

# Identification of Physical Dynamical Processes via Linear Structure Models (Part 1)

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**To cite this article:**

Oleg Yu. Kopysov. (2024). Identification of Physical Dynamical Processes via Linear Structure Models (Part 1). *International Journal of Systems Engineering*, 8(2), 40-65. <https://doi.org/10.11648/j.ijse.20240802.12>

**Received:** 26 July 2024; **Accepted:** 24 September 2024; **Published:** 18 December, 2024

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**Abstract:** The article discusses methods for identifying parameters of partial differential equations. Identification problems are often called poorly conditioned. However, the reason is the ambiguity of the solution, even at the point of minimality of the criterion. In particular, the article discusses: (1) An analysis of singular values for identify the unambiguous solution. The basis of these methods is a singular value decomposition of the matrix of experimental data, what makes it possible to abandon the inversion of matrices and, as a consequence, translate the problem of ill-conditioned problems into the problem of ambiguity of the solution. (2) The issues of anomalous measurements and combination of various experiments. (3) A universal optimization method for identifying parameters by their complete simple enumeration. The method is based on fast calculation of points on a multidimensional sphere. (4) The issues of identifiability of linear structure models and construction of experiments guaranteeing identification. (5) A method for identifying parameters via projecting linear structure model elements onto the plane of guarantors. (6) An approach to constructing histograms of unknown parameters of dynamic systems before calculating them using any algorithm. The approach is based on linear structure models with parameters on a sphere and a rather unexpected application of singular value decomposition. (7) The methods are accompanied by examples of heat equations. The Appendix contains algorithms in the MATLAB language for all examples. (8) The presented optimization, projection and statistical methods based on the concept of linear structure models allow solving the same identification problem in fundamentally different ways, which significantly increases the reliability of the results obtained.

**Keywords:** Identification, Identifiability, Guaranteeing Identification Experiment, Projection onto Planes of Guarantors, Histograms of Unknown Parameters

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## 1. Introduction

The methods of identification of dynamical systems are essentially purely mathematical, however, in this case, when the study of physical processes is involved, they have specific features.

When idealizing real physical processes as dynamic models describing dependencies between physical measurements, partial differential equations, which include constant parameters (equation coefficients) reflecting the properties of physical processes, are most often used. For example, in the heat equation the coefficients characterize such properties of the heated material as heat conductivity, heat capacity, and others.

The parameters of physical processes are usually

determined during experiments. It is very important to conduct such an experiment that the parameters are determined unambiguously based on its results. This is the physical side of the problem.

From the mathematical point of view, a correct mathematical model of the process as well as a stable method and algorithm for calculating the parameters of the model, the results of which do not contradict the physical meaning, are important.

Let's consider a simple example of the heat equation:

$$a_1 w_t(x, t) + a_2 w_{xx}(x, t) = g(x, t).$$

Suppose in the course of an analytical, mental experiment at  $g(x, t)=0.2$  we got  $w(x, t)=t+x(x-1)/2$ , then  $w_t(x, t)=1$

and  $w_{xx}(x, t) = 1$ . Substituting them into the equation, we get

$$a_1 \cdot 1 + a_2 \cdot 1 = 0.2.$$

It is obvious that the parameters identification problem has an ambiguous general solution:  $a_1 + a_2 = 0.2$ . If we choose the normal solution of the least squares method for the numerical solution of this problem, we'll get  $a_1 = 0.1$ ,  $a_2 = 0.1$ . As is known, the normal solution is the only and stable one, it is included in the general solution, however, in this case, it contradicts the physical law of heat propagation from a more heated part of the body to a less heated one, since both  $a_1 > 0$  and  $a_2 > 0$ . I'd like to note that we did not have any physical grounds to choose the normal solution from a set of equivalent solutions only on the mathematical basis that it is unique and stable, although these are very important arguments.

In the following sections, issues concerning correct, from the identifiability point of view, writing of model formulas and searching for experiments that guarantee their identification, will be considered.

## 2. Linear Structure Models

Following [1, 2] let's define the linear space  $\mathbb{A}^{\mathbf{t}}$  over the field  $\mathcal{A}$  as the set of model elements. Let's take the fundamental relation over elements of a linear space – linear dependence relation – as the genus relation of a model. And let's call this model a Linear Structure Model (*LSModel*).

In physics, this relation leads us to equilibrium models such as the energy conservation law.

In mathematics this definition allows us to write the LSModel as a linear algebra formula. The formula symbolizes the model as a whole and also allows us to operate within the limits of mathematical theory.

Let's write the Linear Structure Model Class (or *LSModels* to simplify) by the following symbolic formula

$$\sum_{n \in \mathbf{n}} \alpha_n \varphi_n(t) = 0,$$

where

- $\alpha_n$  is a symbolic model parameter,
- $\varphi_n(t)$  is a symbolic model element,
- $\mathbf{n} = \{n\}$  is a set of indices.

If model elements are linearly dependent, i.e. satisfy the model formula with coefficients  $\alpha_n$ , then  $\alpha_n$  are called model parameters.

Let a LSModel mean one model and LSModels mean all models – the Linear Structure Model Class.

The given set  $\{\varphi_n(t) : n \in \mathbf{n}\}$  of element formula defines the particular Class, that is a subclass of LSModels.

The set  $\mathbf{a} = \{a_n : n \in \mathbf{n}\}$  of values of symbolic model parameters  $\alpha_n$  defines the particular LSModel and is a vector of the space of parameters (*SP*),  $\mathbf{a} \in \mathbb{A}^{\mathbf{n}}$ .

The set  $\mathbf{f}(t) = \{f_n(t) : n \in \mathbf{n}\}$  of values of symbolic model elements  $\varphi_n(t)$  defines the *realization* of LSModel and is

also a vector of the space of parameters (*SP*),  $\mathbf{f}(t) \in \mathbb{A}^{\mathbf{n}}$ . As, according to LSModel formula

$$\sum_{n \in \mathbf{n}} a_n f_n(t) = 0 \quad \text{or} \quad \langle \mathbf{a}, \mathbf{f}(t) \rangle = 0$$

where  $\langle \mathbf{a}, \mathbf{f}(t) \rangle$  is a scalar product in *SP* between vector of parameters  $\mathbf{a}$  and vector of realization  $\mathbf{f}(t)$ .

The set  $\{f_n(t) : n \in \mathbf{n}\}$  is the minimum information necessary for identification of the parameters  $\mathbf{a} = \{a_n : n \in \mathbf{n}\}$ . The set  $A = \{\mathbf{a}_t : \langle \mathbf{a}_t, \mathbf{f}(t) \rangle = 0, t \in \mathbf{t}\}$  is the hyperplane with the normal vector  $\mathbf{f}(t)$  in *SP*.

Since we now display both parameters and realizations in the *SP* space, it is more accurate to call it the space of parameters/realizations (*SPR*) and in it the coordinate axes have a double name  $a_n / f_n$ .

Let's fix the set  $\mathbf{t} = \{t\}$  as a set of values of  $t$ . Then the set  $f_n(\mathbf{t}) = \{f_n(t) : t \in \mathbf{t}\}$  will be an element of the linear space  $\mathbb{A}^{\mathbf{t}}$  ( $f_n(\mathbf{t}) \in \mathbb{A}^{\mathbf{t}}$ ), the dimension of  $f_n(\mathbf{t})$  coincides with the dimension of  $\mathbf{t}$ .

The matrix  $F = \mathbf{f}(\mathbf{t}) = [f_n(\mathbf{t})] = [\mathbf{f}(t)]$  is called a matrix of Experimental Data (*ED*). Usually a column is an element of the LSModel and a row is a realization of the LSModel.

The Problem of Modeling via LSModels consists in searching for the LSModel elements  $f_n(\mathbf{t})$  at the interval  $\mathbf{t}$  according to given parameters  $\mathbf{a} = \{a_n\}$  and the Problem of Identification via the LSModels consists in searching for parameters  $\mathbf{a} = \{a_n\}$  according to given LSModel elements  $f_n(\mathbf{t})$  at the observation interval  $\mathbf{t}$ . To solve the IP via LSModels it is necessary to solve the algebraic matrix equation  $F \cdot \mathbf{a} = 0$ .

The model belonging to the Model Class and containing all, without exception, experiment realizations in its set of realizations will be called a Particular Solution of Identification Problem (*PSIP*) via the Model Class according to the Experiment.

The set of one and all particular solutions of the identification problem (*PSIP*) via the Model Class according to the experiment will be called a General Solution of Identification Problem (*GSIP*) via the Model Class according to the Experiment.

It is obvious that the experiment realizations and the model parameters divide the *SPR* into two orthogonal complements (subspaces): the general solution and the current model plane (linear span of all realizations generated by the experiment). In particular, it is clear that the only solution is a straight line, and the model plane will then be a hyperplane.

### Example

Let's write the Linear Structure Model Class by the following symbolic heat equation:

$$\alpha_1 w_t(x, t) + \alpha_2 w_{xx}(x, t) + \alpha_3 g(x, t) = 0.$$

Let's assume that in the course of three experiments on the same object of our research the measurements  $g(\mathbf{x}, \mathbf{t})$ ,  $w(\mathbf{x}, \mathbf{t})$  were obtained and the immeasurable elements of the model  $w_t(\mathbf{x}, \mathbf{t})$  and  $w_{xx}(\mathbf{x}, \mathbf{t})$  were calculated by formulas of central

difference derivatives:

$$w_t(x, t) = (w(x, t+h) - w(x, t-h))/2h,$$

$$w_{xx}(x, t) = (w(x+2h, t) - 2w(x, t) + w(x-2h, t))/(2h)^2.$$

It is critical that  $h$  be a power of 2, then the computer division of  $/2h$  is performed without additional rounding errors [1].

In experiment #1 obtained measurements  $g(x, t)=0.2$  and  $w(x, t)=x(x-1)/2+t$  look like :

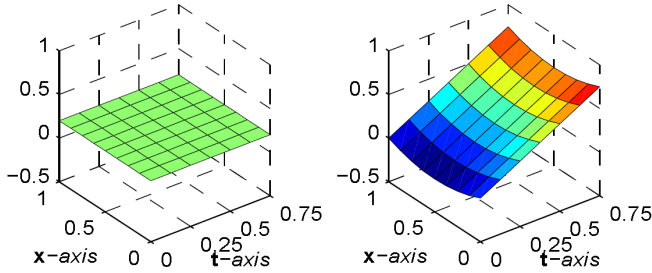


Figure 1.  $g(x, t)$  and  $w(x, t)$  in Ex#1.

and immeasurable  $w_t(x, t)$ ,  $w_{xx}(x, t)$  look like :

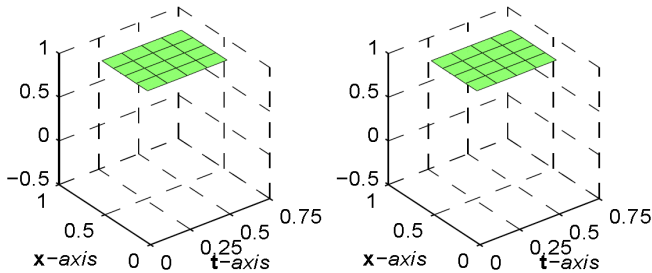


Figure 2.  $w_t(x, t)$  and  $w_{xx}(x, t)$  in Ex#1.

at  $x=\{0, 0.125, \dots, 1\}$ ,  $t=\{0, 0.125, \dots, 0.75\}$  are calculated.

In experiment #2 obtained measurements

$$g(x, t)=0.2+t \text{ and } w(x, t)=x(1-x)/6+0.625t^2$$

look like :

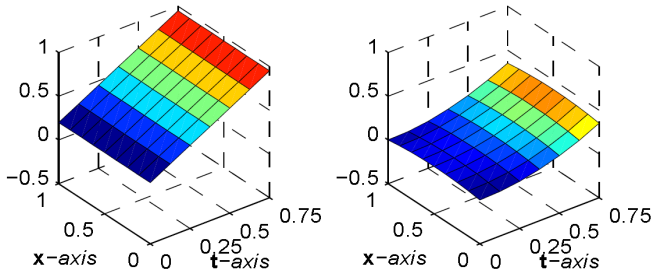


Figure 3.  $g(x, t)$  and  $w(x, t)$  in Ex#2.

and immeasurable  $w_t(x, t)$ ,  $w_{xx}(x, t)$  look like :

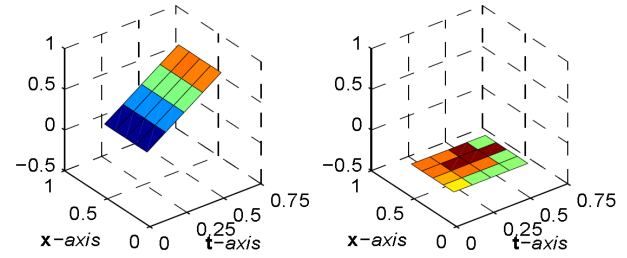


Figure 4.  $w_t(x, t)$  and  $w_{xx}(x, t)$  in Ex#2.

at  $x=\{0, 0.125, \dots, 1\}$ ,  $t=\{0, 0.125, \dots, 0.75\}$  are calculated.

In experiment #3 obtained measurements

$$g(x, t)=\sin(x) \cdot \sin(t) \text{ and } w(x, t)=\sin(x) \cdot \sin(t+\theta)$$

look like :

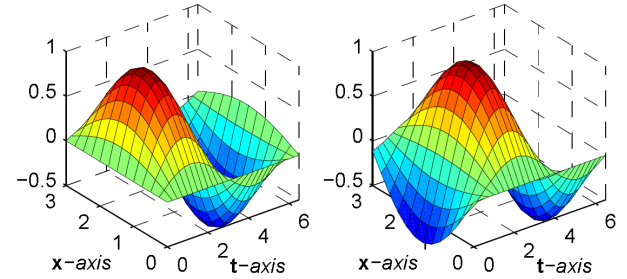


Figure 5.  $g(x, t)$  and  $w(x, t)$  in Ex#3.

and immeasurable  $w_t(x, t)$ ,  $w_{xx}(x, t)$  look like :

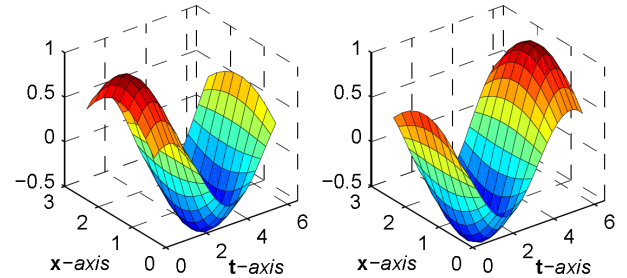


Figure 6.  $w_t(x, t)$  and  $w_{xx}(x, t)$  in Ex#3.

at  $x=\{0, 0.25, \dots, 3\}$ ,  $t=\{0, 0.25, \dots, 6.5\}$  are calculated.

And here's how the same experiments look like in the space of parameters/realizations (SPR):

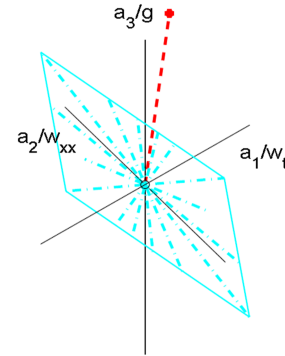


Figure 7. SPR in Ex#1.

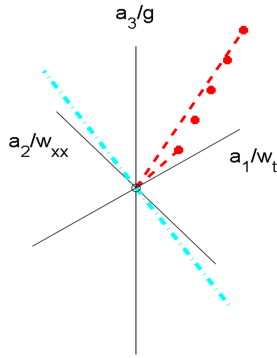


Figure 8. SPR in Ex#2.

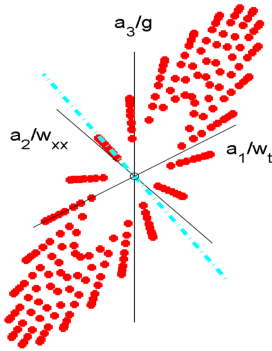


Figure 9. SPR in Ex#3.

