

Total Least Squares Approach to Modeling: A Matlab Toolbox

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This paper deals with a mathematical method known as total least squares or orthogonal regression or error-in-variables method. The mentioned method can be used for modeling of static and also dynamic processes. A wide area of other applications is in signal and image processing. We also present a Matlab toolbox which can solve basic problems related to the total least squares method in the modeling. Several illustrative examples are presented as well.

Key words: total least squares, orthogonal regression, SVD, QR, PCA, Matlab, identification.

1 Introduction

In this paper we present the total least squares method (TLS), which is also known as error-in-variables method or orthogonal regression method. One could hardly name another method which is used as frequently as the method which is known as the least squares method. At the same time, it is difficult to name another method which was accompanied by such strong and long lasting controversy as the least squares method. It is also difficult to find another method, which is so easy and at the same time as artificial as the least squares method. The story of the birth of the least squares method is well covered in the literature and can be summarized as follows [4, 6, 12, 17].

The priority in publication definitely belongs to A. M. Legendre (1805), who also gave the method its famous name, but C. F. Gauss (1809) claimed that he knew and used this method much earlier, about 10 years before the Legendre's publications. Gauss's arguments for his priority were not perfect at all. His diaries with computations claimed to be made by the least squares method were lost. It is also known that when H. C. Schumacher suggested repeating Gauss's lost computations claimed to be done by the least squares method, Gauss totally rejected this idea with the words that such attempts would only suggest that he could not be trusted.

In other words, it is well known which method Legendre used, and it is not clear at all which method was used by Gauss. Assuming that it was Gauss who invented the least squares method, it is hard to believe that he did not realize the huge potential of this method and its importance for applications. Knowing Gauss as a prolific mathematician and looking at the present version of the least squares method, one can see a certain contradiction. Indeed, let us look at the picture which appears frequently in the textbooks, slides, and blackboards as a geometric illustration of the least squares method.

Nowadays, the distance is widely used as an optimal fitting criterion in the field of signal processing, image processing for industrial and scientific applications, especially in problems of shape recognition and curve detection and fitting. In general, the use of orthogonal distance fitting requires the use of numerical routines for minimization of the criteria. However, even in the case of orthogonal distance fitting it is possible to obtain simple formulas for evaluating the parameters of a straight line that fits a given set of points in the plane (orthogonal linear regression problem). For general curve fitting, iteration methods must be used. On the other hand, total least squares approach is a general approach because this approach can be used in n-dimensional space, where we have to minimize the sum of hypervolumes of hyperspheres with radii that are equal to the distances from the data points to the fitting line [12].

The total least squares methods can be characterized by the orthogonal distance as it is depicted in Fig. 1. Mathematically we can express the TLS method by the following relation [2]:

$$R = \sum_{i=1}^n |d_i|$$

where d is the orthogonal distance and the goal is to find a min of R .

For practical calculation with the TLS method, we are able to use the well-known mathematical tools as for example the eigenvalue, SVD, PCA methods. In this paper we present methods, which were proposed for fitting the line and general curves via bounded optimization algorithm, SVD and QR methods, and fitting the line

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and plane via the PCA method. For all above-mentioned mathematical methods the Matlab routines have been created [14].

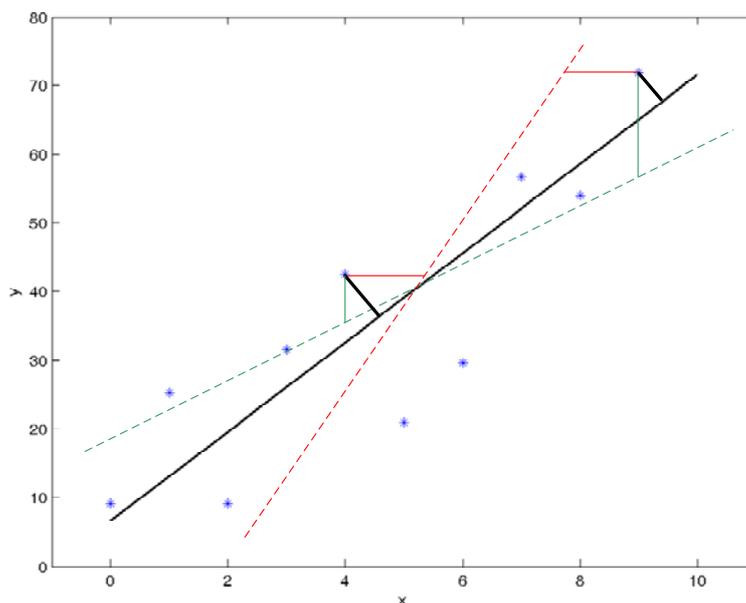


Fig. 1. Principle of the TLS method.

