software package is used to carry out the numerical optimization required periodically for each stage of the analysis. We report computational performance results and offer related insight. Our case study shows the robust and efficient performance of the global scope model calibration approach.

Key words: Regression analysis · Nonlinear model fitting to data · Global optimization · Space engineering applications · Composite periodic functions · Trend analysis · Failure detection.

MSC Classification (2000) 62J02, 90C26, 90C30, 90C90, 90-02, 90-08

1 Introduction

Regression analysis (Bates and Watts, 1988; Seber and Wild, 1989; Björck (1996); Sen and Srivastava 2011; Chatterjee and Hadi, 2012; Greene, 2012; Kleijnen, 2015) is an important subject across a broad range of studies in econometrics, engineering, and the sciences. Nonlinear regression is a general framework for regression analysis in which the observational data are modeled by a postulated nonlinear function: this function is then parameterized according to a stated optimality criterion. A quick Internet search for the key words “Nonlinear Regression” returns close to 2,700,000 results (as of March 2016, using Google’s search engine), clearly indicating a substantial interest towards the subject.

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The most frequently used classical optimization method to find the parameters of a nonlinear regression model (based on the minimization of the corresponding least squares error function) is the Levenberg–Marquardt algorithm (LMA). The LMA is a modification of the Gauss-Newton method, proposed by Levenberg (1944) and rediscovered by Marquardt (1963): consult e.g. the related discussions in Press *et al.* (1992), Björck (1996), and Kelley (1999). In the LMA a linearized local approximation of the nonlinear model is used sequentially, and – based on a suitable initial solution “guess” – the model parameters are iteratively refined.

The model fitting exercise can become a hard numerical challenge when the conjectured regression model includes highly nonlinear functions. This study will discuss such a case with compositions of trigonometric functions in the regression model. In similar cases, the error function can be multi-extremal: hence, different initial solution “guesses” can lead to locally best model fitting results of broadly varying quality – calling for a global scope calibration strategy.

Model development studies in which a proper global optimization approach is required arise in numerous real-world applications: consult e.g., Pintér (1990, 1996, 2003), Van der Molen and Pintér (1993), Finley *et al.* (1998) for related examples and case studies. The substantial advances in global optimization witnessed in recent decades support the application of global optimization algorithms and software to handle challenging nonlinear model fitting problems. Without going into details on the subject of global optimization that are outside of the scope of the present discussion, we refer e.g. to (Horst and Pardalos 1995; Pintér, 1996; Pardalos and Romeijn, 2002; Liberti and Maculan, 2005; Pintér, 2002, 2006, 2009).

The chapter is organized as follows. The subjects of model calibration, global optimization and information regarding the LGO software package are concisely presented and discussed in Section 2. Following these brief expositions that serve as the technical basic of our modeling and solution approach, we present a trend analysis and failure detection case study arising in a current space engineering application (Section 3). Section 4 presents concluding notes, followed by a list of references.

Let us mention that a broad range of space engineering case studies is discussed in the edited volumes Fasano and Pintér (2013, 2016): several of these studies include also various model calibration tasks as important ingredients.

2 Global Optimization for Nonlinear Model Fitting

2.1 The Model Calibration Problem

Model development is an essential research tool in many quantitative studies. In very general terms, the following main phases of such development can be distinguished:

- 1) formulation of model objectives
- 2) determination of the model structure (functional form selection) based on domain specific knowledge and expertise
- 3) data collection and analysis, to support model development
- 4) model fitting to data (calibration, parameterization)
- 5) validation and sensitivity study
- 6) applications in analysis, forecasting, management, and so on.

Hence, model calibration is an important stage of the process of understanding and managing complex (chemical, engineering, environmental, physical, or other) systems.

In order to present a general model calibration problem statement, we introduce the following notation:

$t = 1, \dots, T$	time moments of system observations; T is the number of data used
x	model parameters (to be selected according to some chosen optimality criterion); x is assumed to be a real n -vector
D	set of admissible (feasible) model parameterizations
M	continuous (real-valued, scalar) model function; the values of M depend on x , for each value of $t = 1, \dots, T$
m_t	model output data at time t ; $m_t = M(x, t)$; their sequence is $\{m_t\}$, for $t = 1, \dots, T$
o_t	measurement data at time t corresponding to m_t ; their sequence is $\{o_t\}$, $t = 1, \dots, T$
f	continuous error function that expresses the discrepancy between the sequences $m = \{m_t\}$ and $o = \{o_t\}$: $f = f(\{m_t\}, \{o_t\})$.