Here the dots mean realizations, in the first and second experiments there are 25 of them, in the third one there are 225. However, in the first experiment we see only one, the others are equal to it, because  $w_t(\mathbf{x}, t)=1$ ,  $w_{xx}(\mathbf{x}, t)=1$ ,  $g(\mathbf{x}, t)=0.2$  for all  $\mathbf{x}, t$ . The only realization vector  $[1 \ 1 \ 0.2]'$  (dashed line) means that the general solution is the plane perpendicular to it:  $1 \cdot a_1 + 1 \cdot a_2 + 0.2 \cdot a_3 = 0$  (in the figure it is a set of dot and dash straight lines enclosed in a rectangle). In the introduction, the heat equation was written with  $g(\mathbf{x}, t)$  in the right side of the equation, that is,  $a_3 = -1$ , then  $a_1 + a_2 = 0.2$  and the obtained result is the same as the result from the introduction.

In the second experiment we see five different points, five realization vectors that form a small, but a piece of the plane. This means that the general solution is a straight line perpendicular to all realizations (dot and dash line).

In the third experiment, everything is quite obvious: the points lie in one well-conditioned plane. It is clear that, as in the second experiment, the general solution is a straight line perpendicular to all realizations. However, the third experiment is more credible.

It is intuitively clear that it is easier to look for a general solution in the space of parameters/realizations. There is no such variety of elements as in the space of elements. It seems that since the space of elements, as a functional space, is infinite-dimensional, then the space of realizations is infinite-dimensional as well. However, this is not the case and this is a huge advantage of the space of parameters/realizations.

Theoretically, if the model is identifiable, then all realizations obtained in all conceivable experiments belong to

one model plane, which is a hyperplane of a given space of parameters/realizations (SPR). The subspace of parameters is then a straight line. In the language of the equation, this means that the coefficients may be multiplied by any number, what corresponds to the mathematical spirit of the equation. And now, having fixed any parameter, as in the introduction we took  $a_3 = -1$ , we get a meaningful physically justified unambiguous solution. If the object is not sufficiently excited in the experiment, then the linear span of the realizations of its mathematical model (the current model plane) will no longer be a hyperplane and we will not be able to find an unambiguous solution (a straight line) in the general solution of the identification problem. This is clearly seen in the figure of the space of parameters /realizations of experiment #1. There are infinitely many straight lines belonging to the general solution, and it is impossible to determine which one is correct.

### 3. In Search of a Unique Solution

The task is that according to the given set of realizations determine its dimension and location in the space of parameters/realizations, in other words, to find the current model plane and construct a general solution orthogonal to this current model plane.

Obviously, then the angle of deviation of the current model plane from the ideal model plane will be equal to the angle of deviation of the found general solution from the ideal general solution.

And the more precisely we draw the model plane, the more precisely we will determine the parameters.

#### 3.1. Singular Value Decomposition (SVD)

Any  $m \times n$  complex matrix  $F$  may be represented as a product of three matrices:

$$F = USV^*,$$

here

$U = [\mathbf{u}_1 \dots \mathbf{u}_m]$  –  $m \times m$  complex unitary matrix,

$S = \text{diag}(s_1, \dots, s_n)$  –  $m \times n$  diagonal matrix,

$V = [\mathbf{v}_1 \dots \mathbf{v}_n]$  –  $n \times n$  complex unitary matrix,

$V^*$  – complex conjugate of the matrix  $V$ .

Such a representation is called singular value decomposition (svd), numbers  $s_i$  are singular values and  $s_1 \geq s_2 \geq \dots \geq s_n$ , columns  $\mathbf{u}_i$  of the matrix  $U$ , and columns  $\mathbf{v}_i$  of the matrix  $V$  are left and right singular vectors of the matrix  $F$ , corresponding to  $s_i$ :

$$\mathbf{u}_i^* F = s_i \mathbf{v}_i^*, \quad F \mathbf{v}_i = s_i \mathbf{u}_i, \quad 1 \leq i \leq n.$$

Hereinafter we will consider only matrices consisting of real numbers with a number of rows exceeding the number of columns ( $m > n$ ), then the operation of complex conjugation and transposition  $(\ )^*$  may be replaced by the operation of transposition  $(\ )'$ .

Now the singular value decomposition will look as follows:

$$F = USV',$$

here  $U$  and  $V$  are real orthogonal matrices.

It's also easy to show that

$$F = \sum_{i=1}^n \mathbf{u}_i s_i \mathbf{v}_i' = \sum_{i=1}^n F_i, \quad F_i = \mathbf{u}_i s_i \mathbf{v}_i' = F \mathbf{v}_i \mathbf{v}_i'.$$

It is interesting that the columns of the matrix  $U$  may be interpreted as an orthonormal basis in the space of elements, then the elements of the model in the basis  $U$  will look as follows:

$$F^u = U'F = S V' = \begin{bmatrix} s_1 \mathbf{v}_1' \\ \vdots \\ s_n \mathbf{v}_n' \end{bmatrix}.$$

As the vectors  $\mathbf{v}_i$  are normalized, then  $|v_{ji}| \leq 1$  and  $|f_{ji}^u| \leq s_i$ , in other words, in the  $U$  basis the  $i$ -th coordinates of all model elements modulo are no more than  $s_i$ .

Similarly, in the  $V$  basis, the model realizations will look as follows:

$$F^v = FV = US = [\mathbf{u}_1 s_1 \dots \mathbf{u}_n s_n].$$

And as the vectors  $\mathbf{u}_i$  are normalized, then  $|f_{ij}^v| \leq s_i$ , in other words, in the basis  $V$  the  $i$ -th coordinates of all realizations of the model modulo are no more than  $s_i$ .

We can say that all realizations of the model are enclosed in a multidimensional rectangle with sides  $2s_i$ .

The figure below shows  $f_i^u$  - model elements in the  $U$  basis and  $f_i^v$  - model elements in the  $V$  basis for the experiment #3.

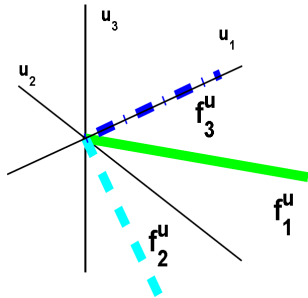


Figure 10. Basis  $U$  in Ex#3.

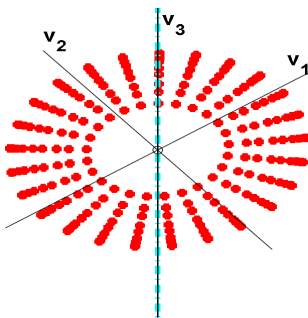


Figure 11. Basis  $V$  in Ex#3.

If  $s_1 \geq s_2 \geq \dots \geq s_r > 0$  and  $s_{r+1} = s_{r+2} = \dots = s_n = 0$ , then

$$F \mathbf{v}_i = s_i \mathbf{u}_i = 0, \quad F_i = \mathbf{u}_i s_i \mathbf{v}_i' = 0, \quad i = r+1, \dots, n.$$

It follows that any linear combination of vectors  $\mathbf{v}_i$

$$\mathbf{a} = \sum_{i=r+1}^n b_i \mathbf{v}_i$$

is the solution of equation  $F\mathbf{a} = 0$  and

$$F = F_r = \sum_{i=1}^r \mathbf{u}_i s_i \mathbf{v}_i' = U_r S_r V_r', \quad r = \text{rank}(F),$$

$$U_r = [\mathbf{u}_1 \dots \mathbf{u}_r], \quad S_r = \text{diag}(s_1, \dots, s_r), \quad V_r = [\mathbf{v}_1 \dots \mathbf{v}_r].$$

In other words, the linear span of vectors  $\mathbf{v}_1 \dots \mathbf{v}_r$  is a model plane in the space of parameters/realizations, and the orthogonal to it linear span of vectors  $\mathbf{v}_{r+1} \dots \mathbf{v}_n$  is a general solution to the identification problem.

The great advantage of this method of obtaining a general solution, or rather a fundamental solution  $\{\mathbf{v}_{r+1} \dots \mathbf{v}_n\}$ , is the presence of an excellent procedure for calculating the singular value decomposition of any matrix. In Matlab, it is enough to write:

```
>> [U, S, V] = svd(F);
```

or

```
>> [U, S, V] = svd(F, 0);
```

in the last case  $U$  has dimension  $m \times n$ ,  $S$  and  $V$  – dimensions  $n \times n$ .

For example, in the three experiments described above, the following singular values were calculated in the absence of measurement noises.

In experiment #1

$$s_1 = 7.1414, \quad s_2 = 9.5467 \cdot 10^{-16}, \quad s_3 = 0,$$

this means that all realizations lie almost on a straight line segment, because two singular values are very close to zero, what indicates the ambiguity of the problem solution.

In experiment #2

$$s_1 = 4.2621, \quad s_2 = 0.6110, \quad s_3 = 5.7812 \cdot 10^{-16},$$

and in experiment #3

$$s_1 = 12.251, \quad s_2 = 8.5309, \quad s_3 = 3.9351 \cdot 10^{-15}.$$

This means that all realizations lie almost on the plane, what points to the obtained unambiguous solution, which should be calculated using the third columns of the corresponding  $V$  matrices.

We need  $a_3$  to be equal to  $-1$ , then  $\mathbf{a} = -\mathbf{v}_3 / v_{33}$ , or in Matlab

```
>> a = -V(:, 3) / V(3, 3)
```

Do not forget that for the stability of calculations,  $v_{33}$ , as a divisor, must be significantly greater than zero, that is,

congruent modulo with  $\max_i |v_{in}|$ .

*Be sure to check it out!*

In experiment #2

$$a_1=0.80000, a_2=-0.60000, a_3=-1,$$

and in experiment #3

$$a_1=0.80839, a_2=-0.61266, a_3=-1.$$

In experiment #2, we obtained accurate theoretical values of the parameters, however in experiment #3, the parameter estimates are much worse. The discrepancies in the parameter values are caused by the chosen method of calculating derivatives, which works fine in the case of linear functions and worse for nonlinear ones. To increase the accuracy, you need to reduce the measurement step.

It is also obvious that it is practically impossible to obtain exact zeros in singular values, especially in conditions of inaccurate measurements and calculations. In other words, the experimental data matrices almost always have a full rank.

However, it is extremely important for approximate calculations that perturbations of matrix elements lead to smaller or equal perturbations of its singular values.

Let  $\tilde{F}=F+\Delta F$  then

$$|\tilde{s}_i - s_i| \leq \|\Delta F\|_2.$$

It is also important that singular values do not depend on the permutation of columns and rows of the experimental data matrix.

But the singular vectors  $\mathbf{v}_{r+1}, \dots, \mathbf{v}_n$  are unstable to calculations, because in the case of an ambiguous solution ( $r+1 < n$ ), even if the ambiguous solution itself is stable, there are infinitely many orthogonal bases of this solution.

In experiment #1 the ambiguous solution – the plane  $a_1 + a_2 + 0.2 \cdot a_3 = 0$  is stable, but you can choose as many orthogonal vectors  $\mathbf{v}_2, \mathbf{v}_3$  lying on this plane, as you want.

If the solution is unambiguous,  $\mathbf{v}_n$  steadily points to the solution, while  $\gamma_0$  is the angle of deviation from the exact solution  $\mathbf{v}_n^-$  ( $\|\mathbf{v}_n^-\|=1$ ) defines a relative error

$$\delta \mathbf{a} = \frac{\|\Delta \mathbf{a}\|}{\|\mathbf{a}\|} = 2 \sin(\gamma_0/2),$$

$$\mathbf{a} = c \mathbf{v}_n, \mathbf{a}^- = c \mathbf{v}_n^-, \Delta \mathbf{a} = \mathbf{a} - \mathbf{a}^-,$$

because triangles with vertices  $\mathbf{v}_n^-, \mathbf{0}, \mathbf{v}_n$  and  $\mathbf{a}_n^-, \mathbf{0}, \mathbf{a}_n$  are isosceles, and their heights are medians and bisectors.

Obviously, we don't know the exact solution. However,  $\gamma_0$  is the angle between the model hyperplane of the *svd*-solution ( $\text{span}\{\mathbf{v}_1, \dots, \mathbf{v}_{n-1}\}$ ) and the hyperplane of the exact solution, as  $\mathbf{v}_n$  and  $\mathbf{v}_n^-$  are their normals. Now assuming that the exact model plane in the basis  $V$  does not extend beyond the boundaries of the rectangle with vertices  $(\pm s_i, \pm s_j)$  we can take the maximum deviation angle  $\gamma = \arctan(s_n/s_{n-1})$ , since all  $s_i$  are ordered. Then, as an estimate of the relative

error of  $\hat{\mathbf{a}}$ , we can take

$$\delta \mathbf{a} = 2 \sin(\arctan(s_n/s_{n-1})/2).$$

If the angle  $\gamma$  is small, such that  $\sin(\gamma) \approx \gamma$ , then

$$\arctan(s_n/s_{n-1}) \approx s_n/s_{n-1},$$

$$\sin(\arctan(s_n/s_{n-1})/2) \approx (s_n/s_{n-1})/2,$$

in the end

$$\hat{\mathbf{a}} \approx s_n/s_{n-1}.$$

In the figure below, in the basis  $V$ , the points represent the realizations of experiment #3 ( $\Delta F \neq 0$ ), while the axis  $\mathbf{v}_1$  is perpendicular to the plane of the figure. Implementations are concentrated near the point  $\mathbf{0}$ .

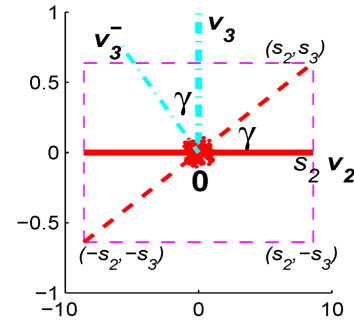


Figure 12. Basis  $V$  Ex#3  $\Delta F \neq 0$ .

The bold line is the current model hyperplane  $\text{span}\{\mathbf{v}_1, \mathbf{v}_2\}$ , within the boundaries of a rectangle with vertices:  $(s_2, s_3)$ ,  $(s_2, -s_3)$ ,  $(-s_2, -s_3)$ ,  $(-s_2, s_3)$ . The dashed line is an exact model hyperplane maximally deflected by an angle  $\gamma$ , passes within the boundaries of the above specified rectangle. Dot and dash lines denote vectors  $\mathbf{v}_3^-$  and  $\mathbf{v}_3$ , which make up the angle  $\gamma$  and an isosceles triangle with vertices:  $\mathbf{v}_3^-, \mathbf{0}, \mathbf{v}_3$ .

### 3.2. Total Least Squares (TLS)

Following [3], but staying in our notation, the Total Least Squares (TLS) problem involves finding a perturbation matrix  $\Delta F$  having minimal Frobenius norm  $\|\Delta F\|_F$  such that  $\text{rank}(F + \Delta F)$  is rank deficient and a vector  $\mathbf{a}$  such that

$$(F + \Delta F) \mathbf{a} = \mathbf{0}.$$

Let

$$F = U S V'.$$

If  $s_1 \geq s_2 \geq \dots \geq s_r > s_{r+1} = s_{r+2} = \dots = s_n > 0$ , then

$$s_n = \min_{\text{rank}(F + \Delta F) < n} \|\Delta F\|_F.$$

Moreover, the minimum is attained by setting  $\Delta F = -F \mathbf{a} \mathbf{a}'$ , where  $\mathbf{a}$  is any unit vector in the  $\text{span}\{\mathbf{v}_{r+1}, \dots, \mathbf{v}_n\}$ .

It follows that if  $s_n/s_{r+1} = 1$ , then we got one hundred percent ambiguity of solutions, and each solution gives a deviation having the same minimum of the Frobenius norm



$\|\Delta F\|_F$ , in other words, no method using this optimality criterion, will be able to choose the right solution.