This article is organized as follows: In Section 1 we present a brief introduction to the history of the total least square method. In Section 2 are some preliminaries. Some known mathematical tools and statistical indexes are defined. Section 3 is oriented to the application of the total least squares method. Static and dynamical models are presented there together with created Matlab functions. Section 4 concludes this article with some remarks. The list of references contains the supporting material for further reading.

2 Preliminaries

2.1 Eigenvalue and Eigenvector

Given a linear transformation (or matrix) \mathbf{A} , a non-zero vector \mathbf{v} is defined to be an eigenvector of the transformation if it satisfies the eigenvalue equation

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v} \Leftrightarrow (\mathbf{A} - \lambda\mathbf{E})\mathbf{v} = 0, \quad |\mathbf{v}| = 1$$

for some scalar λ . In this situation, the scalar λ is called an eigenvalue of \mathbf{A} corresponding to the eigenvector \mathbf{v} , where \mathbf{E} is the identity matrix.

When a transformation is represented by a square matrix \mathbf{A} , the eigenvalue equation can be expressed as $(\mathbf{A} - \lambda\mathbf{E})\mathbf{v} = 0$ with the trivial solution $\mathbf{v} = 0$. Thus by assuming properties from linear algebra that the determinant equals zero, we obtain characteristic equation: $\det(\mathbf{A} - \lambda\mathbf{E}) = 0$.

2.2 Singular Value Decomposition (SVD)

SVD is a factorization process, which leads to decomposition of matrix \mathbf{D} to its left and right singular vectors \mathbf{U} and \mathbf{V} , which are orthogonal matrices and a diagonal matrix \mathbf{S} , with singular values for which we have

$$\mathbf{D} = \mathbf{U}\mathbf{S}\mathbf{V}^T.$$

Generally we will consider an SVD method, where if \mathbf{D} is matrix of type $m \times n$, then \mathbf{U} is matrix of type $m \times m$, \mathbf{S} is diagonal matrix of type $n \times m$ and \mathbf{V} is a matrix of type $n \times n$. If \mathbf{D} is a real $m \times n$ matrix, then orthogonal matrices

$$\mathbf{U} = [u_1 \dots u_n] \in R^{m \times n} \quad \text{where} \quad \|\mathbf{U}\| = \mathbf{E}$$

$$\mathbf{V} = [v_1 \dots v_n] \in R^{n \times n} \quad \text{where} \quad \|\mathbf{V}\| = \mathbf{E}$$

exist such that

$$\mathbf{U}^T \mathbf{D} \mathbf{V} = \mathbf{S} = \text{diag} \{ \sigma_1 \dots \sigma_p \} \in R^{p \times p} \quad \text{for} \quad p = \min \{ m, n \},$$

where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0$, and where this condition guarantees exactness of the solution.

Similar to the SVD method, but easier, is decomposition which is called QR method.

2.3 Principal Component Analysis (PCA)

The principle of this method is based on the reduction of data dimensions to a representative number of principal components.

A technique known as SVD can be used for their calculation, because matrix \mathbf{V} consists of eigenvectors and the diagonal matrix \mathbf{S} consists of eigenvalues. The PCA transformation for data matrix \mathbf{X} is given as

$$\mathbf{Y}^T = \mathbf{X}^T \mathbf{W} = \mathbf{V} \mathbf{S},$$

where $\mathbf{V} \mathbf{S} \mathbf{W}^T$ is SVD of data matrix \mathbf{X} .

3 Applications of the TLS method

There exist many areas of applications, where the TLS method was used, such as for instance signal processing [18], image processing [7], economics [9, 11, 15], and several possible applications and open problems [1, 5, 8, 16], etc. In this section we show some applications of the TLS method in static and dynamical modeling by using the created Matlab functions [14].

3.1 Linear regression model

For linear regression model (see simple example depicted in Fig. 1 – black line) of the form:

$$y = bx + a, \tag{1}$$

we can derive the following relations for the calculation of the coefficients a and b :

$$a = \frac{\sum_{i=1}^n y_i - b \sum_{i=1}^n x_i}{n} = \bar{y} - b \bar{x}, \tag{2}$$

$$B = \frac{1}{2} \frac{\left(\sum_{i=1}^n y_i^2 - n \bar{y}^2 \right) - \left(\sum_{i=1}^n x_i^2 - n \bar{x}^2 \right)}{n \bar{x} \bar{y} - \sum_{i=1}^n x_i y_i}, \tag{3}$$

where $b = -B \pm \sqrt{B^2 + 1}$ and it depends on line slope. It can be determined from correlation coefficient r . Both lines go through the centroid and there is a relation: $b_1 b_2 = -1$.