Applying these notations, the generic model calibration problem can be formulated as

$$\begin{aligned} \min f(\{m_t\}, \{o_t\}) & \tag{1} \\ m_t = M(x, t) \quad t = 1, \dots, T & \\ x \in D \subset R^n. & \end{aligned}$$

In order to specify the general model (1), next we present some frequently used model types. The set of feasible parameter settings D can be defined by explicit finite lower and upper bounds (n -vectors l and u) regarding x , as well as by an optional set of $k \geq 0$ additional constraints written in summary form as $g(x) \leq 0$ (g denotes a continuous k -dimensional vector function when such constraints are present):

$$D = \{x: l \leq x \leq u, g(x) \leq 0\}. \tag{2}$$

Based on these conditions, D is a bounded subset of the n -dimensional Euclidean space; we will assume that D is non-empty.

The aggregate model error function f is often defined using a suitably chosen l_p -norm to measure the discrepancy between the vectors m and o :

$$f = f(\{m_t\}, \{o_t\}) = \|m - o\|_p \quad 1 \leq p \leq \infty. \tag{3}$$

Various extensions of this model can be introduced to handle more general formulations, including consideration for uncertainties and/or for multiple model calibration objectives: consult, e.g. Van der Molen and Pintér (1993), Pintér (1996).

In the context of our discussion, let us point out that the general nonlinear model calibration problem (1)-(3) could well be multi-extremal: cf. e.g. Pintér (1996) Chapter 4.5, and several

environmental modeling case studies discussed in the same work that illustrate this aspect. For this reason, we have been introducing and using global optimization technology to handle nonlinear model calibration problems across a range of application areas.

2.2 *The Global Optimization Model*

The model calibration problem (1)-(3) belongs to the general class of continuous global optimization models stated as

$$\min f(x) \tag{4}$$

$$D = \{x: l \leq x \leq u, g(x) \leq 0\} \tag{5}$$

$$f \text{ and } g \text{ (the latter component-wise) are continuous functions in } [l, u]. \tag{6}$$

Notice the absence of the usual convexity assumptions in the above general model formulation that would justify the use of local optimization tools. In (4)-(6) not only the objective f could be multi-extremal, but the feasible region D could also be non-convex. At the same time, the above stated key assumptions already guarantee that the optimal solution set X^* of model (1)-(3) is non-empty. For additional technical details, we refer to Pintér (1996).

2.3 *LGO Solver Suite for Nonlinear Optimization*

The traditional numerical optimization methods used for model calibration seek only for local optima (tacitly assuming the availability of a sufficiently good initial parameter vector). In the general framework presented here this may not be a realistic assumption: therefore global scope search strategies will be required to parameterize (possibly multi-extremal) nonlinear regression models.

Specifically, we will use the Lipschitz Global Optimizer (LGO) solver suite for constrained nonlinear – both global and local – optimization. LGO can handle models with merely continuous structure (without asking for higher order – gradient, Hessian – information); and its operations are based on model function values. This feature makes LGO a suitable choice to tackle a broad range of model calibration problems, including completely “black box” models, in addition to standard (analytically defined) models.

LGO has been discussed in other works, cf. e.g. Pintér (1996, 1997, 2009, 2015): therefore here we present only a summary description. The design of LGO is based on the flexible combination of several nonlinear optimization algorithms, each with corresponding theoretical (provable) global and local convergence properties. It should be noted that the name LGO reflects the original (first) global solver component embedded in the software. (Note in passing that even this solver component uses only model function values, without requiring exact – typically unknown – Lipschitz-continuity information.)