To simulate measurement noises, values from a normal distribution with mean 0 and standard deviation 0.001 were added to the calculated temperature  $w(\mathbf{x}, \mathbf{t})$ .

In experiment #1

$$s_1=7.1291, s_2=0.1067, s_3=0.0061,$$

at that  $\mathbf{a}=-\mathbf{v}_3/v_{33}$

$$a_1=0.1862, a_2=-0.0139, a_3=-1.$$

And we got a wrong solution, although the ratio  $s_n/s_{r+1}=s_3/s_2=0.0572$  is quite satisfactory, only 5.72% are for ambiguity. However, we know for sure that there must be an ambiguity. But as with the chosen method of calculating derivatives, the noise intensity in the first derivative is much less than in the second one, we cannot expect equality of singular numbers. Practice always makes changes to theoretical results, and this is normal.

In experiment #2

$$s_1=4.2664, s_2=0.6160, s_3=0.0838,$$

then  $s_3/s_2=0.1360$  and only 13.6% are for ambiguity and the solution  $\mathbf{a}=-\mathbf{v}_3/v_{33}$

$$a_1=0.8168, a_2=-0.5682, a_3=-1$$

is satisfactory.

In experiment #3

$$s_1=12.2510, s_2=8.5313, s_3=0.0715,$$

then  $s_3/s_2=0.0084$  or 0.84% are for ambiguity. The experiment is quite convincing, the solution is unambiguous

$$a_1=0.8085, a_2=-0.6125, a_3=-1.$$

### 3.3. Matrix Approximation Theorem (MAT)

Following [4], but staying in our notation and conditions  $m>n$  and  $\text{rank}(F)=n$ , we obtain the following writing of theorem 2.3 (Eckart-Young-Mirsky):

Let the SVD of  $F \in \mathbb{R}^{m \times n}$  be given by

$$F = \sum_{i=1}^n \mathbf{u}_i s_i \mathbf{v}_i' = \sum_{i=1}^n F_i.$$

If  $r < n$  and

$$\hat{F} = F_r = \sum_{i=1}^r \mathbf{u}_i s_i \mathbf{v}_i',$$

then

$$\min_{\text{rank}(D)=r} \|F - D\|_2 = \|F - \hat{F}\|_2 = s_{r+1},$$

and

$$\min_{\text{rank}(D)=r} \|F - D\|_F = \|F - \hat{F}\|_F = \sqrt{\sum_{i=r+1}^n s_i^2}.$$

The theorem says that the best approximation of the matrix  $F$  of rank  $n$  by the matrix  $\hat{F}$  of a given rank  $r < n$  consists in cutting off the last  $n-r$  terms from the sum of the singular value decomposition of the matrix  $F$ . At the same time, the choice of any rank  $r$  leads to an optimal solution.

Now the task is to choose the rank  $r$ , which will also lead us to an unambiguous assessment of parameters. Otherwise, we will consider the performed experiment unconvincing.

To estimate the effective rank, I use the inverse of the condition number  $\text{cond}(F)=s_{\max}/s_{\min}$ . The convenience is that  $\text{cond}(F)$  varies from 1 to  $\infty$ , and  $1/\text{cond}(F)$  – from 0 to 1, what makes it possible to use the familiar concept of percent (%). In this case, the matrix  $F$  will be from 0% to 100% a matrix of full rank.

In experiment #1

$$s_1=7.1291, s_2=0.1067, s_3=0.0061,$$

then  $s_{\min}/s_{\max}=s_3/s_1=0.0008556$  bespeaks that only 0.08% are for the fact that  $F=F_r=F_1+F_2+F_3$  has the rank  $r=3$ . This is good, it means the problem of finding parameters for 99.92% has a solution.

Further  $s_2/s_1=0.0150$  bespeaks that only 1.5% are for the fact that  $F_r=F_1+F_2$  has the rank  $r=2$ . At that  $\|F - F_r\|_2=s_{r+1}=0.0061$ , what indicates an excellent approximation of the matrix  $F$  by the matrix  $F_1+F_2$ . However, the solution  $\mathbf{a}=-\mathbf{v}_3/v_{33}$

$$a_1=0.1928, a_2=0.0052, a_3=-1$$

is unsatisfactory and even contradicts the physical meaning.

Considering both factors, we come to the conclusion that the rank of the matrix  $F$  is closer to  $r=1$  (98.5%), what means the ambiguity of the solution and therefore  $\mathbf{a}=-\mathbf{v}_3/v_{33}$  cannot consistently point to the right solution.

In experiment #2

$$s_1=4.2664, s_2=0.6160, s_3=0.0838,$$

then  $s_3/s_1=0.0196$  and  $s_2/s_1=0.1444$ . In other words 1.96% are for  $r=3$  and that's good, meaning there is a solution. But 14.44% are for  $r=2$ , that is 85.56% are for  $r=1$ , what means ambiguity, although  $s_3/s_2=0.1360$  and only 13.6% are for ambiguity according to TLS. The experiment is inconclusive, but the solution  $\mathbf{a}=-\mathbf{v}_3/v_{33}$ :

$$a_1=0.8168, a_2=-0.5682, a_3=-1$$

turned out to be satisfactory.

In experiment #3

$$s_1=12.2510, s_2=8.5313, s_3=0.0715,$$

then  $s_3/s_1=0.0058$  or 0.58% are for  $r=3$  and  $s_2/s_1=0.6964$  or 69.64% are for  $r=2$ , as well as  $s_3/s_2=0.0084$  or 0.84% are for ambiguity. The experiment is quite convincing, the solution is unambiguous

$$a_1=0.8085, a_2=-0.6125, a_3=-1.$$

Let's increase the noise deviation by 10 times, then in experiment #1 we'll get:

$$s_1=7.0542, s_2=1.6244, s_3=0.0456,$$

then  $s_3/s_1=0.0065$  and  $s_2/s_1=0.2303$ . In other words 0.65% are for  $r=3$  and 23.03% are for  $r=2$ , at that  $s_3/s_2=0.0281$ . The experiment is still controversial.

In experiment #2

$$s_1=4.2930, s_2=1.9915, s_3=0.3830,$$

then  $s_3/s_1=0.0892$  and  $s_2/s_1=0.4639$ . In other words 8.92% are for  $r=3$  and 46.39% are for  $r=2$ , at that  $s_3/s_2=0.1923$  and 19.23% are for ambiguity according to TLS. Still an unconvincing experiment  $\mathbf{a}=-\mathbf{v}_3/v_{33}$ :

$$a_1=1.1385, a_2=-0.0508, a_3=-1$$

does not point to the correct solution.

In experiment #3

$$s_1=12.2853, s_2=8.6178, s_3=0.6473,$$

then  $s_3/s_1=0.0527$  and  $s_2/s_1=0.7015$ . In other words 5.27% are for  $r=3$  and 70.15% are for  $r=2$ , at that  $s_3/s_2=0.0751$  and 7.51% are for ambiguity according to TLS. The experiment is still very convincing and  $\mathbf{a}=-\mathbf{v}_3/v_{33}$ :

$$a_1=0.8106, a_2=-0.5955, a_3=-1$$

points to the correct solution.

It is clearly seen that with a 10-fold increase in noise the third singular numbers  $s_3$ , which in an ideal experiment should be equal to zero, also increased by 10 times or slightly less.

So far, only experiment #3 demonstrates good stable results. Let's increase the noise deviation by another 10 times. I'd like note that for all  $x, t$  the exact values  $|w_t(x, t)| \leq 1$  and  $|w_{xx}(x, t)| \leq 1$  and  $|g(x, t)| \leq 1$ , while the standard noise deviation is already 0.1. Then in experiment #3 we'll get:

$$s_1=17.8796, s_2=11.9318, s_3=4.5130,$$

and  $s_3/s_1=0.2524$ ,  $s_2/s_1=0.6673$ . In other words 25.24% are for  $r=3$  and 66.73% are for  $r=2$ , while  $s_3/s_2=0.3782$  and 37.82% are for ambiguity according to TLS.

25.24% are for  $r=3$ , In other words, all elements of the model are 25.24% linearly independent and the identification problem has no solution at all already at 25.24%. Besides 37.82% are for the ambiguity. The experiment becomes inconclusive. At the same time  $\mathbf{a}=-\mathbf{v}_3/v_{33}$ :

$$a_1=0.8219, a_2=-0.1441, a_3=-1$$

of course, does not point to the correct solution.

As the performed experiments have shown, an increase in the noise intensity leads to an increase in the last singular number and its approach to the penultimate one, what leads to the ambiguity of the solution or to the absence of a solution. An excessively intense noise can ruin even a good experiment.

To explain the discrepancies in the estimates of ambiguity by the two methods given above, let's take, as in the previous subsections, as a solution

$$\mathbf{a} = \sum_{i=r+1}^n b_{i-r} \mathbf{v}_i = \mathbf{V}_{r+} \mathbf{b},$$

$$\mathbf{V}_{r+} = [\mathbf{v}_{r+1} \dots \mathbf{v}_n], \quad \mathbf{b} = [b_1 \dots b_{n-r}]',$$

then

$$\hat{F} \mathbf{a} = 0, \quad F \mathbf{a} = \mathbf{e} = \sum_{i=r+1}^n \mathbf{u}_i s_i \mathbf{v}_i' \mathbf{a} = \mathbf{U}_{r+} \mathbf{S}_{r+} \mathbf{b}.$$

In the TLS subsection we got the solution in the form of  $(F + \Delta F_{tls}) \mathbf{a} = 0$  or  $F \mathbf{a} = -\Delta F_{tls} \mathbf{a}$  or  $F \mathbf{a} = \mathbf{e}_{tls}$ .

It's easy to show that

$$F \mathbf{V}_{r+} = \mathbf{U}_{r+} \mathbf{S}_{r+},$$

here

$$\mathbf{U}_{r+} = [\mathbf{u}_{r+1} \dots \mathbf{u}_n], \quad \mathbf{S}_{r+} = \text{diag}(s_{r+1}, \dots, s_n).$$

Then

$$\mathbf{e}_{tls} = F \mathbf{a} \mathbf{a}' \mathbf{a} = \mathbf{U}_{r+} \mathbf{S}_{r+} \mathbf{b} \mathbf{b}' \mathbf{V}_{r+}' \mathbf{V}_{r+} \mathbf{b} = \mathbf{U}_{r+} \mathbf{S}_{r+} \mathbf{b} = \mathbf{e}$$

at  $\|\mathbf{b}\|=1$ , in other words at  $\|\mathbf{a}\|=1$ , what corresponds to the conditions of the TLS theorem.

However

$$F \mathbf{a} \mathbf{a}' = \mathbf{U}_{r+} \mathbf{S}_{r+} \mathbf{b} \mathbf{b}' \mathbf{V}_{r+}' \neq \mathbf{U}_{r+} \mathbf{S}_{r+} \mathbf{V}_{r+}' = F - \hat{F},$$

in other words,

$$F \mathbf{a} \mathbf{a}' = -\Delta F_{tls} \neq \Delta F_{mat} = F - \hat{F}.$$

Moreover,  $\text{rank}(F + \Delta F) = n-1$ , however it follows from the theorem  $\text{rank}(F - (F - \hat{F})) = \text{rank}(\hat{F}) = r$ . But if the solution  $\mathbf{a} = \mathbf{v}_n$  is unambiguous, that is  $r = n-1$ ,  $s_1 \geq \dots \geq s_n > 0$  and  $s_n/s_{n-1} \ll 1$  and  $s_{n-1}/s_1 \approx 1$ , then

$$-\Delta F_{tls} = F \mathbf{v}_n \mathbf{v}_n' = \mathbf{u}_n s_n \mathbf{v}_n' = F - \hat{F} = \Delta F_{mat}.$$

It is very important that  $\Delta F_{mat}$  may be calculated before calculating the parameters themselves, and therefore used to improve their values.

### 3.4. Anomalous Measurements

It is known that parameter estimates deteriorate significantly in the presence of even single anomalous measurements. It is also clear that  $\Delta F_{mat}$  are measurement and calculation errors, and therefore the analysis of this value is of a certain interest.

Assume that in experiment #3 (standard deviation 0.001) the measurements failed, and one value  $w(1.25, 3)$  increased by 1.5 times. Having calculated the derivatives we need and calculated the singular value decomposition of the matrix of experimental data, we obtain:

$$s_1=12.7798, s_2=10.0656, s_3=2.5892,$$

and  $s_3/s_2=0.2572$ ,  $s_2/s_1=0.7876$ . In other words 25.72% are for  $r=1$  and 78.76% are for  $r=2$ ,

while  $\mathbf{a} = -\mathbf{v}_3/v_{33}$ :

$$a_1=0.8413, a_2=-0.4062, a_3=-1.$$

It can be seen that  $a_1$  has changed a little, but  $a_2$  has changed quite a lot, what is not surprising, because the second derivative suffers more than the first one.

Let's calculate

$$\Delta F_{mat} = \mathbf{u}_3 s_3 \mathbf{v}_3' = [\mathbf{u}_3 s_3 v_{13} \quad \mathbf{u}_3 s_3 v_{23} \quad \mathbf{u}_3 s_3 v_{33}].$$

In the figure below, this matrix is represented graphically, where each column  $\Delta f_i = \mathbf{u}_3 s_3 v_{i3}$  is depicted as a plot of  $\Delta f_i$  against  $j=1 \dots m$ . Next to it is the plot  $s_3 \mathbf{u}_3$  of the third column



of the matrix  $U$  multiplied by the third singular number  $s_3$ . The first thing that catches your eye, the peak values on the plots are the impact of a single measurement failure.

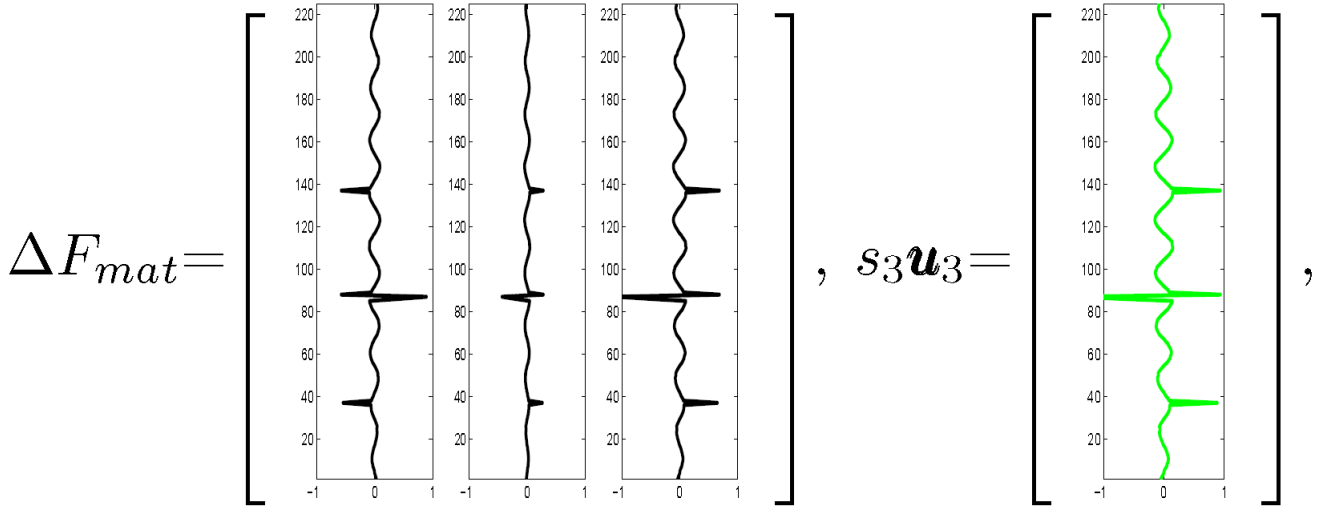


Figure 13.  $\Delta F_{mat}$  and  $s_3 u_3$  in Ex#3.