The relations (2) and (3) can also be used for the modified model of the form:

$$y = \frac{1}{a + bx}, \tag{4}$$

By substituting $yt = 1/y$ in (4) we obtain the mathematical model of the form:

$$yt = a + bx,$$

and similarly the model in the form

$$y = \frac{x}{a + bx} \quad (5)$$

can be solved as well. Substituting $yt = x/y$ we obtain a mathematical model (5) of the form

$$yt = a + bx.$$

By using the TLS method, we can derive the statistical indexes for linear regression models, which can be presented by the following definitions:

Definition 2.1: Residual dispersion for linear regression model computed by total least squares (TLS) method is defined as [2,3]:

$${}_{TLS}S_{rez}^2 = \frac{\sum_{i=1}^n d_i^2}{n-p} = \frac{\sum_{i=1}^n \left(\frac{y_i - (a + bx_i)}{\sqrt{1+b^2}} \right)^2}{n-p} = \frac{\sum_{i=1}^n \left(\frac{y_i - Y_i}{\sqrt{1+b^2}} \right)^2}{n-p}, \quad (6)$$

where p is the number of model parameters.

Definition 2.2: Total dispersion (complex) for linear regression model computed by total least squares (TLS) method is defined as [2,3]:

$${}_{TLS}S_{celk}^2 = \frac{\sum_{i=1}^n \left(\sqrt{(y_i - \bar{y})^2 + (x_i - \bar{x})^2} \right)^2}{n-1} = \frac{\sum_{i=1}^n (y_i - \bar{y})^2 + (x_i - \bar{x})^2}{n-1}. \quad (7)$$

Definition 2.3: Following Definition 2.1 and Definition 2.2 it is possible to derive a relation to calculate the value of F test criteria for adequacy validation of linear regression model computed by total least squares (TLS) method, which can be defined as

$$F = \frac{S_{celk}^2}{S_{rez}^2}.$$

After substituting the relations from Definition 2.1 and Definition 2.2 we obtain the formulae for calculating the F test criteria value defined as [2,3]:

$${}_{TLS}F = \frac{(n-p) \left(\sum_{i=1}^n (y_i - \bar{y})^2 + (x_i - \bar{x})^2 \right)}{(n-1) \sum_{i=1}^n \left(\frac{y_i - Y_i}{\sqrt{1+b^2}} \right)^2}, \quad (8)$$

which can be used, under some conditions, for the adequacy validation of linear regression model.

For linear regression model and its statistical indexes Matlab routines [14] were developed:

- function [Err, P] = fit_2D_data(XData, YData, vizualization)
- function [Err, P] = fit_2D_data_SVD(XData, YData, vizualization)
- function [Err, P] = orm(X, Y, order)
- function [F, Srez, Scel] = statindexes(XData, YData, a, b)

Function `fit_2D_data` uses relations (2) and (3). Further functions `fit_2D_data_SVD` and `orm` use the SVD and QR methods, respectively. Functions `statindexes` returns the appropriate statistical indexes as for instance both dispersions and F test.

An illustrative example of the linear regression model (1) computed from measured data stored in file `dataLRM.txt`, via TLS method and the classical least square (LS) method together with the statistical indexes calculation for both cases we can find in work [14].

3.2 Nonlinear regression model

In the case of nonlinear regression model it is not possible to derive an exact mathematical relation for the calculation of model parameters and therefore we used an optimization algorithm for the solution of this problem. For this purpose was created a Matlab function [14]:

- ```
function [Err, min_param] = numerFminS(fun, p, LBa, UBa, xdata, ydata)

% Input parameters:
% - fun: name of file where is the model defined
% - p: number of optimized parameters (same as in the file 'fun')
% - LBa: lower bound vector or array for parameters
% - UBa: upper bound vector or array for parameters
% - xdata: input data block -- x: axis
% - ydata: input data block -- y: axis
%
% Return parameters:
% - Err: error - sum of squared orthogonal distances
% - min_param: vector of model parameters
```

where the model should be defined by a function (second degree polynomial), e.g.

```
function [yM] = model(xm, a)
yM = zeros(3,1);
yM = a(1)*xm.^2+a(2)*xm+a(3);
```

and for finding the model parameters from measured data stored in file `dataNRM.txt`, we can use the following commands:

```
load dataNRM.txt;
xdata=dataNRM(1,:);
ydata=dataNRM(2,:);
[ErrTLS,P]=numerFminS(@model,3,[-0.05 0.5 9.5], [-0.04 0.7 10.0], xdata,
ydata)
YhatTLS=polyval(P(1:3),xdata);
plot(xdata, ydata, '*');
hold on
plot(xdata,YhatTLS,'k');
```