Next, we briefly describe the overall algorithmic structure of LGO. LGO includes a local solver (LS) option which precedes all global search options. LS can be started either from an initial solution point provided by the user, or from a default point determined by LGO. The LS search mode can be also used without a subsequent global search phase. Following the LS phase,

two quick global pre-solvers are launched: each of these is followed by LS from the current best point, if an improved solution has been found. The overall purpose of these solver components is to provide a reasonable quality solution with a relatively small global search effort. Next, one of three theoretically “exhaustive” global search options is invoked based on the LGO user’s preference: the methods to choose from are branch-and-bound (BB), single-start partially randomized search (RS), and multi-start partially randomized search (MS). Each of BB and RS is followed by a LS phase, while each major MS iteration is followed by a corresponding LS phase.

Based on the solver options summarized above, LGO – as a stand-alone solver suite – can be used for both global and local constrained nonlinear optimization. Without going into further details, we refer to Pintér (1996) for an in-depth discussion of the theoretical results leading to the global search options BB, RS and MS. The relatively inexpensive first global pre-solver is described in Pintér and Horváth (2013); the second one is an unpublished heuristic strategy. The LS method is a generalized reduced gradient algorithm implementation: for background, consult e.g. Edgar *et al.* (2001).

In the practical context of numerical optimization – that is, in resource-limited computations – each one of LGO’s “exhaustive” global search options generates a global solution estimate(s) that is (are) refined by the seamlessly following local search mode(s). This way, the expected overall result of using LGO is global and/or local search based high-quality feasible solution that satisfies at least the local optimality criteria. (To guarantee theoretical local optimality, standard local smoothness conditions need to apply – at least whenever LS is invoked.)

At the same time, one should keep in mind that no global – or, in fact, any other – optimization software will always work satisfactorily, with default settings and under resource limitations related to model size, time, model function evaluation, or other usage limits. With this cautionary remark in mind, extensive numerical tests and a growing range of practical applications demonstrate that LGO and its platform-specific implementations can find high-quality numerical solutions to complicated and sizeable GO problems. For details, consult e.g. Pintér (1996, 2002, 2014, 2015), Pintér and Kampas (2013), with references to a range of applications – including also real-world model fitting problems.

LGO is available for use with a range of compiler platforms (C/C++/C#, Fortran 77/90/95), with seamless links to several optimization modeling languages (currently, AMPL, GAMS, MPL), to Excel, and to the leading high-level technical computing systems Maple, *Mathematica*, and MATLAB.

The structure of the compiler-based core LGO implementation used in our study is shown by Fig. 3: a brief explanation of the symbols displayed follows below.

LGOMAIN is a driver program that defines or retrieves from the input file (called LGO.IN) LGO’s static calling parameters before activating LGO. The adjective static refers to model descriptor and solver option information that is defined (or read) only once and then remains unchanged during a specific LGO run. LGOMAIN may also include additional user actions such as links to other program files and to external applications, to report generation and to the further optional use of LGO results.

LGOFCT serves to define the dynamic components of an optimization problem: these are defined by the model objective f and constraint functions g . Here dynamic means that this file will be called at every algorithmic iteration step of LGO, to evaluate its functions depending on the algorithmically generated sequence of input variable arguments x . Again, this file may include calls to other application programs (as needed), in order to evaluate the model functions.

LGO.IN is an optionally used LGO input parameter (text) file that stores LGO's static calling parameters (unless these are directly defined by LGOMAIN).

The source code files LGOMAIN and LGOFACT are to be compiled and linked to the LGO (object or dynamic link library) file. Upon launching the generated executable program, LGOMAIN invokes the LGO solver suite; then LGO iteratively calls LGOFACT.

LGO's operations can be partially controlled by the static input parameter file LGO.IN, or by changing LGOMAIN: this structure supports repeated LGO runs under various model specifications and/or solver option settings. Of course, LGOFACT can also be changed if necessary to test different model variants. LGOMAIN optionally reads LGO.IN when launched; in the opposite case all calling parameters are directly defined in LGOMAIN.

LGO optionally generates result text files, on different levels of detail specified by the user. The first one of these files, called LGO.SUM, presents only a concise summary of the results obtained. The second file, called LGO.OUT, provides more detailed information pertinent to the optimization process. The third file, called LGO.LOG, reports the entire sequence of all arguments x generated and the resulting function values f and g .