The location of these peaks on all plots is the same, what corresponds to the formulas  $\Delta f_i = u_3 s_3 v_{i3}$ . On the other hand:  $\Delta f_1$  are errors in calculations of  $w_t(x, y)$ ,  $\Delta f_2$  are errors in  $w_{xx}(x, y)$ , and  $\Delta f_3$  are errors in  $g(x, y)$ . But  $g(x, y)$  is known for sure. We will fix this shortcoming of the TLS method a little later.

What is proposed to correct the situation with anomalous measurements. You just need to remove the corresponding bad realizations from the matrix  $F$ , and specify the numbers of these realizations by the column  $u_3$ . If there are not very many anomalous measurements, this will not greatly affect the number of  $F$  matrix rows, but can seriously improve the definition of parameters.

For example, the cut-off level can be taken  $1/\sqrt{m}$  (or slightly higher), what corresponds to the assumption of uniformity of noise throughout the experiment. In other words, if  $|u_{j3}| > 1/\sqrt{m}$ , then the row  $f_j$  is removed from the matrix  $F$ . As a result of removing only five realizations ( $j=37, 86, 87, 88, 137$ ) in experiment #3 (standard deviation 0.001) with one anomalous measurement, values of singular numbers and parameters close to the previous ones were obtained.

### 3.5. The Best Fitting for a System of Points

In 1901, Karl Pearson [5] solved the problem of the best fitting of a system of points to a plane in the sense of minimizing the sum of squares of the lengths of the perpendiculars from the points to the desired plane, and at the same time he proved the fundamentally important theorem:

*The best-fitting straight line for a system of points in a space of any order goes through the centroid of the system.*

We will not repeat the method of calculating the best fitting plane given in [5], but before calculating the singular value

decomposition of the matrix  $F$ , we will make a parallel transfer of all realizations so that their centroid coincides with the coordinate origin.

Then we get:

$$F_c = \begin{bmatrix} f_1 - f_{cen} \\ \vdots \\ f_m - f_{cen} \end{bmatrix} = \begin{bmatrix} f_1^c \\ \vdots \\ f_m^c \end{bmatrix}, \quad f_{cen} = \sum_{j=1}^m f_j / m,$$

here  $f_j$  –  $j$ -realization ( $j$ th row of the matrix  $F$ ),

$f_{cen}$  – centroid of the matrix  $F$  realizations.

And then, as we did earlier, as a solution, we will take a linear combination of number of columns we need  $v_i^c$  of the matrix  $V_c$  of singular value decomposition of the matrix  $F_c = U_c S_c V_c'$ :

$$a_c = \sum_{i=r+1}^n b_i v_i^c, \quad \hat{F}_c = \sum_{i=1}^r u_i^c s_i^c (v_i^c)' = \begin{bmatrix} \hat{f}_1^c \\ \vdots \\ \hat{f}_m^c \end{bmatrix},$$

$$F = \begin{bmatrix} f_1^c + f_{cen} \\ \vdots \\ f_m^c + f_{cen} \end{bmatrix}, \quad \hat{F} = \begin{bmatrix} \hat{f}_1^c + f_{cen} \\ \vdots \\ \hat{f}_m^c + f_{cen} \end{bmatrix},$$

and for all  $j$

$$\hat{f}_j^c a_c = (\hat{f}_j - f_{cen}) a_c = 0, \quad \hat{f}_j a_c = f_{cen} a_c = const.$$

This method makes it possible to analyze the unambiguity of solutions and thus obtain more accurate results than the method given in the article; it also fully corresponds to

Pearson's results, because it minimizes the Frobenius norm  $\|F_c - \hat{F}_c\|_F$  or, in other words, the square root of the sum of the squares of deviations. And as all  $\mathbf{v}_i^c$  are orthogonal, the deviations are perpendicular to the model plane  $\text{span}\{\hat{F}_c\}$ .

What is the difference between Pearson's results and the previous ones? First of all, he considered the matrix  $F$  as a system of points, and not vectors of the space of parameters/realizations, what made it possible to obtain model planes in the form of linear manifolds and equations of linear structure models of the following form:

$$\sum_{n \in \mathbf{n}} \alpha_n \varphi_n(t) = \text{const.}$$

From the point of view of physics, we have received many new models that also reflect the physical laws of conservation.

However, if the solution is unambiguous, then

$$\mathbf{v}_n = \pm \mathbf{v}_n^c \quad \text{and} \quad \mathbf{f}_{cen} \mathbf{a}_c = 0,$$

because all realizations lie in the same hyperplane and the centroid of realizations also lies in it, what means that it is perpendicular to any unambiguous solution.

These two equalities may be used to check the unambiguity of the solution. However, it must be remembered that in practice these equalities are fulfilled approximately.

Let's see how it looks on the example of our 3 experiments with pseudo noise with standard deviation 0.001.

In experiment #1 the following singular values of matrices  $F$ ,  $F_c$  and their third right singular vectors  $\mathbf{v}_3$ ,  $\mathbf{v}_3^c$  were obtained:

$$\begin{aligned} s_1 &= 7.1291, & s_2 &= 0.1067, & s_3 &= 0.0061; \\ s_1^c &= 0.6137, & s_2^c &= 0.0915, & s_3^c &= 10^{-14}; \end{aligned}$$

$$\mathbf{v}_3 = \begin{bmatrix} -0.1930 \\ -0.0033 \\ 0.9812 \end{bmatrix}, \quad \mathbf{v}_3^c = \begin{bmatrix} 0 \\ -0.0000 \\ 1.0000 \end{bmatrix}.$$

As we expected  $\mathbf{v}_3 \neq \mathbf{v}_3^c$  and the solutions are ambiguous. However,  $s_3^c = 10^{-14}$ , what clearly indicates the unambiguity of the solution of the equation  $F_c \phi \mathbf{v}_3^c = 0$ . At the same time  $\mathbf{f}_{cen} = [1.0000 \ 0.9998 \ 0.2000]$  and  $\mathbf{f}_{cen} \mathbf{v}_3^c = 0.2000$  (this is another sign of the ambiguity of the solution) and the equation looks as follows:

$$0 \cdot w_t(x, t) - 0 \cdot w_{xx}(x, t) + 1 \cdot g(x, t) = 0.2$$

and this is again due to the fact that  $g(x, t)$  is measured accurately, and  $w_t(x, t)w_{xx}(x, t)$  is measured inaccurately. As a result, the points  $\mathbf{f}_c$  are spread out over two coordinates, forming a small piece of the third coordinate plane. You can estimate the size of this piece by calculating the maximum absolute values of the elements (T-norm) of each column of the matrix  $F_c$ :

$$\max_{1 \leq j \leq m} |f_{j1}^c| = 0.0211, \quad \max_{1 \leq j \leq m} |f_{j2}^c| = 0.1217,$$

$$\max_{1 \leq j \leq m} |f_{j3}^c| = 7 \cdot 10^{-16}.$$

Therefore, the vector of the exact solution perpendicular to all realizations has the form  $\mathbf{v}_3^c = [0 \ 0 \ 1]'$ . These estimates look

like singular values of the matrix  $F_c$  only in a different order and smaller in values. Correlating the obtained values with the accuracy of calculating the derivatives, we can admit that the piece approximately is the zero point.

In experiment #2 the following results were obtained:

$$\begin{aligned} s_1 &= 4.2664, & s_2 &= 0.6160, & s_3 &= 0.0838; \\ s_1^c &= 1.4083, & s_2^c &= 0.2190, & s_3^c &= 0.0145; \end{aligned}$$

$$\mathbf{v}_3 = \begin{bmatrix} -0.5976 \\ 0.3778 \\ 0.7072 \end{bmatrix}, \quad \mathbf{v}_3^c = \begin{bmatrix} 0.6275 \\ 0.0075 \\ -0.7785 \end{bmatrix}.$$

The first sign of ambiguity  $\mathbf{v}_3 \neq \pm \mathbf{v}_3^c$ . The second one  $\mathbf{f}_{cen} = [0.4672 \ -0.3325 \ 0.5750]$  and  $\mathbf{f}_{cen} \mathbf{v}_3^c = -0.1570 \neq 0$  also points to ambiguity.

The singular values of the matrix  $F_c$  indicate that most likely the set of realizations is a smeared segment:  $s_3^c/s_1^c = 0.0103$  and  $s_2^c/s_1^c = 0.1555$ . It means that 84.45% are for  $\text{rank}(F_c) = 1$ . It is also possible to calculate the T-norm of matrix  $F_c$  columns, but everything is already clear from the values of singular numbers. The TLS test  $s_3^c/s_2^c = 0.0662$  has not worked.

If we take from the general ambiguous solution the solution  $\mathbf{a}_c = -\mathbf{v}_3^c/v_{33}^c = [0.8060 \ -0.0096 \ -1]$ , then  $\mathbf{f}_{cen} \mathbf{a}_c = -0.2017$ , and we will get one of the possible models:

$$0.8060 w_t(x, t) - 0.0096 w_{xx}(x, t) = g(x, t) - 0.2017.$$

I remind that in experiment  $w_t(x, t) = 1.25 \cdot t$  and  $g(x, t) = 0.2 + t$ .

If we round the model parameters (coefficients) to the tenth shares we'll get:

$$0.8(1.25 \cdot t) = 0.2 + t - 0.2.$$

The model is quite accurate from a mathematical point of view, but is strange from a physical point of view. And this is always the case when the experiment does not give an unambiguous mathematical answer.

In experiment #3 the following results were obtained:

$$\begin{aligned} s_1 &= 12.2510, & s_2 &= 8.5313, & s_3 &= 0.0715; \\ s_1^c &= 12.2529, & s_2^c &= 8.5326, & s_3^c &= 0.0655; \end{aligned}$$

$$\mathbf{v}_3 = \begin{bmatrix} -0.5676 \\ 0.4298 \\ 0.7022 \end{bmatrix}, \quad \mathbf{v}_3^c = \begin{bmatrix} -0.5676 \\ 0.4298 \\ 0.7022 \end{bmatrix}.$$

and  $\mathbf{f}_{cen} \mathbf{v}_3^c = 0.000073637$ , both signs of unambiguity are satisfied. A good experiment, it is by all signs a good one.

### 3.6. Mixed LS & TLS

A big disadvantage of the above described methods for obtaining a general solution is the distortion of exactly known model elements in the resulting approximation of the initial data. This unpleasant moment is absent in the classical least squares method, which we will use now.

Following the strategy of mixed least squares and total least squares method (mixed LS & TLS) [4] let's write the equation of the model as:

$$\bar{F}\mathbf{b} + \tilde{F}\mathbf{a} = \mathbf{0} \quad \text{§Ü§Ý§Ü} \quad \left[ \begin{array}{c|c} \bar{F} & \tilde{F} \end{array} \right] \begin{bmatrix} \mathbf{b} \\ -\mathbf{a} \end{bmatrix} = \mathbf{0}$$

here in  $\bar{F}$  all columns known with certainty are collected, and in  $\tilde{F}$  – those that are not known with certainty.

In experiments  $g(x, t)$  is known with certainty, and  $w(x, t)$  is measured inaccurately, then:

$$\bar{F} = \begin{bmatrix} g(x_0, t_0) \\ \vdots \\ g(x_f, t_f) \end{bmatrix}, \quad \tilde{F} = \begin{bmatrix} w_t(x_0, t_0) & w_{xx}(x_0, t_0) \\ \vdots & \vdots \\ w_t(x_f, t_f) & w_{xx}(x_f, t_f) \end{bmatrix},$$

$$\mathbf{b} = [a_3], \quad \mathbf{a} = [a_1 \ a_2]'$$

QR decomposition of the matrix  $\bar{F}$ , if the number of rows exceeds the number of columns, will look as follows:  $\bar{F} = Q \begin{bmatrix} T \\ O \end{bmatrix}$ , here  $Q$  is orthogonal,  $T$  is nonsingular square upper triangular and  $O$  - null matrices.

Having multiplied the equation of the model by  $Q'$  we get

$$Q' \left[ \begin{array}{c|c} \bar{F} & \tilde{F} \end{array} \right] \begin{bmatrix} \mathbf{b} \\ -\mathbf{a} \end{bmatrix} = Q' \mathbf{0} \quad \text{§Ü§Ý§Ü} \quad \begin{bmatrix} T & P_1 \\ O & P_2 \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ -\mathbf{a} \end{bmatrix} = \mathbf{0},$$

here  $Q'\tilde{F} = [P_1 | P_2]'$ ,  $P_1$  are projections of inaccurate LSModel elements (columns of matrix  $\tilde{F}$ ) onto the linear shell of columns of matrix  $\bar{F}$ , and  $P_2$  are perpendiculars to this linear shell.

And so we've got two equations

$$P_2 \mathbf{a} = \mathbf{0} \quad \text{and} \quad T \mathbf{b} + P_1 \mathbf{a} = \mathbf{0}.$$

For the first one, we will search for an unambiguous solution using the previously described methods and substitute the necessary particular solution  $\hat{\mathbf{a}}$  into the second equation, which has the following solution  $\hat{\mathbf{b}} = -T^{-1} P_1 \hat{\mathbf{a}}$ .

Let's use the obtained approximation  $\hat{P}_2$  to obtain the approximation  $\hat{F}$ :

$$\hat{F} = Q \begin{bmatrix} T & P_1 \\ O & \hat{P}_2 \end{bmatrix} = \left[ \begin{array}{c|c} \bar{F} & Q \begin{bmatrix} P_1 \\ \hat{P}_2 \end{bmatrix} \end{array} \right].$$

Now the exact initial data  $\bar{F}$  are not distorted in the resulting approximation  $\hat{F}$ .

As examples, let's turn to our three experiments with a standard deviation of noise equal to 0.01. Only this time I combined the realizations of the first and second ones into one matrix  $F$ . First of all, I want to show that it's possible not only to delete but also add realizations, provided that the experiments were carried out on the same object of our research. Secondly, that two dubious experiments, being combined, can produce a very decent result.

In the figures, the symbol \* denotes the rows  $\mathbf{p}_j^2 = [p_1 \ p_2]$  of the corresponding matrices  $P_2$ , as points in the space of parameters/realizations. In the combined experiment #(1+2)

the points related to the first experiment are additionally circled.

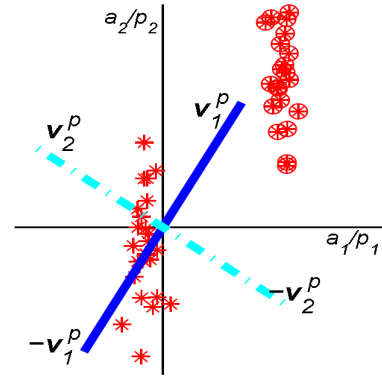


Figure 14. Mixed LS&TLS. SPR in Ex#(1+2).

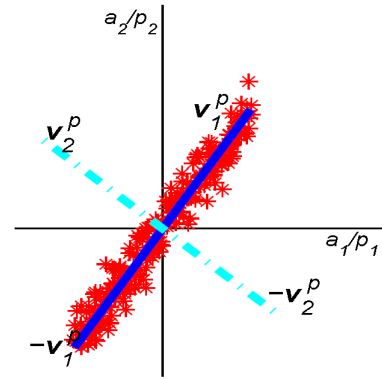


Figure 15. Mixed LS&TLS. SPR in Ex#3.

After the matrix  $P_2$  was calculated, its singular value decomposition was obtained  $P_2 = U_p S_p V_p'$ .

In the combined experiment #(1+2) singular numbers and their ratio

$$s_1^p = 7.1240, \quad s_2^p = 1.5210, \quad s_2^p / s_1^p = 0.2135$$

indicate that 79% are for unambiguity and the second column  $\mathbf{v}_2^p = [-0.8459 \ 0.5333]'$  of the matrix  $V_p$  can be taken as the basis of the solution.

In the figure, the dot and dash line shows vectors  $\mathbf{v}_2^p$  and  $-\mathbf{v}_2^p$  as a general solution and the solid line – vectors  $\mathbf{v}_1^p$  and  $-\mathbf{v}_1^p$  as a model hyperplane.