For a demonstration of the above sequence the comparison of two nonlinear polynomial models of the form

$$y = ax^2 + bx + c \quad (9)$$

is depicted in Fig. 2. The model parameters obtained by the classical least square (LS) method with an approximation error 16.90 are:

$$a = -0.0335, \quad b = 0.2998, \quad c = 10.8836$$

and parameters obtained by the TLS method with an approximation error 15.01 are:

$$a = -0.0422, \quad b = 0.5092, \quad c = 10.0000.$$

In Fig. 2 is depicted a comparison of two mathematical nonlinear models expressed in equation (9) with the above parameters, respectively. We can see that obtained models are appropriate for the measured

data and the numerical error is lower for the TLS model, which is more accurate than the classical one. Correlation index can be computed by Matlab function

- `function [I] = corrindex(XData, YData, YDataM, par_number)`

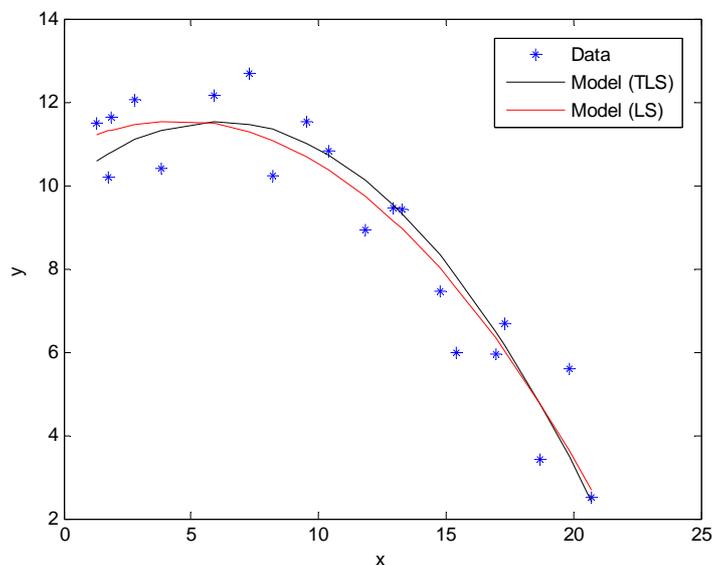


Fig. 2. Comparison of two nonlinear models (9).

### 3.3 Fitting data in 3D space

For fitting data by plane (see Fig. 3) or by line in 3D a Matlab routine [10] was created:

- `function [Err,N,P] = fit_3D_data(XData, YData, ZData, geometry, visualization, sod)`

With the same function we are able to use a line instead of plane. It depends on the option `geometry`. In Fig. 3 is depicted a model (plane) of state economy in the state space for 1980-2008. Normal vector of the plane is  $n = [-0.32, -0.5, -0.8]$  and an approximation error is 18.89.

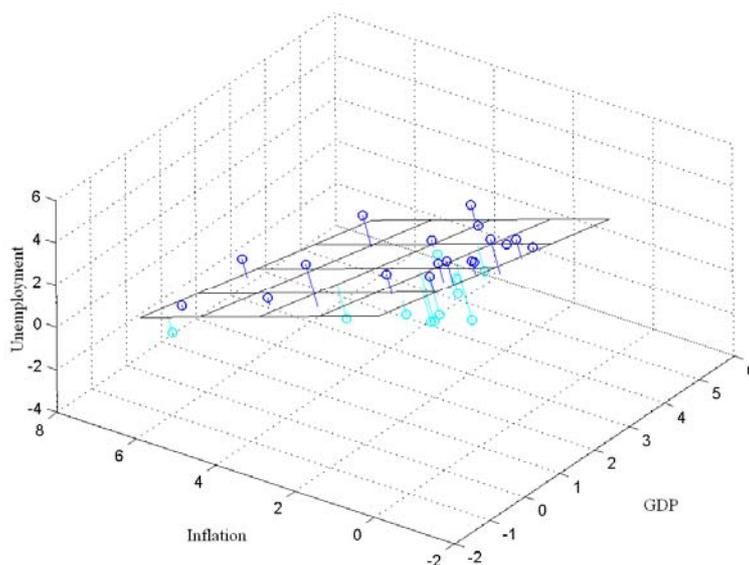


Fig. 3. Approximation of Swiss economy in 3D state space (GDP, Inflation, Unemployment).

### 3.4 Identification of dynamical system

The principle of new identification method is depicted in Fig.4 and Fig. 5. It is based on minimization of functional [13]:

$$\min(J) = \sum_{i=1}^N [y_i^* - y_{i^m}]^2, \quad N = \frac{T_{ident}}{T_{vz}}$$

with the number of samples  $N$ , where  $T_{ident}$  is total identification time and  $T_{vz}$  is sampling period. That means, that during identification of dynamical system in the state space we evaluate the state trajectory. It can be mathematically written as

$$\min(J) = \sum_{i=1}^N |d_i| \quad \text{or} \quad \sum_{i=1}^N d_i^2$$

where  $d$  is orthogonal distance.