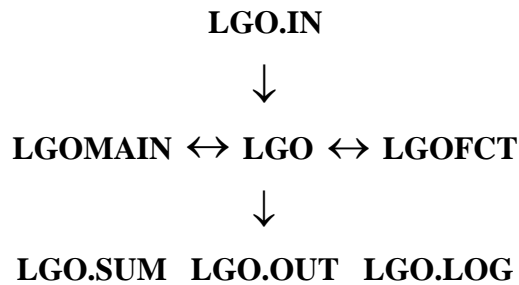


Fig. 1 LGO application program structure

For additional details, we refer to the earlier listed references, especially to the current LGO manual (Pintér, 2015).

3 A Regression Model Case Study in Space Engineering

3.1 Introduction

Columbus is a science laboratory that is part of the International Space Station (ISS): it is the largest contribution to the ISS made by the European Space Agency (ESA). For information related to the ISS, consult NASA (2016a); regarding Columbus, see ESA (2016a). The Columbus laboratory carries an extensive collection of instruments. These instruments – referred to as payloads – are aimed at performing various requested scientific experiments, and can be located either internally or externally.

The SOLAR (external) payload (ESA 2016b, see Fig. 2 below) has the scope of studying the Sun with extremely high accuracy across most of its spectral range. Its scientific contributions are mainly focused on solar and stellar physics, as well as on the Sun's interaction with the

Earth's atmosphere. Its monitoring activity has been in continuous operation since its installation outside the ESA Columbus module in February 2008.

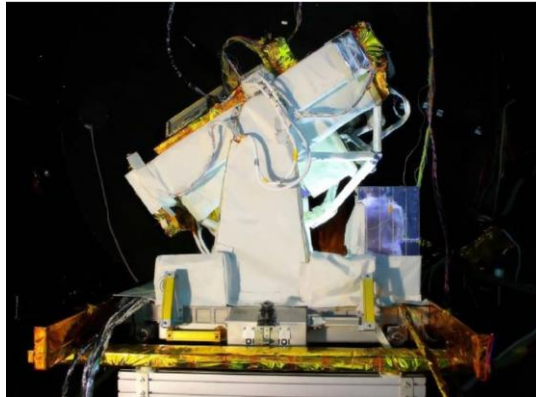


Fig. 2 SOLAR

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SOLAR consists of three instruments that complement each other, to allow measurements of the solar spectral irradiance virtually throughout the whole electromagnetic spectrum (from 17 nm to 100 μm) in which 99% of all solar energy is emitted. These instruments are referred to as SOL-ACES (SOLar Auto-Calibrating Extreme UV/UV Spectrophotometers; see NASA, 2016b), SOLSPEC (SOLar SPECTral Irradiance measurements; see NASA, 2016c) and SOVIM (Solar Variable and Irradiance Monitor; see NASA, 2016d).

The present discussion is focused on monitoring the SOLAR sensor temperature. Relevant data are retrieved continuously from the ISS to the Earth, in order to carry out a dedicated trend analysis and failure detection activity. This is accomplished periodically (every three months), applying regression analysis as described in the following subsections.

3.2 Trend Analysis and Failure Detection

From the point of view of regression modeling, the trend analysis and failure detection activity essentially consists of deriving (repeatedly) the analytical expression representing the sensor temperature trend, from the data available for each time period analysed. (Actually, for safety reasons – in order to increase data reliability – two sensors are utilized and the average of their measurements is considered.) This analysis is then used in conjunction with a reference function to identify possible deviations from the nominal state, together with the identification of possibly occurring anomalies, as well as to predict (through extrapolation) the future behaviour of the system, with respect to the temperature control. A further goal is to verify that the expected temperature trend stays inside the admissible operational range.

At its nominal state, the temperature trend is expected to have two leading modes: a primary (carrier) and a secondary (modulating) periodic mode, as depicted by Fig. 3.