Before calculating  $\mathbf{b}$ , pay attention to the matrix  $T$ , it must be nonsingular.

In this combined experiment #(1+2)  $T = 3.1697$ . The matrix is good, you can calculate  $\mathbf{b}$ .

$$\mathbf{b} = -T^{-1} P_1 \mathbf{v}_2^p = 1.1019.$$

And so

$$a_1 = -0.8459, \quad a_2 = 0.5333, \quad b = 1.1019,$$

but we need  $b = -1$ , then

$$a_1 = 0.7677, \quad a_2 = -0.4840, \quad b = -1.0000.$$

In experiment #3:

$$s_1^p=8.6034, \quad s_2^p=0.9067, \quad s_2^p/s_1^p=0.1054,$$

$$\mathbf{v}_2^p = [-0.8029, 0.5961]',$$

$$T=8.7239, \quad b=0.9852,$$

finally

$$a_1=0.8150, \quad a_2=-0.6051, \quad b=-1.0000.$$

## 4. Objective Functional

Use of a generalized residual indicator, which is then minimized (maximized) under various constraints, is typical for optimization setting of object identification problem.

Often the following objective functional

$$\left( \sum_{m \in \mathbf{m}} |\varepsilon_m|^q \right)^{1/q}, \quad q \geq 1$$

is taken as the indicator. MATLAB makes it possible to calculate such norms using the m-function `norm` (see Appendix line 184).

And the minimum of this objective functional in the set of model parameters is considered as the quality criterion of the taken decision:

$$\min_{\mathbf{a}} \left( \sum_{m \in \mathbf{m}} |\varepsilon_m|^q \right)^{1/q}.$$

Previously, we considered methods for solving identification problems for objective functionals minimizing the Frobenius norm and spectral or 2-norm. Next, a method is proposed for a simple enumeration of all parameters, which allows you to search for solutions for any objective functionals.

LSModel with parameters on a sphere makes it possible to calculate the values of the target functional for all parameters, because the set of parameters on a sphere is compact.

To do this, you have to be able to quickly calculate a certain set of points on a sphere of any dimension  $N$ . The essence of the calculation is that in an  $(N-1)$ -dimensional unit ball or some area of it, a uniform, absolutely accurate binary grid is taken, each point of which is the first  $(N-1)$  coordinates of a point of the sphere. The last  $N$ th coordinate is calculated using the formula:

$$a_N = \sqrt{1 - \sum_{n=1}^{N-1} a_n^2}.$$

Thus we get a point

$$\mathbf{a} = \{a_1, a_2, \dots, a_N\},$$

on the sphere,

only one latest coordinate of this point is calculated with an error.

This digitization produces exactly a hemisphere, and then unambiguous solutions will have one point on the hemisphere with the minimum value of the residual norm.

But it is also possible to consider the full sphere of parameters, then we should consider the points with

$$a_N = -\sqrt{1 - \sum_{n=1}^{N-1} a_n^2},$$

and then unambiguous solutions will have two points on the sphere.

$T$ -norm of the residual was calculated for our 3 experiments with measurements with standard deviation 0.001

$$\|\mathbf{e}\|_{\infty} = \max_{1 \leq m \leq M} |e_m|,$$

here  $\mathbf{e} = F\mathbf{a}$ ,  $\|\mathbf{a}\|=1$ ,  $\mathbf{e} = [e_1 \dots e_M]'$ .

Below are given graphs of  $\|\mathbf{e}\|_{\infty}$  depending on the number of the point on the hemisphere of parameters for our three experiments.

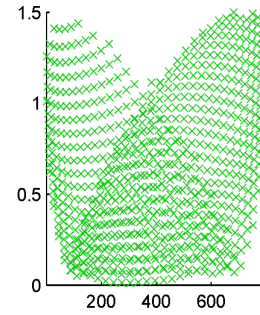


Figure 16. Ex#1.

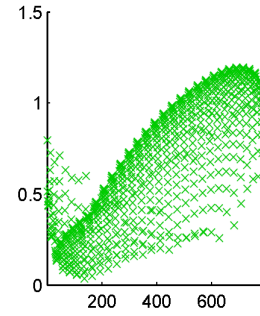


Figure 17. Ex#2.

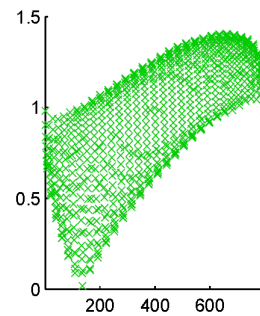


Figure 18. Ex#3.

It is clearly seen that in experiment #1, the unambiguous minimum of the norm is not obvious, although the computer will certainly find the minimum from approximately equal ones. As we know, such ambiguity leads to instability in the calculation of the minimum.

Experiment #3 demonstrates the existence of an explicit unambiguous minimum.

Experiment #2 occupies an intermediate position, because the minimum it is not clearly seen.

Pay attention to how anomalous measurements affect the target functional of the criterion:

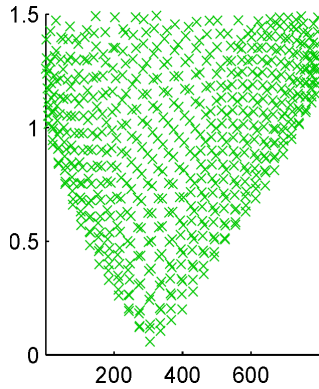


Figure 19. Anomalous measurements. Ex#1.

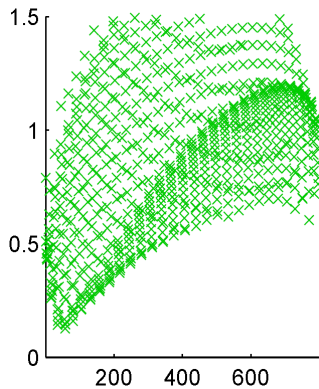


Figure 20. Anomalous measurements. Ex#2.

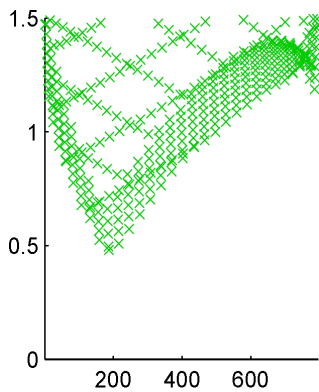


Figure 21. Anomalous measurements. Ex#3.

and how the minimums of the target functionality have

sharpened, but they point to false targets.

See the appendix for details of calculations. The method of pass around points on the parameter sphere, proposed therein, allows us to obtain a completely understandable image of both the multidimensional parameter sphere itself and the target functionals of criteria based on it.

It is important that such graphs may be drawn at any dimension of the space of parameters. And also the parameters themselves may be calculated with given accuracy, gradually reducing the digitization area of the sphere of parameters and as well as the digitization step in this area, close to the minimum [1].

## 5. Identifiability and Guaranteeing Identification Experiment

Earlier it has been convincingly demonstrated that a properly conducted experiment is of paramount importance for qualitative identification. It is equally important to construct the model formula correctly, from physical as well as from mathematical points of view. Further we will consider the mathematical side of the matter.

Following [1,2], let's write the formula for LSModels as a sum of two structural parts:

$$\mathfrak{S}_\alpha(\varphi) + \mathfrak{S}_\beta(\psi) = 0, \quad (0)$$

where  $\mathfrak{S}_\alpha(\varphi)$  is a structural element of the LSModel,

applied to atom  $\varphi$  with parameters  $\alpha$ ;

$\mathfrak{S}_\beta(\psi)$  is another structure over guarantor  $\psi$ ;

$\alpha, \beta$  are two parts of model parameters.

Let's write the general solution (GS) of the identification problem (IP) according to the experimental data  $\{f, g\}$  as a sum of a certain particular solution  $\{\alpha, \beta\}$  and its variations  $\{\Delta\alpha, \Delta\beta\}$ .

Owing to the linear structure of the LSModels we can write two structural equations of the IP

$$\mathfrak{S}_\alpha(f) + \mathfrak{S}_\beta(g) = 0, \quad (1)$$

$$\mathfrak{S}_{\Delta\alpha}(f) + \mathfrak{S}_{\Delta\beta}(g) = 0. \quad (2)$$

Our problem now consists in making  $\Delta\alpha = \Delta\beta = 0$  in any solution according to the guaranteeing experiment  $\{f, g\}$ , or in other words, in discovering of a subclass, i.e. restrictions on parameters of each model in a class, and the conditions on guarantors, so that the identification problem had the unique solution  $\{\alpha, \beta\}$ .

Having applied the structure  $\mathfrak{S}_{\Delta\alpha}$  to the equation of IP (1) and the structure  $\mathfrak{S}_\alpha$  to the equation of IP (2) we get:

$$\mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\alpha(f) + \mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\beta(g) = 0, \quad (3)$$

$$\mathfrak{S}_\alpha\mathfrak{S}_{\Delta\alpha}(f) + \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\beta}(g) = 0. \quad (4)$$

Let's subtract one expression from the other and require that

the structures  $\mathfrak{S}_\alpha$  and  $\mathfrak{S}_{\Delta\alpha}$  are commutative, in other words, that  $\mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\alpha = \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\alpha}$ , then we see that

$$\mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\beta(\mathbf{g}) - \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\beta}(\mathbf{g}) = 0. \quad (5)$$

This expression is the LSModel for guarantors:

$$\mathfrak{U}_\gamma(\mathbf{g}) = 0 \quad (6)$$

where  $\mathfrak{U}_\gamma = \mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\beta - \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\beta}$ .

This structural relation defines the relation of recalculation of parameters  $\gamma$  to parameters  $[\Delta\alpha \ \Delta\beta]^T$  through a matrix  $\mathfrak{J}(\alpha, \beta)$  composed of parameters  $\alpha, \beta$ :

$$\gamma = \mathfrak{J}(\alpha, \beta) \cdot \begin{bmatrix} \Delta\alpha \\ \Delta\beta \end{bmatrix}. \quad (7)$$

Having required nondegeneracy of the recalculation relation matrix  $\mathfrak{J}(\alpha, \beta)$  for all LSModels in the subclass and the unique null solution  $\gamma=0$  of identification problem via the LSModel of guarantors according to the planned experiment, we get  $\Delta\alpha=0, \Delta\beta=0$  in the GSIIP according to this experiment. Earlier, these experiments were called the guaranteeing identification experiments (*GIEperiments*).

### 5.1. Example

Let's consider the following LSModels

$$\alpha_1 w_t(\mathbf{x}, \mathbf{t}) + \alpha_2 w_{xx}(\mathbf{x}, \mathbf{t}) + \beta g(\mathbf{x}, \mathbf{t}) = 0.$$

Let's choose  $g(\mathbf{x}, \mathbf{t})$  as a guarantor, then

$$\mathfrak{S}_\alpha(\ ) = \alpha_1(\ )_t + \alpha_2(\ )_{xx},$$

$$\mathfrak{S}_{\Delta\alpha}(\ ) = \Delta\alpha_1(\ )_t + \Delta\alpha_2(\ )_{xx},$$

$$\mathfrak{S}_\beta(\mathbf{g}) = \beta g(\mathbf{x}, \mathbf{t}), \quad \mathfrak{S}_{\Delta\beta}(\mathbf{g}) = \Delta\beta g(\mathbf{x}, \mathbf{t}).$$

Let's make sure that  $\mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\alpha(\mathbf{w}) = \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\alpha}(\mathbf{w})$ .

$$\begin{aligned} \mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\alpha(\mathbf{w}) &= \Delta\alpha_1(\alpha_1(\mathbf{w})_t + \alpha_2(\mathbf{w})_{xx})_t \dots \\ &\quad + \Delta\alpha_2(\alpha_1(\mathbf{w})_t + \alpha_2(\mathbf{w})_{xx})_{xx} \\ &= \Delta\alpha_1 \alpha_1 \mathbf{w}_{tt} + \Delta\alpha_1 \alpha_2 \mathbf{w}_{xxt} \dots \\ &\quad + \Delta\alpha_2 \alpha_1 \mathbf{w}_{txx} + \Delta\alpha_2 \alpha_2 \mathbf{w}_{xxxx}, \\ \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\alpha}(\mathbf{w}) &= \alpha_1(\Delta\alpha_1(\mathbf{w})_t + \Delta\alpha_2(\mathbf{w})_{xx})_t \dots \\ &\quad + \alpha_2(\Delta\alpha_1(\mathbf{w})_t + \Delta\alpha_2(\mathbf{w})_{xx})_{xx} \\ &= \alpha_1 \Delta\alpha_1 \mathbf{w}_{tt} + \alpha_1 \Delta\alpha_2 \mathbf{w}_{xxt} \dots \\ &\quad + \alpha_2 \Delta\alpha_1 \mathbf{w}_{txx} + \alpha_2 \Delta\alpha_2 \mathbf{w}_{xxxx}, \end{aligned}$$

and taking into account that  $\mathbf{w}_{xxt} = \mathbf{w}_{txx}$ , we get an equality.

The LSModels of guarantors (6) will be as follows:

$$\begin{aligned} 0 &= \mathfrak{U}_\gamma(\mathbf{g}) = \mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\beta(\mathbf{g}) - \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\beta}(\mathbf{g}) \dots \\ &= \Delta\alpha_1(\beta g(\mathbf{x}, \mathbf{t}))_t + \Delta\alpha_2(\beta g(\mathbf{x}, \mathbf{t}))_{xx} \dots \\ &\quad - \alpha_1(\Delta\beta g(\mathbf{x}, \mathbf{t}))_t + \alpha_2(\Delta\beta g(\mathbf{x}, \mathbf{t}))_{xx} \\ &= (\Delta\alpha_1\beta - \alpha_1\Delta\beta) g_t(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_2\beta - \alpha_2\Delta\beta) g_{xx}(\mathbf{x}, \mathbf{t}) \\ &= \gamma_1 g_t(\mathbf{x}, \mathbf{t}) + \gamma_2 g_{xx}(\mathbf{x}, \mathbf{t}), \end{aligned}$$

where the relations of the recalculation of parameters (7) are

$$\begin{aligned} \gamma_1 &= \Delta\alpha_1\beta - \alpha_1\Delta\beta, \\ \gamma_2 &= \Delta\alpha_2\beta - \alpha_2\Delta\beta. \end{aligned}$$

In the matrix notation the last expressions of recalculation

of parameters are:

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} \beta & 0 & -\alpha_1 \\ 0 & \beta & -\alpha_2 \end{bmatrix} \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \\ \Delta\beta \end{bmatrix}.$$

Now it is necessary to ensure a trivial solution for the Identification Problem via the LSModel of guarantors  $\gamma=0$  according to the guaranteeing experiment  $\mathbf{f}, \mathbf{g}$ . For this purpose all elements of the heat equation of IP via the LSModels of guarantors  $\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\}$  should be linearly independent.

Then the inverse recalculation will give  $\Delta\alpha_1 = \Delta\alpha_2 = \Delta\beta = 0$  at the transformation of nonsingular matrix  $\mathfrak{J}$ .

Let the subclass of LSModels, for which the matrix  $\mathfrak{J}$  has a completed rank, be called *Linear Identifiable Structure Models* or *LISModels*. Let the matrix  $\mathfrak{J}$  be called the *Structural Identifiability Matrix* as a characteristic of identifiable structures of the LSModels.

We have already noted that in order to properly understand the heat equation, it is necessary that  $\beta = -1$ .

*Attention, a variation of the fixed parameter is equal to zero!*

In other words  $\Delta\beta=0$ , then

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} -1 & 0 & -\alpha_1 \\ 0 & -1 & -\alpha_2 \end{bmatrix} \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \end{bmatrix}$$

and regardless of the value of the parameters, we got a LISModel.

Let the LISModels, whose structural identifiability matrix does not depend on unknown parameters, be called *canonical LISModels* and let the structure of such models be called *Canonical Identifiable Structure*.