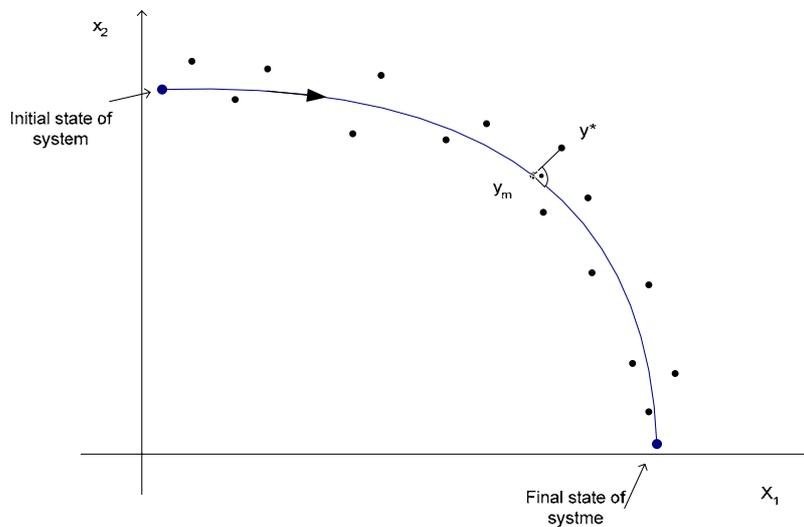


Fig. 4. Graphical interpretation of proposed principle based on the TLS method.

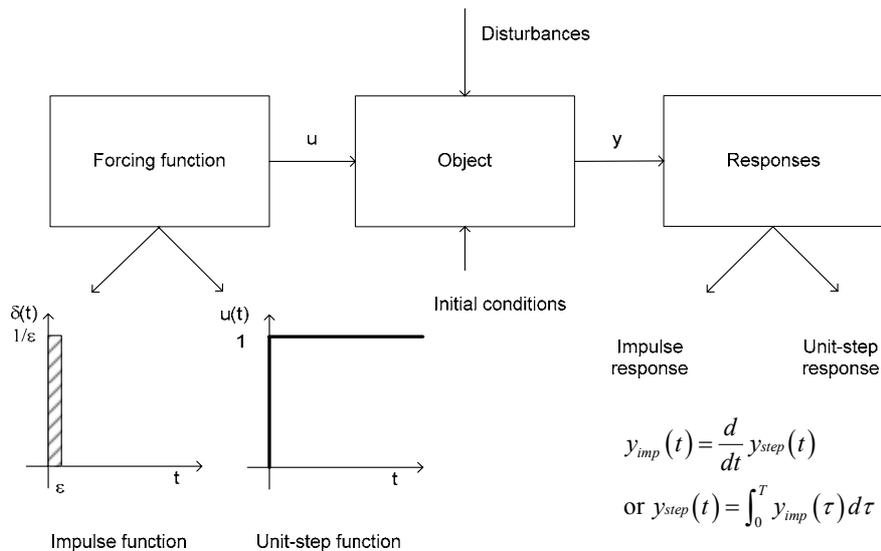


Fig. 5. Block diagram of proposed method.

Let us consider the mathematical model described by the transfer function in the form

$$G(s) = \frac{Y(s)}{U(s)} = \frac{K}{a_n s^n + \dots + a_1 s + a_0}$$

or by its corresponding differential equation

$$a_n y^{(n)}(t) + \dots + a_1 y'(t) + a_0 y(t) = Ku(t) \quad (10)$$

with the initial conditions:

$$y(0), y'(0), \dots, y^{(n-1)}(0).$$

The differential equation (10) can be rewritten to the canonical form

$$\begin{aligned} \frac{dx_1}{dt} &= x_2 \\ \frac{dx_2}{dt} &= x_3 \\ &\vdots \\ \frac{dx_n}{dt} &= \frac{Ku(t) - \dots - a_1 x_2 - a_0 x_1}{a_n}, \quad (y \equiv x_1). \end{aligned} \quad (11)$$

We assume that the independent time variable  $t$  is not influenced by measurement error and therefore we can use a TLS approach.

The state space trajectory is created by measuring the unit step response and impulse response of object as it is depicted in Fig. 5. Both responses are plotted in the state space and then the TLS approach is used to find the best parameters of the dynamical mathematical model (11).

For this purpose was created a Matlab function [14]:

- ```
function [Err, min_param]=numerFminD(fun, p, LBa, UBa, xdata, ydata,
FTIME, Tvz)
%
% Input parameters:
% - fun: name of file where is the model defined
% - p: number of optimized parameters (same as in the file 'fun')
% - LBa: lower bound vector or array for parameters
% - UBa: upper bound vector or array for parameters
% - xdata: input data block -- x: axis
% - ydata: input data block -- y: axis
% - FTIME: final time of computation [0, Tident]
% - Tvz: sampling period
%
% Return parameters:
% - Err: error - sum of squared orthogonal distances
% - min_param: vector of model parameters
```

Suggested method for identification of the dynamical system was verified on the laboratory object (electrical heater depicted in Fig. 6) connected to the PC by PCL BR 2005 with actuator and temperature sensor LM35, which is installed in the Laboratory of Industrial Control Systems (LPRS), Faculty of BERG, Technical University of Košice.