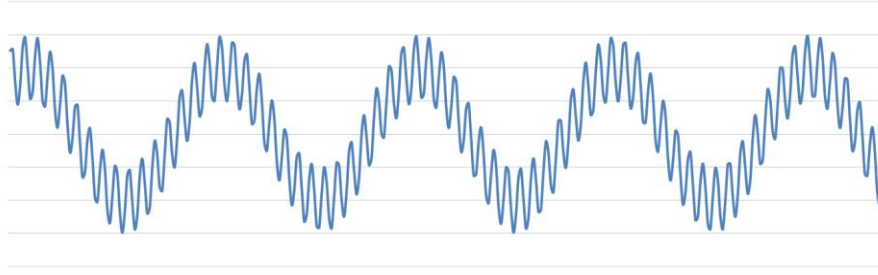


Fig. 3 Primary periodical (carrier) mode and secondary periodical (modulating) mode

The first mode is associated with the nodal precession of the ISS, with a period of about two months (NASA, 2016a). The secondary mode is determined by the orbital motion of the ISS around the Earth, with a period of about 90 minutes. Both modes are therefore assumed to have approximately a sinusoidal nominal trend. A possible systematic physical degradation of the SOLAR thermal protection system (due to ambient radiation) is hypothesized next: for the sake of simplicity, the corresponding trend function is assumed to be linear, see Fig. 4.

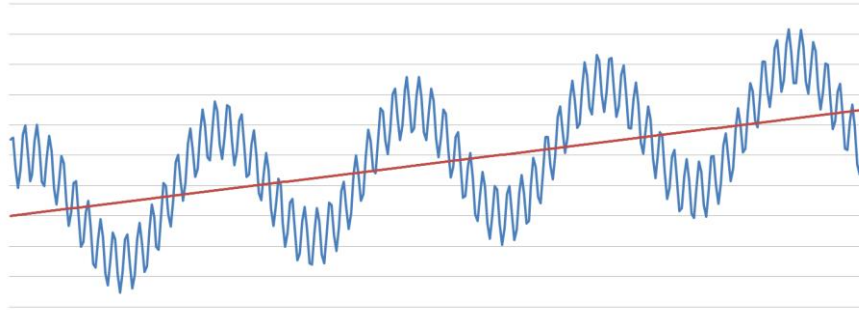


Fig. 4 Possible systematic (linear) degradation function: an example

3.3 *The Model Calibration Problem*

The analytical formulation of the regression model outlined above leads to an optimization problem, defined by the following objective function

$$\min_{\substack{A_1, A_2, \\ T_{01}, T_{02}, \\ K_1, K_2, \\ R, S}} \sum_{i \in I} \{D_i - [A_1 \sin(T_{01} + K_1 T_i) + A_2 \sin(T_{02} + K_2 T_i) + R T_i + S]\}^2 \quad (7)$$

We also consider the following box constraints:

$$\begin{aligned} A_1 &\in [A_1, \bar{A}_1], A_2 \in [A_2, \bar{A}_2], T_{01} \in [T_{01}, \bar{T}_{01}], T_{02} \in [T_{02}, \bar{T}_{02}], \\ K_1 &\in [K_1, \bar{K}_1], K_2 \in [K_2, \bar{K}_2], R \in [R, \bar{R}], S \in [S, \bar{S}]. \end{aligned} \quad (8)$$

In model (7)-(8) $A_1, T_{01}, K_1, A_2, T_{02}, K_2, R, S$ are model parameters to estimate; I denotes the set of sampling time moments, and D_i are the corresponding temperature measurements. The objective function terms $A_1 \sin(T_{01} + K_1 t)$ are related to the primary mode, the terms $A_2 \sin(T_{02} + K_2 t)$ are related to the secondary mode, and $Rt + S$ is the possible linear degradation.

The computational difficulty of this global optimization problem is dictated by its highly multi-modal objective function. Evidently (after considering the specific notations), model (7)-(8) is a special case of both generic model formulations (1)-(3) and (4)-(6).

3.4 Solving the Regression Model

This section provides some insights and details regarding the actual application of the globally optimized model calibration approach. Our experimental results will be merely outlined, due to confidentiality restrictions: nonetheless, what follows will suffice to illustrate the efficiency of the methodology adopted.

Let us point out that the amount of telemetry data to handle is huge. Approximately 150 million sample points (observations affected by abnormal gaps and spikes that are to be properly filtered) have been retrieved since 2011. This circumstance has induced the need to develop a dedicated pre-processing package which will not be discussed here.