And so we've learned to write the heat equation in a canonical identifiable form:

$$\alpha_1 w_t(\mathbf{x}, \mathbf{t}) + \alpha_2 w_{xx}(\mathbf{x}, \mathbf{t}) = g(\mathbf{x}, \mathbf{t}).$$

Now let's turn to the guarantors and see if  $g(\mathbf{x}, \mathbf{t})$  have been correctly selected in the three experiments described in the first part of the article.

In the first experiment  $g(\mathbf{x}, \mathbf{t}) = 0.2$  and

$\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\} = \{0(\mathbf{x}, \mathbf{t}), 0(\mathbf{x}, \mathbf{t})\}$  are linearly dependent, and we have not got an unambiguous solution.

In the second experiment  $g(\mathbf{x}, \mathbf{t}) = 0.2 + t$  and

$\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\} = \{1(\mathbf{x}, \mathbf{t}), 0(\mathbf{x}, \mathbf{t})\}$  also are linearly dependent, but we've got an unambiguous solution. Why? We were lucky with the object behavior! In this case, for  $g(\mathbf{x}, \mathbf{t}) = 0.2 + t$  there are other behaviors, for example,  $w(\mathbf{x}, \mathbf{t}) = 0.25t + 0.625t^2$  and then  $w_{xx}(\mathbf{x}, \mathbf{t}) = 0$  and  $a_2$  can be anything. In other words, in this case, unambiguous identification is not guaranteed to us, maybe we will be lucky, or maybe we will not.

In the third experiment  $g = \sin(\mathbf{x}) \sin(\mathbf{t})$  and

$\{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\} = \{\sin(\mathbf{x}) \cos(\mathbf{t}), -\sin(\mathbf{x}) \sin(\mathbf{t})\}$  are linearly independent, and now, in any case, we are guaranteed to get an unambiguous solution.



## 5.2. Example of a Nonlinear LSModel

The presence of nonlinear elements in the model and their inclusion in the structures  $\mathfrak{S}_\alpha$ ,  $\mathfrak{S}_{\Delta\alpha}$  most often leads to the noncommutativity of these structures. The exception is, for example, the element of delay. Therefore, I recommend to include nonlinear elements in the structures of guarantors  $\mathfrak{S}_\beta$ ,  $\mathfrak{S}_{\Delta\beta}$ , whose commutativity is not required.

Let's consider the following nonlinear LSModel  $\alpha_1 w_t(\mathbf{x}, \mathbf{t}) + \alpha_2 w_{xx}(\mathbf{x}, \mathbf{t}) + \alpha_3 w(\mathbf{x}, \mathbf{t}) + \beta_1 (w_x(\mathbf{x}, \mathbf{t}))^2 + \beta_2 g(\mathbf{x}, \mathbf{t}) = 0$ .

Let's choose  $w_x^2(\mathbf{x}, \mathbf{t})$  and  $g(\mathbf{x}, \mathbf{t})$  as guarantors, then

$$\begin{aligned}\mathfrak{S}_\alpha(\cdot) &= \alpha_1(\cdot)_t + \alpha_2(\cdot)_{xx} + \alpha_3(\cdot) \\ \mathfrak{S}_{\Delta\alpha}(\cdot) &= \Delta\alpha_1(\cdot)_t + \Delta\alpha_2(\cdot)_{xx} + \Delta\alpha_3(\cdot) \\ \mathfrak{S}_\beta(g) &= (\beta_1 w_x^2 + \beta_2 g), \\ \mathfrak{S}_{\Delta\beta}(g) &= (\Delta\beta_1 w_x^2 + \Delta\beta_2 g).\end{aligned}$$

The LSModels of guarantors (6) will be as follows:

$$\begin{aligned}0 &= \mathfrak{L}_\gamma(g) = \mathfrak{S}_{\Delta\alpha}\mathfrak{S}_\beta(g) - \mathfrak{S}_\alpha\mathfrak{S}_{\Delta\beta}(g) \dots \\ &= \Delta\alpha_1(\beta_1 w_x^2 + \beta_2 g)_t + \Delta\alpha_2(\beta_1 w_x^2 + \beta_2 g)_{xx} \dots \\ &\quad + \Delta\alpha_3(\beta_1 w_x^2 + \beta_2 g) - \alpha_1(\Delta\beta_1 w_x^2 + \Delta\beta_2 g)_t \dots \\ &\quad - \alpha_2(\Delta\beta_1 w_x^2 + \Delta\beta_2 g)_{xx} - \alpha_3(\Delta\beta_1 w_x^2 + \Delta\beta_2 g) \dots \\ &= (\Delta\alpha_1\beta_1 - \alpha_1\Delta\beta_1)(w_x^2)_t(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_2\beta_1 - \alpha_2\Delta\beta_1)(w_x^2)_{xx}(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_3\beta_1 - \alpha_3\Delta\beta_1)w_x^2(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_1\beta_2 - \alpha_1\Delta\beta_2)g_t(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_2\beta_2 - \alpha_2\Delta\beta_2)g_{xx}(\mathbf{x}, \mathbf{t}) \dots \\ &\quad + (\Delta\alpha_3\beta_2 - \alpha_3\Delta\beta_2)g(\mathbf{x}, \mathbf{t}) \dots \\ &= \gamma_1(w_x^2)_t(\mathbf{x}, \mathbf{t}) + \gamma_2(w_x^2)_{xx}(\mathbf{x}, \mathbf{t}) + \gamma_3 w_x^2(\mathbf{x}, \mathbf{t}), \\ &\quad + \gamma_4 g_t(\mathbf{x}, \mathbf{t}) + \gamma_5 g_{xx}(\mathbf{x}, \mathbf{t}) + \gamma_6 g(\mathbf{x}, \mathbf{t}).\end{aligned}$$

In the matrix notation the last expression of recalculation of parameters is:

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \\ \gamma_5 \\ \gamma_6 \end{bmatrix} = \begin{bmatrix} \beta_1 & 0 & 0 & -\alpha_1 & 0 \\ 0 & \beta_1 & 0 & -\alpha_2 & 0 \\ 0 & 0 & \beta_1 & -\alpha_3 & 0 \\ \beta_2 & 0 & 0 & 0 & -\alpha_1 \\ 0 & \beta_2 & 0 & 0 & -\alpha_2 \\ 0 & 0 & \beta_2 & 0 & -\alpha_3 \end{bmatrix} \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \\ \Delta\alpha_3 \\ \Delta\beta_1 \\ \Delta\beta_2 \end{bmatrix},$$

at  $\beta_2 = -1$

$$\begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \gamma_3 \\ \gamma_4 \\ \gamma_5 \\ \gamma_6 \end{bmatrix} = \begin{bmatrix} \beta_1 & 0 & 0 & -\alpha_1 \\ 0 & \beta_1 & 0 & -\alpha_2 \\ 0 & 0 & \beta_1 & -\alpha_3 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} \Delta\alpha_1 \\ \Delta\alpha_2 \\ \Delta\alpha_3 \\ \Delta\beta_1 \end{bmatrix}.$$

It's evident that the structural identifiability matrix has a full rank at  $\alpha_1 \neq 0$  or  $\alpha_2 \neq 0$  or  $\alpha_3 \neq 0$  while  $\beta_1$  can be equal to zero and all the same this model will be a LISModel. We have not got a canonical form, but we have got three conditions and it

is enough to fulfill one of them.

Now the parameter recalculation relation is as follows:  $\gamma_1 = \beta_1 \Delta\alpha_1 - \alpha_1 \Delta\beta_1$ ,  $\gamma_2 = \beta_1 \Delta\alpha_2 - \alpha_2 \Delta\beta_1$ ,  $\gamma_3 = \beta_1 \Delta\alpha_3 - \alpha_3 \Delta\beta_1$ ,  $\gamma_4 = -\Delta\alpha_1$ ,  $\gamma_5 = -\Delta\alpha_2$ ,  $\gamma_6 = -\Delta\alpha_3$ .

It is clear that  $\gamma_4 = \gamma_5 = \gamma_6 = 0$  guarantees that  $\Delta\alpha_1 = \Delta\alpha_2 = \Delta\alpha_3 = 0$ . In order for  $\Delta\beta_1 = 0$ , it is enough that either  $\gamma_1 = 0$ , or  $\gamma_2 = 0$ , or  $\gamma_3 = 0$ . Often in physical experiments  $g(\mathbf{x}, \mathbf{t}) = g(\mathbf{x}) + g(\mathbf{t})$  and as a consequence  $w(\mathbf{x}, \mathbf{t}) = w(\mathbf{x}) + w(\mathbf{t})$ , and then  $(w_x^2)_t(\mathbf{x}, \mathbf{t}) = 0$  and  $\gamma_1$  in the model of guarantors may be anything. But the linear independence of  $w_x^2(\mathbf{x}, \mathbf{t})$ ,  $g(\mathbf{x}, \mathbf{t})$ ,  $g_t(\mathbf{x}, \mathbf{t})$ ,  $g_{xx}(\mathbf{x}, \mathbf{t})$  is easier to ensure. Then  $\gamma_3 = 0$  and  $\Delta\beta_1 = 0$ .

This bespeaks that the nonlinearity in the model gives more options for choosing guarantors than for the linear model.

Now that we have learned how to choose LISModels and guarantors for experiments, let's return to calculating parameters in conditions of inaccurate measurements.

## 6. Projection onto the Hyperplane of Guarantors

From algebra it is known that the projection of the sum of vectors onto any subspace is equal to the sum of projections of vectors onto this subspace  $\mathbf{pr}(\mathbf{f}_1 + \mathbf{f}_2) = \mathbf{pr}(\mathbf{f}_1) + \mathbf{pr}(\mathbf{f}_2)$ , and also the projection of a vector multiplied by a number is equal to this number multiplied by the projection of the vector  $\mathbf{pr}(a \cdot \mathbf{f}) = a \cdot \mathbf{pr}(\mathbf{f})$ .

Finally a projection of a linear combination onto a subspace is equal to a linear combination of projections with the same coefficients.

Following [1,6] let's take a linear span of the set of guarantors  $\text{span}(\mathbf{G})$  as a subspace, then the identification problem in m-dimensional space  $\mathbb{A}^m$

$$\sum_{n \in \mathbf{n}} a_n \cdot \mathbf{f}_n = 0, \quad \mathbf{f}_n \in \mathbb{A}^m$$

may be replaced with the identification problem in  $(n-1)$ -dimensional space  $\text{span}(\mathbf{G}) = \mathbb{A}^{(n-1)}$

$$\sum_{n \in \mathbf{n}} a_n \cdot \mathbf{pr}(\mathbf{f}_n) = 0, \quad \mathbf{pr}(\mathbf{f}_n) \in \mathbb{A}^{(n-1)}.$$

If the guarantors are also chosen so that the noises in the measurements are perpendicular to the subspace of guarantors  $\text{span}(\mathbf{G})$ , then very good identification results can be achieved. This additional requirement further complicates the search for guarantors and requires some knowledge about noises in measurements.

For experiments in which the supposed guarantors are not expressed by mathematical formulas (of course, such experiments most often happen in practice) is very important to check them for linear independence.

In our three experiments from the first part of the article, the set of guarantors

$$\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\}$$

may be calculated by formulas of central difference derivatives having measurements  $g(\mathbf{x}, \mathbf{t})$ . And the check for linear independence may be carried out with the help of singular value decomposition as well as with the help of QR-decomposition.

With the help of QR-decomposition, it is also easy to calculate the needed projections of LSModel elements onto the linear span of the guarantors.

Let  $G = [\mathbf{g}_1 \dots \mathbf{g}_{n-1}]$  is  $(m \times n-1)$ -matrix whose columns are measured or calculated guarantors. For  $m > n-1$  its QR-decomposition will have the form:  $G = Q_g \begin{bmatrix} T_g \\ - \\ O \end{bmatrix}$ , here  $Q_g$  is orthogonal,  $T_g$  is nonsingular square upper triangular and  $O$  is null matrices.

The orthogonal matrix  $Q_g$  can be considered as a new orthonormal basis. The transition to this basis is carried out by multiplying any vector  $\mathbf{f}_i$  on the right by the transposed matrix  $Q'_g$ .

From QR-decomposition it follows that

$$Q'_g G = \begin{bmatrix} T_g \\ - \\ O \end{bmatrix}$$

or

$$\begin{aligned} Q'_g \mathbf{g}_1 &= [t_{11}^g & 0 & \dots & 0 & | & 0 \dots 0]', \\ Q'_g \mathbf{g}_2 &= [t_{12}^g & t_{22}^g & \dots & 0 & | & 0 \dots 0]', \\ &\vdots \\ Q'_g \mathbf{g}_{n-1} &= [t_{1,n-1}^g & t_{2,n-1}^g & \dots & t_{n-1,n-1}^g & | & 0 \dots 0]', \end{aligned}$$

or in other words, the coordinates, starting from the number  $n$ , of all vectors  $\mathbf{g}_i$  in the new basis are zero. This means that the subspace consisting of  $n-1$  coordinate is a linear span of guarantors.

Thus, the first  $n-1$  coordinates of any vector in the new basis  $Q'_g \mathbf{f}_i$  are a projection onto  $\text{span}(\mathbf{G})$  and the other coordinates are a perpendicular.

Let's turn to our three experiments again. Let's calculate the matrix of guarantors  $G = [\mathbf{g}_t \mathbf{g}_{xx}]$  and its QR-decomposition in every experiment.

In experiment #1 matrix  $T_g = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$  and therefore  $\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\}$  are not guarantors.

In experiment #2 matrix  $T_g = \begin{bmatrix} 5 & 0 \\ 0 & 0 \end{bmatrix}$  and again  $\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\}$  are not guarantors.

In experiment #3 matrix

$$T_g = \begin{bmatrix} 8.5882 & 0.0099 \\ 0 & 8.5436 \end{bmatrix}$$

and  $\mathbf{G}(g(\mathbf{x}, \mathbf{t})) = \{g_t(\mathbf{x}, \mathbf{t}), g_{xx}(\mathbf{x}, \mathbf{t})\}$  are almost orthogonal

guarantors with a good length and we continue.

Let's calculate the projections of LSModel elements:

$$\begin{aligned} \mathbf{pr}(w_t(\mathbf{x}, \mathbf{t})) &= Q'_g w_t(\mathbf{x}, \mathbf{t})|_{1:2} = [4.9971 & -6.8849]', \\ \mathbf{pr}(w_{xx}(\mathbf{x}, \mathbf{t})) &= Q'_g w_{xx}(\mathbf{x}, \mathbf{t})|_{1:2} = [7.0822 & 5.5698]', \\ \mathbf{pr}(g(\mathbf{x}, \mathbf{t})) &= Q'_g g(\mathbf{x}, \mathbf{t})|_{1:2} = [0.0075 & -8.7258]', \end{aligned}$$

then the matrix of the projections of LSModel elements will be:

$$\begin{aligned} P_r &= [\mathbf{pr}(w_t(\mathbf{x}, \mathbf{t})) \quad \mathbf{pr}(w_{xx}(\mathbf{x}, \mathbf{t})) \quad \mathbf{pr}(g(\mathbf{x}, \mathbf{t}))] \\ &= \begin{bmatrix} 4.9971 & 7.0822 & 0.0075 \\ -6.8849 & 5.5698 & -8.7258 \end{bmatrix}. \end{aligned}$$

Let's calculate its singular value decomposition  $P_r = U_p S_p V'_p$  and perform a singular analysis

$$s_1^p = 12.4449, \quad s_2^p = 8.6497, \quad s_2^p/s_1^p = 0.6950,$$

and based on it calculate parameters  $\mathbf{a}_p = -\mathbf{v}_3^p/v_{33}^p$

$$a_1^p = 0.8074, \quad a_2^p = -0.5686, \quad a_3^p = -1.0000.$$

Why should we perform the singular analysis, after all we have chosen the canonical LISModel, checked a set of guarantors for linear independence. All correct, indeed, mathematical model obeys mathematical theory, but the object of our research does not know what a good model we've come up with and what a super guaranteed experiment we've conducted. As a result, there may not be an unambiguous solution. And then it's necessary either to study the noise or change the initial model and look for a guaranteed experiment again.