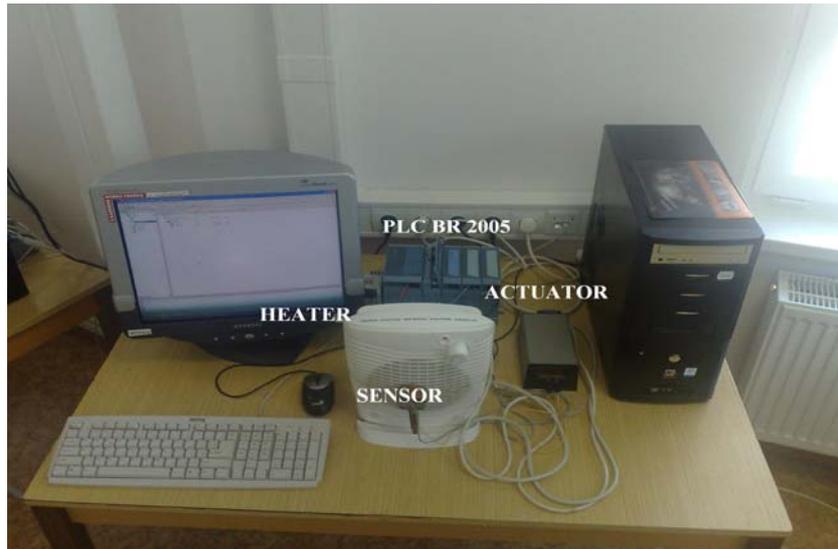


Fig. 6. Laboratory object (electrical heater).

Measured unit step response of the laboratory object is depicted in Fig. 7.

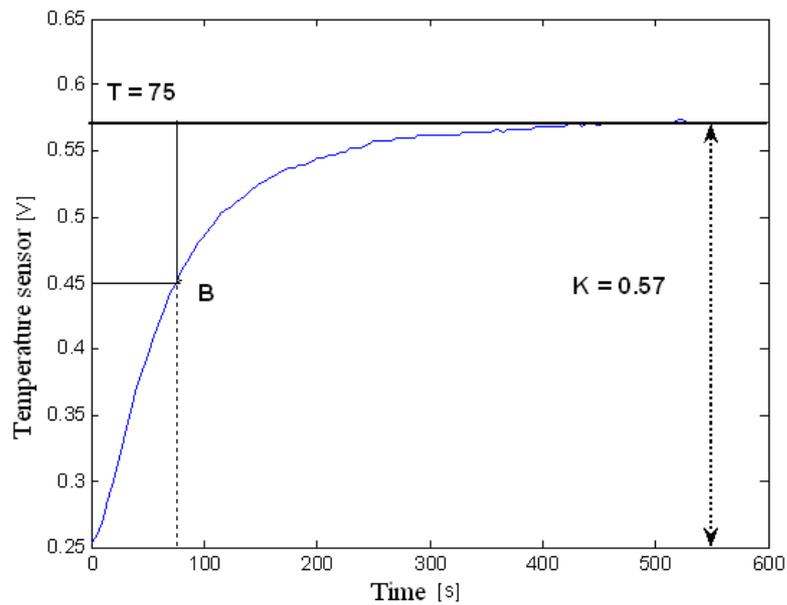


Fig. 7. Unit step response of the electrical heater.

The mathematical model of the electrical heater obtained by graphical identification method is:

$$75y'(t) + y(t) = 0.57u(t), \quad (12)$$

or it can be rewritten to the following form:

$$133.6y'(t) + 1.75y(t) = u(t) \quad (13)$$

Comparison of obtained mathematical model (12) or (13) and measured unit step response is depicted in Fig. 8. We can observe a good consistency of both responses.

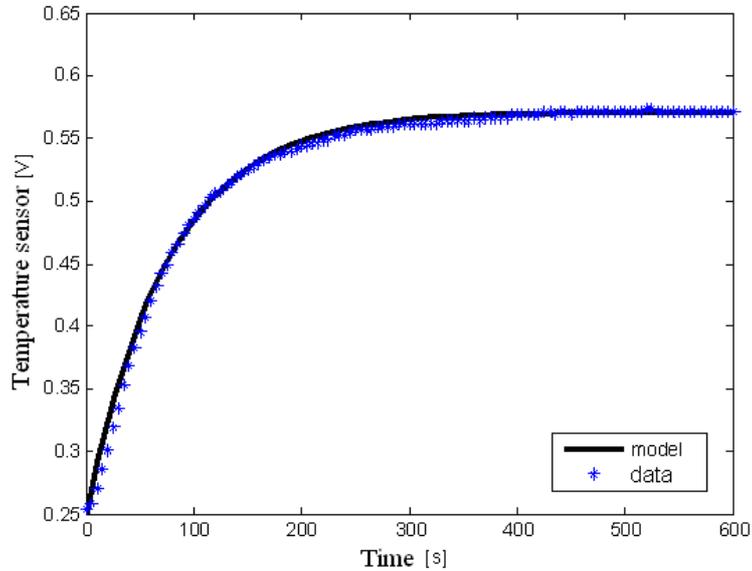


Fig. 8. Comparison of model and measurement.