Fig. 5 illustrates a typical solution extracted from the set of those obtained so far, considering 365 days of observation on the horizontal axis and temperature trend expressed in centigrade degrees on the vertical axis.

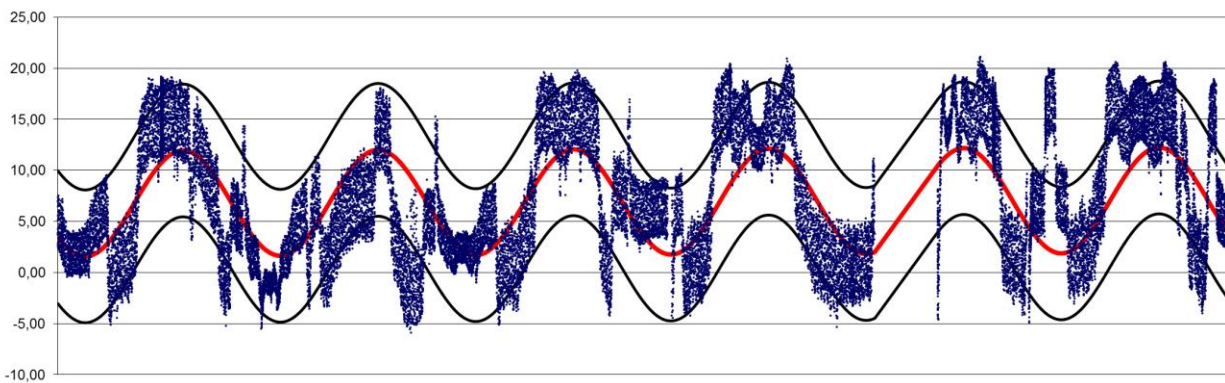


Fig. 5 Solution typology: graphical representation

The experimental analysis that has been performed since 2008 to date has highlighted a slight increment of the amplitude A_1 of the primary mode. A linear degradation rate of about 1.35 degC/year has furthermore been detected based on the mean value since 2008 to date. By extrapolating the latter information, compliance with the currently given tolerance limits would be guaranteed until 2025, well beyond the mission deadline.

No actual anomalies have been identified so far, although apparently some occurred: in fact, these were related to non-nominal manoeuvres of the ISS itself. Fig. 6 shows an example of such

explainable anomalies, pointing out the supposed deviation by circling the relevant two sets of measurements. In all observed cases, the event times corresponded exactly to specific non-standard control actions performed by the ISS.

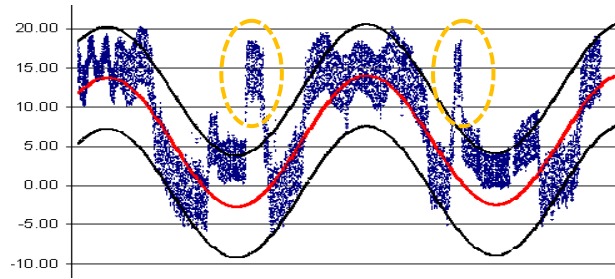


Fig. 6 An example of explained anomalies

In our study, the LGO solver suite has been regularly (sequentially) used to solve model calibration problems of the type (7)-(8). Since the frequencies and amplitudes corresponding to the primary and secondary modes respectively are characterized by pronouncedly different scales, in practice the relevant parameters could be estimated separately. A first analysis is therefore performed regarding the primary set of terms including a possible degradation A_1, T_{01}, K_1, R, S , while neglecting the secondary terms A_2, T_{02}, K_2 . Next, a number of short-term sub-intervals is selected, and then an evaluation of the secondary parameters can be carried out, while keeping the results obtained for the primary terms. The average values of the secondary terms, derived considering the entire set of sub-intervals selected, will yield the final estimation. At each step of this analysis, the numerical results obtained in the previous step for the entire set of model parameters $(A_1, T_{01}, K_1, A_2, T_{02}, K_2, R, S)$ have been utilized as initial solution “guess” values.