If the object does not obey the stated theory for the model we invented, then the model is redundant (insufficient), In other words, it has an extra (missing) element.

The methods described in the previous part of the article, especially the method using Pearson's centroid theorem, will help to search for a new model.

Now about the noise. In this experiment, to simulate measurement noises, values from a normal distribution with standard deviation 0.1 were added to the calculated temperature  $w(\mathbf{x}, \mathbf{t})$ . The methods from the first part of the article could not cope with such a value of standard deviation.

Obviously, by taking  $\sin(x)\cos(t)$  and  $\sin(x)\sin(t)$  as guarantors on their period, we ensured that the high-frequency noises were perpendicular to our guarantors span. Hence such good results.

It is interesting to see how the projections and perpendiculars of the elements of the initial LSModel look like in the element space.

In the subspace of guarantors

$$\mathbf{pr}(w_t(\mathbf{x}, \mathbf{t})) = Q'_g w_t(\mathbf{x}, \mathbf{t})|_{1:2},$$

$$\mathbf{per}(w_t(\mathbf{x}, \mathbf{t})) = Q'_g w_t(\mathbf{x}, \mathbf{t})|_{3:225},$$

and to translate into the space of LSModel elements, they

should be supplemented with the necessary number of zeros and multiplied by the matrix  $Q_g$  on the left:

$$Q_g [pr(w_t(\mathbf{x}, t))' \ 0 \dots 0]',$$

$$Q_g [0 \ 0 \ per(w_t(\mathbf{x}, t))']'.$$

These are 225-dimensional vectors and I will represent them as graphs. Such graphs are very useful for practitioners to look at, they can be drawn for models of any complexity and any dimension of space-time  $(\mathbf{x}, t)$ .

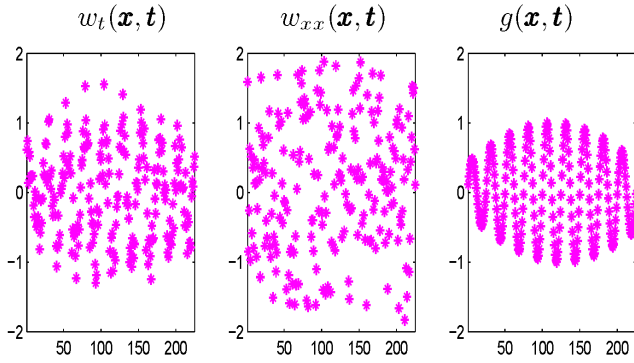


Figure 22. LSModel elements.

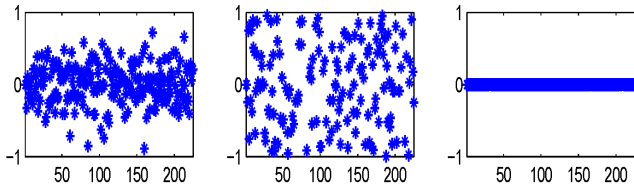


Figure 23. ...their perpendiculars.

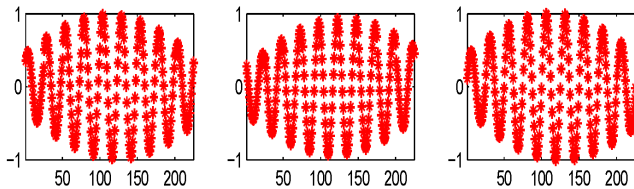


Figure 24. ...and projections in Experiment #3.

Note that the element  $g(\mathbf{x}, t)$  has a zero perpendicular and its projection is in no way different from the element, because it is set without noise.

The success of application of the method of projection onto the hyperplane of guarantors of course depends on the accuracy of measurement of guarantors. Therein, the method is very similar to the least squares method. Therefore, in the example of a nonlinear LSModel, where the guarantor  $w_x^2(\mathbf{x}, t)$  is calculated with large errors, the method works inefficiently.

In the third part of the article, a projection method for guarantors measured with errors will be proposed. And we will also abandon the calculation of derivatives from measurements and move on to filtering these measurements.

## 7. Histograms of Unknown Parameters

The idea of constructing histograms is very simple. Let's consider it on the example of experiment #2. Let me remind that the LSModel and its elements look as follows:

$$\alpha_1 w_t(\mathbf{x}, t) + \alpha_2 w_{xx}(\mathbf{x}, t) = g(\mathbf{x}, t),$$

$$w_t(\mathbf{x}, t) = 1.25t, \quad w_{xx}(\mathbf{x}, t) = -1/3, \quad g(\mathbf{x}, t) = 0.2 + t.$$

Having taken the measurements at  $x=0, t=0$ , we substitute them into the equation of the model and get the equation in the space of parameters:

$$a_1 \cdot w_t(0, 0) + a_2 \cdot w_{xx}(0, 0) = g(0, 0),$$

or

$$a_1 \cdot (0) + a_2 \cdot (-1/3) = 0.2, \quad \text{or} \quad a_2 = -0.6.$$

Below in the left graph, this straight line (hyperplane or general solution according to the first realization) is shown by a bold line. Similarly, other hyperplanes were obtained for  $\mathbf{x} = \{0, 0.125, \dots, 1\}, t = \{0, 0.125, \dots, 0.75\}$ .

In total, 25 straight lines are given in the graph (only 7 of them are visible). All these hyperplanes intersect at one point  $\mathbf{a} = (a_1, a_2) = (0.8, -0.6)$ , because all measurements and calculations are absolutely accurate.

However, if the measurements are inaccurate, we will get a completely different picture of the intersections of these 25 lines in the right graph. And now we can construct histograms of parameter values in the points of all possible intersections of these lines.

Hyperplanes in experiment #2:

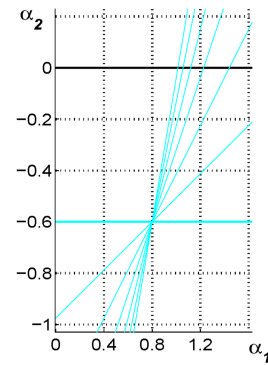


Figure 25. Deviation 0.

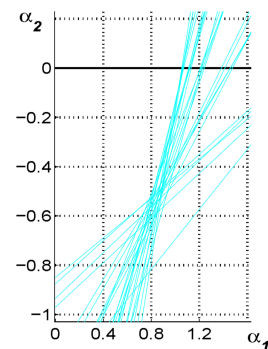


Figure 26. Deviation 0.001.

The intersection points  $\mathbf{a}_k$  or, in other words, the outcomes of a random experiment are the solutions of the following equations:

$$\begin{bmatrix} w_t(m_1) & w_{xx}(m_1) \\ w_t(m_2) & w_{xx}(m_2) \end{bmatrix} \begin{bmatrix} a_1^k \\ a_2^k \end{bmatrix} = \begin{bmatrix} g(m_1) \\ g(m_2) \end{bmatrix},$$

where  $m_1, m_2$  are numbers of different realizations.

The main advantage of this method is obtaining of a sufficiently large number of outcomes of a random experiment, even with few measurements. In the example with 25 measurements we got  $C_{25}^2 = 25 \cdot 24 / 2 = 300$  intersections.

It is also very important that completely different, and not only identical, experiments may be combined to calculate histograms, as the parameters of the same object do not depend on experimental data. The disadvantage of the algorithm considered in the example is a large dispersion of intersection points  $\mathbf{a}_k$  across the space of parameters. Therefore, to correct this shortcoming, a restriction, for example  $\|\mathbf{a}_k\|=1$ , is imposed on the norm of the parameter vector. I call such models LSModels with parameters on the sphere.

Then, solving the equations

$$\begin{bmatrix} w_t(m_1) & w_{xx}(m_1) & g(m_1) \\ w_t(m_2) & w_{xx}(m_2) & g(m_2) \end{bmatrix} \begin{bmatrix} a_1^k \\ a_2^k \\ a_3^k \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

using singular value decomposition and taking the last column of the matrix  $V_k$  of right singular vectors as a solution, we get a solution on the unit sphere. This is a very important restriction for us, because we have obtained a compact set of parameters and now the intersection points will not scatter over the entire space of parameters, but will always lie on a unit sphere. Below, the left graphs show the intersection points  $\mathbf{a}_k$  in 3-dimensional space of parameters, and the right ones – hyperplanes (straight lines) of general solutions according to the LSModel realization for two levels of measurement noises.

The graphs clearly show that the set  $A$  of elementary events (the set of intersection points  $\mathbf{a}_k$ ) has the shape of a ring. The plane of the ring is located at some angle to the axes and therefore the histograms of the coordinates of the parameter vectors  $\mathbf{a}_k$  do not reflect the true distribution of points  $\mathbf{a}_k$  across the sphere.

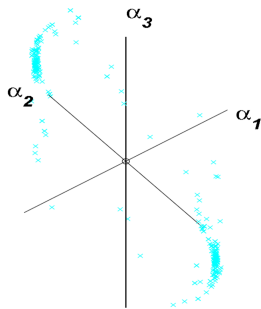


Figure 27. Points  $\mathbf{a}_k$  (deviation 0.001).

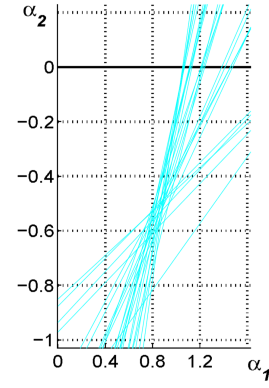


Figure 28. Hyperplanes (deviation 0.001).

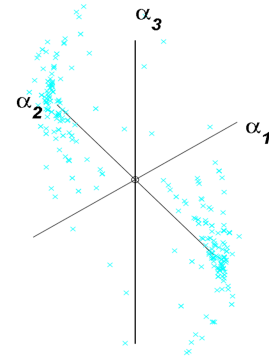


Figure 29. Points  $\mathbf{a}_k$  (deviation 0.01).

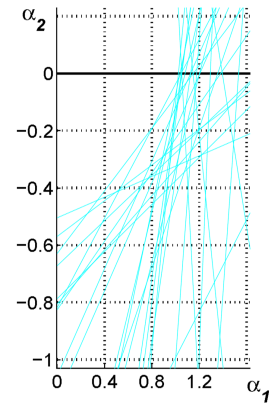


Figure 30. Hyperplanes (deviation 0.01)

To match the histograms on the sphere to the histograms on the axes (which we can calculate), it is necessary that: 1) the diameters of the set  $A$  of elementary events coincide with the coordinate axes and 2) the division points  $a_n(i)$  of the Cartesian axis  $a_n$  when calculating histograms have the form:

$$\{a_n(i) = \cos(\theta_i) : \theta_i = -\pi, -\pi + \pi/I, \dots, 0\},$$

where  $I$  is a number of intervals (bins). After all, the sizes of histogram sectors should be the same on the circle, not on the Cartesian axis.

In the MATLAB Programm it looks as follows:

```
I=64; axis_a=cos(-pi:pi/I:0); % 68
```

### 7.1. Algorithm

Let's assume that the following matrix of experimental data was obtained during the Experiment

$$F=[f_{mn}], \quad m=1, \dots, M, \quad n=1, \dots, N, \quad M>N.$$

Let's form all possible, including random, samples  $\{f(m_1), \dots, f(m_{N-1})\}$ , consisting of  $(N-1)$ -th realization of the experimental data matrix  $F$  and let's make up the matrices:

$$F_k = \begin{bmatrix} f(m_1) \\ \dots \\ f(m_{N-1}) \end{bmatrix}, \quad k=1, \dots, K.$$

Let's obtain their singular value decompositions

$$F_k = U_k S_k V_k$$

and let's take the last column  $v_N^k$  of the matrix  $V_k$  as the exact solution of the system  $F_k a_k = 0$ . If the solution is unambiguous, then  $a_k = v_N^k$  and  $-a_k = -v_N^k$  will be the intersection points of the unit sphere with the straight line of the general solution of this system.

Let's take the set

$$A = \{a_k = v_N^k, \quad k=1, \dots, K\}.$$

as a set of elementary events.

Statistical formulation is reasonable when there is a lot of same-type information obtained as a result of a sufficiently large number of outcomes of a random experiment. In this case, for  $M>N$  we have  $K = C_M^{N-1}$  various samples and exact solutions  $a_k$  on the unit sphere of parameters.

Let singular value decomposition of the matrix of elements  $F$  be as follows:

$$F = U S V',$$

where

$U = [u_1 \dots u_M]$ ,  $V = [v_1 \dots v_N]$  are orthogonal  $(M \times M)$  and  $(N \times N)$  matrices consisting of  $u_i$  – left and  $v_i$  – right singular vectors, respectively;

$S = \text{diag}(s_1, \dots, s_N)$  is the diagonal  $(M \times N)$ -matrix with singular numbers  $s_1, \dots, s_N$  on the main diagonal.

Let  $M>N$ , then the equation of the LSModel in matrix notation will look as follows:

$$U S V' a_k = e_k, \quad \forall a_k \in A, \quad A = [a_1 \dots a_K].$$

Having denoted

$$P = U S, \quad b_k = V' a_k$$

we get

$$P b_k = e_k, \quad \forall b_k \in B, \quad B = [b_1 \dots b_K],$$

then

$$B = V' A, \quad A = V B, \quad P = F V, \quad P' = V' F'.$$

This means that having moved to a new basis  $\{v_1, \dots, v_N\}$  in the space of parameters or, in other words, having rotated the points of sets  $A$  and  $F'$  by an orthogonal matrix  $V'$ , we'll get a new equation of the LSModel. It is fundamentally important for us that at the same time the relative position of points in the space of parameters/realizations does not change, but only the coordinates of these points change:  $a_n$  to  $b_n$  and  $f_{mn}$  to  $p_{mn}$ .

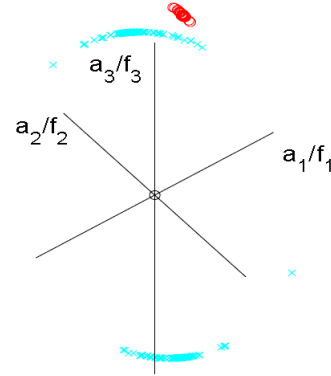


Figure 31. Experiment #1, deviation 0.001 (initial bases).

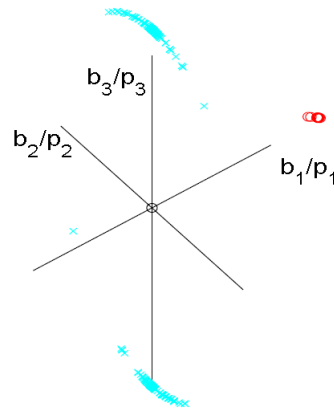


Figure 32. Experiment #1, deviation 0.001 (V bases).

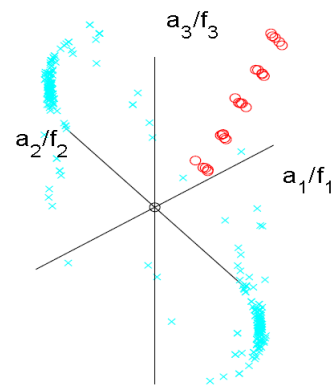


Figure 33. Experiment #2, deviation 0.001 (initial bases).

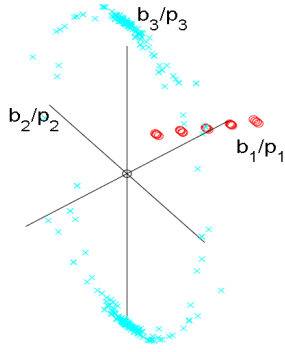


Figure 34. Experiment #2, deviation 0.001 (V bases).