Let us consider mathematical model of the form

$$\begin{aligned} \frac{dx_1(t)}{dt} &= x_2(t) \\ \frac{dx_2(t)}{dt} &= \frac{u(t) - a_1 x_2(t) - a_0 x_1(t)}{a_2}, \end{aligned} \quad (14)$$

and we use a new identification method, where unknown parameters are a_0 , a_1 , a_2 , and where $x_1(t)$ is unit step response and $x_2(t)$ is impulse response under the following conditions $y(t) = x_1(t)$ a $y'(t) = x_2(t)$.

We have measured unit step response depicted in Fig. 8 and the measured impulse response is shown in Fig. 9.

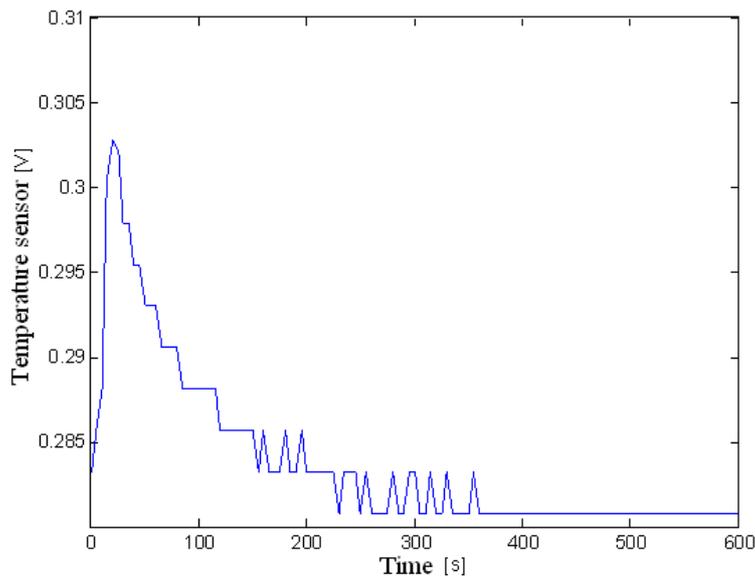


Fig. 9. Impulse response of the electrical heater.

The state space trajectory can be obtained by plotting the measured unit step response and impulse response to 2D state space according to relation (14). Such trajectory is depicted in Fig. 10.

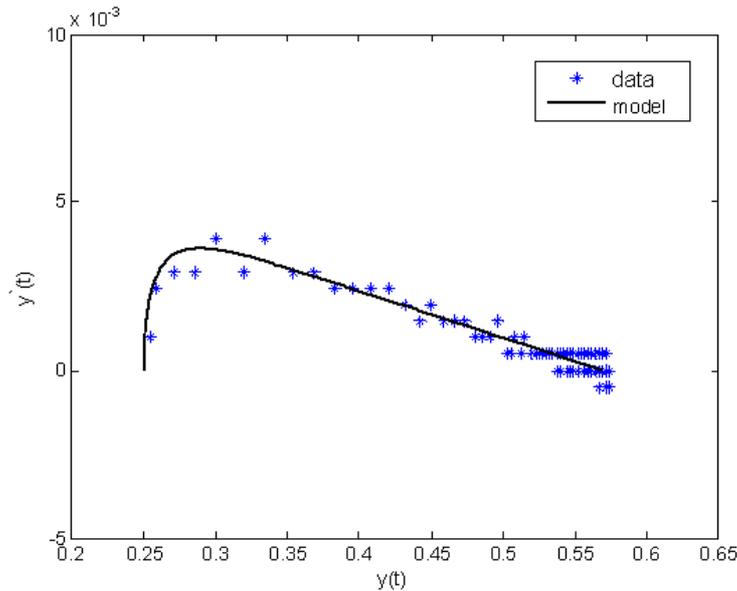


Fig. 10. Measured state space trajectory.