Test Case Number	Number of Variables	Time Period		Number of Data Entries	Program Execution Time	Normalized Least Squares Error	Global Optimality Status
		Days	Dates				
TEST 1	5	365	01/01/2013 → 12/31/2014	2186	01:42:06	21.97	Optimum Reached
TEST 2	5	365	04/01/2013 → 03/31/2014	2191	03:16:28	22.17	Optimum Reached
TEST 3	5	365	07/01/2013 → 06/30/2014	2270	02:24:37	25.92	Optimum Reached
TEST 4	5	365	10/01/2013 → 09/30/2014	2193	01:07:01	23.24	Optimum Reached
TEST 5	5	365	01/01/2014 → 12/31/2014	2183	00:43:04	23.12	Optimum Reached
TEST 6	5	90	01/01/2014 → 03/31/2014	542	05:52:42	20.04	Optimum Reached
TEST 7	5	90	04/01/2014 → 06/30/2014	1083	11:53:49	23.96	Optimum Reached
TEST 8	5	90	07/01/2014 → 09/30/2014	1636	18:08:29	18.65	Optimum Reached
TEST 9	5	90	10/01/2014 → 12/31/2014	2183	02:12:37	13.88	Optimum Reached

Table 1 Illustrative experimental results

In order to provide an overview of the solution quality obtained by the LGO solver, observational data related to the time period January 2013 to December 2014 have been considered and analysed according to two different temporal frameworks: 365 days and 90 days. A set of 9 model fitting test case results is summarized in Table 1, indicating also the number of observational data used, the computational effort (expressed as hours:minutes:seconds), and the solution quality obtained. The number of the optimized (primary) variables is 5, in each case shown.

For both timeframes considered, LGO finds parameter settings that lead to remarkably well-fitted models. Two examples of the solutions found are shown by Fig. 7 and Fig. 8 respectively: the scattered dots (representing actual data) are compared with the continuous line representing the expected trend according to the parameterized model resulting from the analysis.

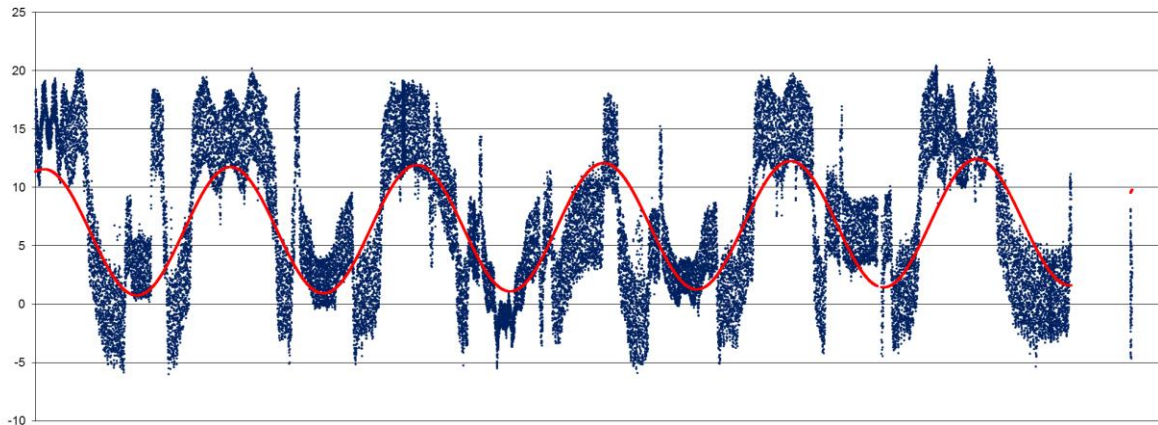


Fig. 7 Example of analysis for the carrier mode (TEST 1, 365 days)

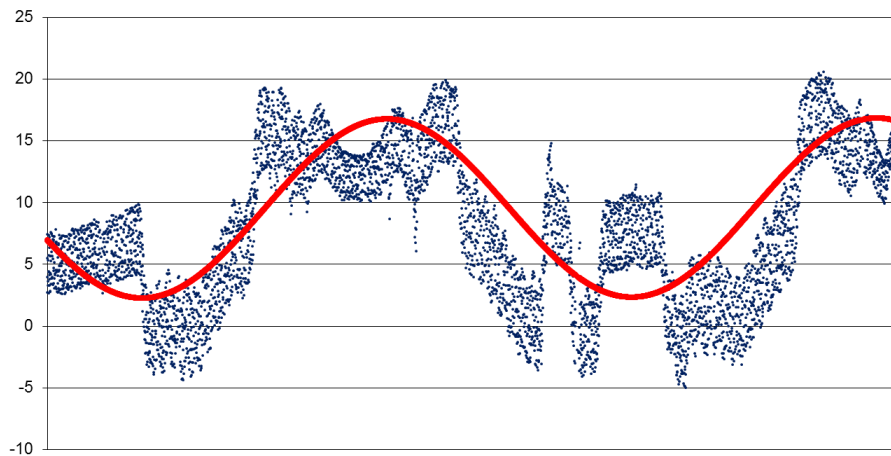


Fig. 8 Example of analysis for the carrier mode (TEST 9, 90 days)

In all examples presented, a high-quality numerical global optimum is reached. Additional statistical analysis of the residuals (normalized with respect to the mean value of the model function) exhibits an apparently “normal-like” distribution: see Fig. 9. This finding is in line with the underlying statistical assumptions of the least squares based model fitting paradigm.

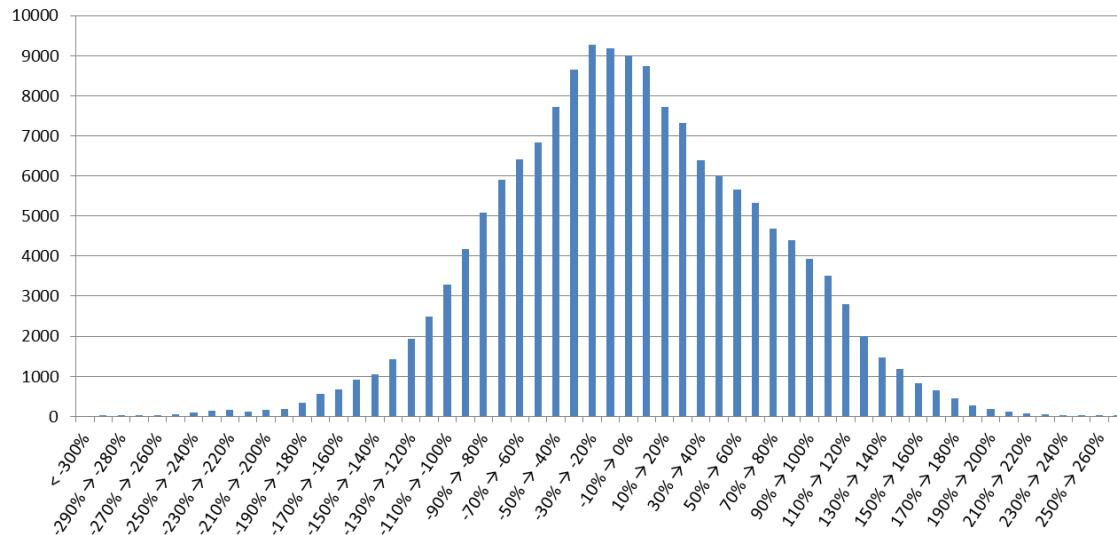


Fig. 9 Normal-like distribution of residuals for carrier mode

4 Conclusions

This work discusses a nonlinear regression model development and calibration study in the context of an application in space engineering. We study the SOLAR payload, installed on-board of the International Space Station. This scientific device is aimed at studying the Sun's effect on the Earth's atmosphere. Due to the apparent non-convexity of the underlying mathematical model, a global optimization approach has been proposed for model calibration. The LGO solver suite is used to carry out the numerical optimization required periodically for each analysis stage. Insights regarding the experimental results and computational performance are provided. Our case study demonstrates the efficiency of the approach proposed, as well as of the software used.

Regarding the SOLAR mission, future research can be directed towards optimizing further model parameters relevant to the payload, such as the voltage/current involved. Extensions to other scientific instruments on-board the International Space Station can also be foreseen, as well as applications related to future scenarios including the anticipated challenge of interplanetary missions.

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