For finding the parameters of the mathematical models we used the created Matlab routines and the following syntax for data stored in `dataHeater.txt`:

```

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
function [dy] = dmodel2D(t,y,a)
dy = zeros(2,1);
dy(1) = y(2);
dy(2) = (1 - a(2)*y(2)-a(1)*y(1))/a(3);
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

load dataHeater.txt
XData=dataHeater(:,1);
YData=dataHeater(:,2);
FTime = 600; Tvz=5;
LBa=[1.75 125 550]; UBa=[1.75 135 570];
[Err, min_param]=numerFminD(@dmodel2D, 3, LBa, UBa, XData, YData, FTime,
Tvz)
[time, Yhat] = ode45(@(time,Yhat)dmodel2D(time,Yhat,min_param),
[0:Tvz:FTime],[XData(1,1) YData(1,1)]);
plot(XData,YData,'*');
hold on
plot(Yhat(:,1),Yhat(:,2),'k');

```

It is necessary to note that for various estimates of parameters interval, we get different values of the parameters. We have found the following values of the parameters:

$$a_0 = 1.75, \quad a_1 = 129.57, \quad a_2 = 565.00, \quad (15)$$

with an approximation error $1.29 \cdot 10^{-4}$.

Next we will compare a measured unit step response with the models. In Fig. 11 is compared a unit step response with the model where parameters were obtained by standard Matlab functions `iddata()` and `pem()`. In Fig. 12 is depicted a comparison of the measured unit step response with the model, where parameters (15) were obtained by new identification method based on the TLS approach. As we can see, proposed method works and we get good model parameters for given estimate of the intervals.

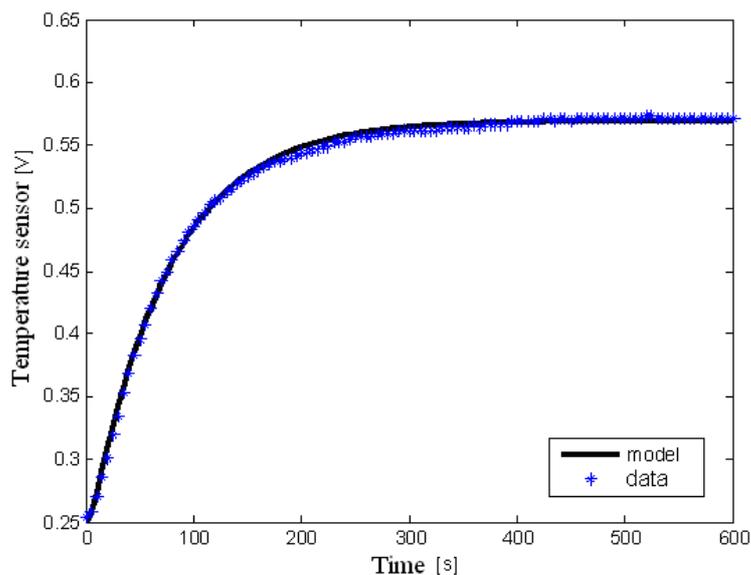


Fig. 11. Comparison of measured unit step response with the model obtained by $pem()$.

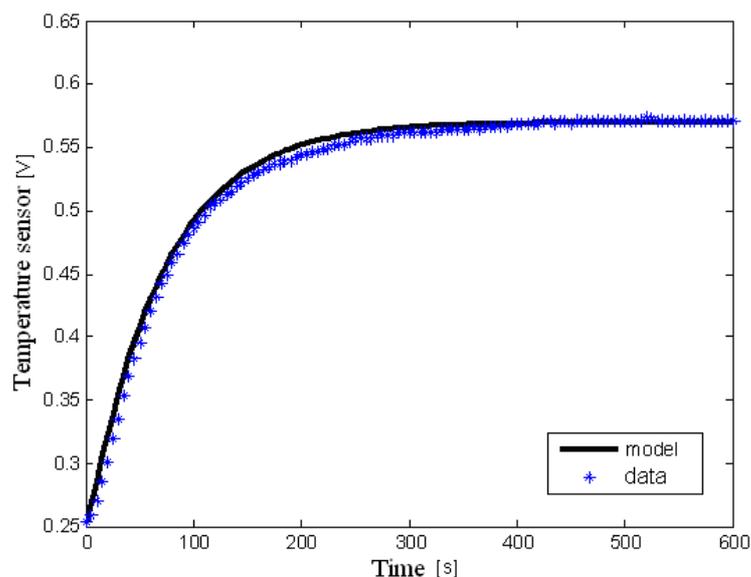


Fig. 12. Comparison of measured unit step response with the model (15).

4 Conclusion

In this paper we have presented a total least square method and its utilization in static and dynamical models. We defined statistical indexes for linear regression model together with F test criteria. For both, linear and nonlinear, regression models the Matlab functions were created which use the total least squares method. In the case of dynamical system, we proposed a new identification method in the state space, which uses the total least squares method as well and a Matlab function was also created. The suggested applications of the total least squares method are presented by the illustrative examples with good results.

Acknowledgements: This work is partially supported by grants VEGA 1/0390/10 and APVV-0040-07.

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