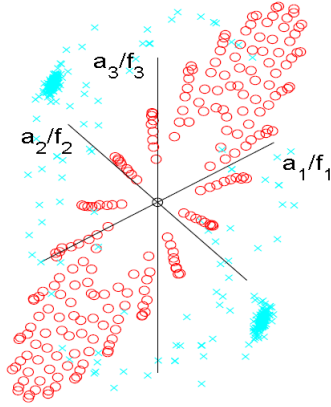


Figure 35. Experiment #3, deviation 0.001 (initial bases).

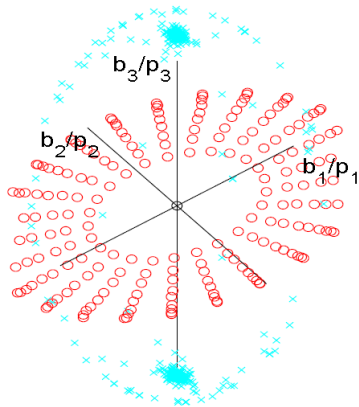


Figure 36. Experiment #3, deviation 0.001 (V bases).

Let me remind that in basis  $V$  for all realization  $\mathbf{p}_m$   $|p_{mi}| \leq s_i$ , as  $FV = P = US = [s_1 \mathbf{u}_1, \dots, s_N \mathbf{u}_N]$  and  $\mathbf{u}_i$  are orthonormal.

Then for example when  $s_3 = 0.08$ , the third coordinates of all realizations  $|p_{m3}| \leq 0.08$ , in other words, the realizations (denoted by 'o' in the graphs) almost lie in the plane of Cartesian axes  $b_1/p_1$  (before replacement of the basis  $\mathbf{v}_1$ ) and  $b_2/p_2$  (before replacement of  $\mathbf{v}_2$ ), and almost perpendicular to them parameters  $\mathbf{b}_k$  are close to Cartesian axis  $b_3/p_3$  ( $\mathbf{v}_3$  before replacement). The graphs clearly show the concentration of 300 intersection points (denoted by 'x')

mainly around  $b_3/p_3$  and  $-b_3/p_3$  in experiments #1 and #2 and  $C_{225}^2 = 225 \cdot 224 / 2 = 25200$  points in experiment #3.

The concentration of intersections near two points  $[0 \ 0 \ 1]$  (before replacement of  $\mathbf{v}_3$ ) and  $[0 \ 0 \ -1]$  (before replacement of  $-\mathbf{v}_3$ ) creates inconveniences when interpreting histograms of parameters, therefore it is better to fix the sign of the last coordinate of the calculated solution  $\mathbf{b}_k$ . To do this, when  $b_{Nk} < 0$ , you need to assign the value  $-\mathbf{b}_k$  to  $\mathbf{b}_k$ . Then the concentration of points on the last axis will be only near the point  $[0 \dots 0 \ 1]$ .

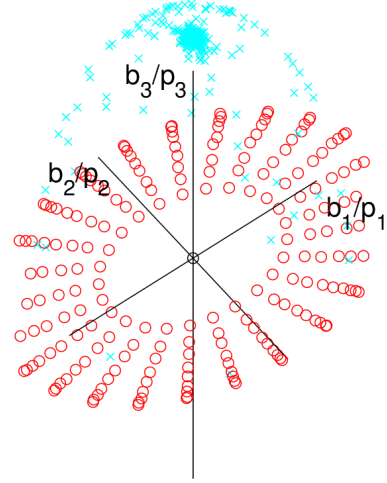


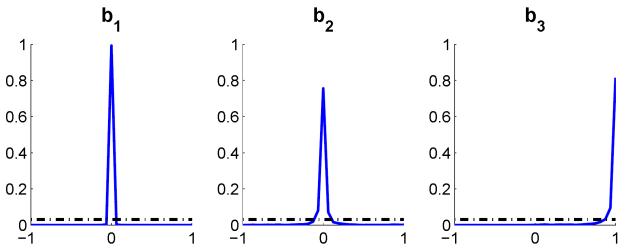
Figure 37. V bases.

Now it is possible to calculate the histograms [7] of coordinates of parameters  $\mathbf{b}_k$ . To do this, we will use the MATLAB function *hist* with two arguments:

$$H_n = \text{hist}(B_n, \text{axi})$$

where  $H_n$  is an array of dimension  $I$ , which contains the distribution of values of random variables from array  $B_n$  ( $n$ th row of matrix  $B$ ) among  $I$  intervals (bins) with centers, specified by values from array  $\text{axi}$ , the dimension of which also determines the dimension of  $I$ .

In the figure below you can see the normalized histogram  $H_n/K$  for our three experiments.

Figure 38. Histograms of coordinates of parameters  $\mathbf{b}$  in experiment #1 ( deviation 0.001).



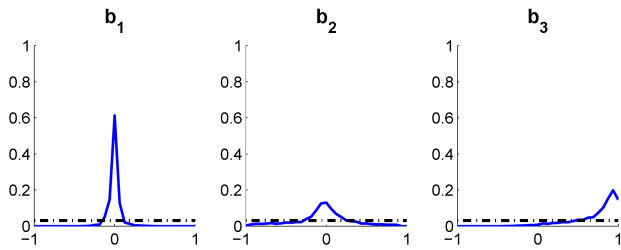


Figure 39. Histograms of coordinates of parameters  $\mathbf{b}$  in experiment #2 ( deviation 0.001).

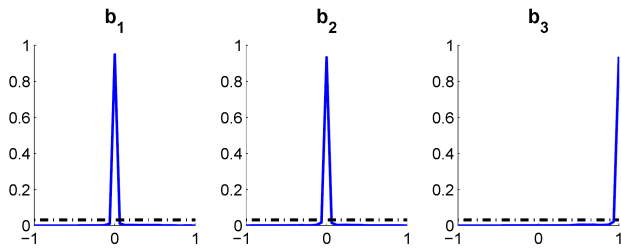


Figure 40. Histograms of coordinates of parameters  $\mathbf{b}$  in experiment #3 ( deviation 0.001).

Histograms of coordinates of vectors  $\mathbf{b}_k$  clearly indicate the most probable solution  $\hat{\mathbf{b}} = [0 \ 0 \ 1]'$ . Then  $\hat{\mathbf{a}} = V\hat{\mathbf{b}} = V[0 \ 0 \ 1]' = \mathbf{v}_3$ , only with different probabilities and different vectors  $\mathbf{v}_3$ .

If in experiment #2 it is apparent that the solution  $\mathbf{v}_3$  is questionable, then in experiment #1, the solution does not cause any doubts, although we know that it is not unambiguous. We discussed the reason for this in the first part of the article. Experiment #3, as before, is the best of all. But as noise intensity increases, the situation changes and the probability that  $\mathbf{v}_3$  is a solution, decreases.

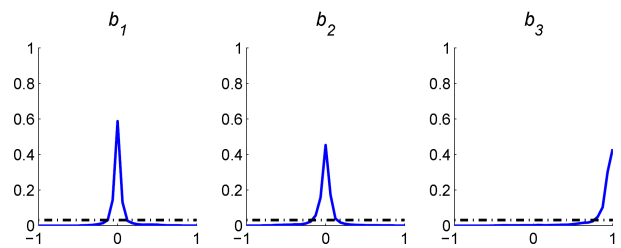


Figure 41. Histograms of coordinates of parameters  $\mathbf{b}$  in experiment #3 ( deviation 0.01).

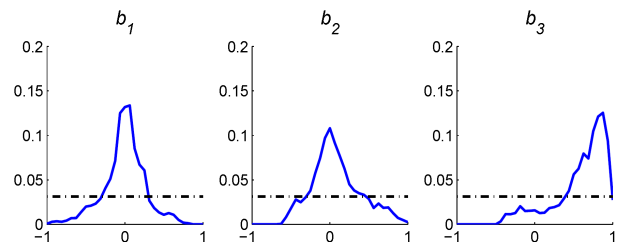


Figure 42. Histograms of coordinates of parameters  $\mathbf{b}$  in experiment #3 ( deviation 0.1).

Here I just want to emphasize that it is necessary to apply several methods to determine the uniqueness of the solution. And construction of histograms is one more of them.

## 8. Conclusion

In conclusion of the first part of the article, I offer brief recommendations on the use of the methods described above.

You should start by dividing the identification problem into two subproblems using the Mixed LS & TLS method. This is very important, since it is often possible to get serious errors in parameter estimates by mixing accurate data with approximate ones. This will also reduce the dimension of the general identification problem using the TLS method and it will be easier to perform singular analysis.

Then cut off the anomalous realizations in the first subproblem of the Mixed LS& TLS method and solve it in two ways: with and without the involvement of the centroid, with a complete singular analysis of both.

It is very useful to have a look at what we discard when deciding on an effective rank.  $\Delta F_{mat}$  plots can be drawn at any dimension of the space of parameters/realizations, in contrast to pictures in the space itself. It is also useful to combine various experiments and compare the results obtained.

Additional possibilities are provided by studying the graph of all values of the functional used to obtain the optimal solution. The use of other functionals, including non-norm, can change your approach to solving the identification problem.

We need to evaluate soberly the experimental data we have: how stable calculation of parameters they can give. The optimality of estimates is not a guarantee of their unambiguous stable calculation.

Projection methods are fundamentally different from optimization methods. The latter are insensitive to small changes in the source data. Projection methods, as resonant in fact, have wider possibilities for the selection of small identifying guarantor signals perpendicular to the measurement noise.

The search for guarantors and the structure of the LSModel used is a separate very important problem.

The histogram calculation method will help to investigate the effect of noise on parameter identification.

It is very good when there are several different methods of studying the same experimental data. There is something to compare, there is something to choose from.

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## Abbreviations

ED	Experimental Data
GIExperiments	Guaranteeing Identification Experiments
GSIP	General Solution of Identification Problem
IP	Identification Problem
LISModels	Linear Identifiable Structure Models
LSModel	Linear Structure Model
LSModels	Linear Structure Model Class
mat	Matrix Approximation Theorem
mixed LS&TLS	Mixed least Squares and Total Least Squares
PSIP	Particular Solution of Identification Problem
SP	Space of Parameters
SPR	Space of Parameters/Realizations
SVD	Singular Value Decomposition
TLS	Total Least Squares

## Appendix: MATLAB Program

```

clear; clf; format short e; % 1
colormap('jet'); % 2
% % HEAT EQUATION % 3
% % 0.8 w_t(x,t) - 0.6 w_xx(x,t) = g(x,t) % 4
% % % 5
Experiment=3 % 6
% % % 7
% % % 8
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% % % 46

```

```

w_t(i-2,j-1)=... % 47
    (w(i,j+1)-w(i,j-1))/(t(j+1)-t(j-1)); % 48
w_xx(i-2,j-1)=... % 49
    (w(i+2,j)-2*w(i,j)+w(i-2,j))... % 50
    /((x(i+1)-x(i-1))^2); % 51
m=m+1; % 52
F(m,1)=w_t(i-2,j-1); % 53
F(m,2)=w_xx(i-2,j-1); % 54
F(m,3)=g(i,j); % 55
end; end; % 56
[M,N]=size(F); % 57
% 58
subplot(241); surf(t,x,g); % 59
    title('{\it g(x,t)}'); % 60
subplot(242); surf(t,x,w); % 61
    title('{\it w(x,t)}'); % 62
% 63
xm=x(3:sx-2); tm=t(2:st-1); % 64
subplot(245); surf(tm,xm,w_t); % 65
    title('{\it w_t(x,t)}'); % 66
subplot(246); surf(tm,xm,w_xx); % 67
    title('{\it w_xx(x,t)}'); % 68
subplot(122); % 69
    plot3(F(:,1),F(:,2),F(:,3),'r*'); % 70
    title('{\it F}'); grid on; % 71
% 72
%% SVD %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 73
[U,S,V]=svd(F,0); % 74
a=-V(:,3)/V(3,3) % 75
[U_,S_,V_]=svd([F(:,3) F(:,1) F(:,2) ],0); % 76
pause; % 77
% 78
%% U and V BASES %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 79
UF=U'*F; FV=F*V; % 80
subplot(222); % 81
    plot3([0],[0],[0],'k.');
```

$$\text{hold on;}$$

```

    plot3([-5. 10.],[0 0],[0 0],'k'... % 82
        ,[0 0],[ -6. 0.],[0 0],'k'... % 83
        ,[0 0],[0 0],[ -1 1],'k'); % 84
    plot3([0 UF(1,1)],[0 UF(2,1)]... % 85
        ,[0 UF(3,1)],'g','LineWidth',3); % 86
    plot3([0 UF(1,2)],[0 UF(2,2)]... % 87
        ,[0 UF(3,2)],'c--','LineWidth',3); % 88
    plot3([0 UF(1,3)],[0 UF(2,3)]... % 89
        ,[0 UF(3,3)],'b-','LineWidth',3); % 90
    title('{\bf U^*F}'); grid on; % 91
    axis([-5. 10. -6. 0. -1 1]); % 92
subplot(224); % 93
    plot3([0],[0],[0],'k.');
```

$$\text{hold on;}$$

```

    plot3([-2. 2.],[0 0],[0 0],'k'... % 94
        ,[0 0],[ -2. 2.],[0 0],'k'... % 95
        ,[0 0],[0 0],[ -1. 1.],'k'); % 96
    plot3(FV(:,1),FV(:,2),FV(:,3),'r*'); % 97
    title('{\bf FV}'); grid on; % 98
    zlim([-1. 1]); % 99
pause; % 100
% 101
%% Selection of realisations %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% 102
L=1/sqrt(M); F1=zeros(size(F)); % 103
j=0; % 104
for i=1:M, % 105
    if abs(U(i,3))<L, % 106
        j=j+1; F1(j,:)=F(i,:); % 107
    end; % 108
end; % 109
[U1,S1,V1]=svd(F1(1:j,:),0); % 110
a1=-V1(:,3)/V1(3,3) % 111
subplot(122); % 112
plot3(F1(1:j,1),F1(1:j,2),F1(1:j,3),'r*'); % 113
title('{\bf F_1}'); grid on; pause; clf; % 114
% 115
% 116
% 117
% 118

```

```

%% Pearson centroid
fcen=sum(F,1)/M;
for m=1:M, Fc(m,:)=F(m,:)-fcen; end;
[Uc,Sc,Vc]=svd(Fc,0); fcenVc3=fcen*Vc(:,3)
if Experiment==3, r=2; else r=1; end;
Fc_r=Uc(:,1:r)*Sc(1:r,1:r)*Vc(:,1:r)';
for m=1:M, Fpea(m,:)=Fc_r(m,:)+fcen; end;
TnormDeltaFpea=max( abs(F-Fpea), [], 1);

%% Mixed LS & TLS
[Q,T]=qr(F(:,3)); T1=T(1:1,1:1)^(-1);
P=Q'*F(:,1:2); [Up,Sp,Vp]=svd(P(2:M,:),0);
am=[ Vp(:,2); -T1*P(1:1,:) *Vp(:,2)]';
am=-am/am(3)
r=1; P2r=Up(:,1:r)*Sp(1:r,1:r)*Vp(:,1:r)';
Fpr=Q*([P(1:1,:); P2r] T );
subplot(231); hold on;
plot(P(2:M,1),P(2:M,2),'r*');
plot([-Vp(1,1),Vp(1,1)]...
      ,[-Vp(2,1),Vp(2,1)],'b');
title('\itP'); grid on;
subplot(232);
plot(2:M, Sp(1,1)*Up(:,1),'g*');
title('\it s^p_1{\bfu}^p_1');
subplot(233); hold on;
plot(2:M,Sp(2,2)*Up(:,2),'c*');
title('\it s^p_2{\bfu}^p_2');
L=1.3*Sp(2,2)/sqrt(M-1);
plot([0 M],[L L],'k',[0 M],[-L -L],'k');
%% Selection of realisations %%
Po=zeros(size(P)); j=0; s2=Sp(2,2);
for i=1:M-1,
    if abs(s2*Up(i,2))<L,
        j=j+1; Po(j,:)=P(i+1,:);
    end;
end;
[Uo,So,Vo]=svd(Po(1:j,:));
ao=[ Vo(:,2); -T1*P(1:1,:) *Vo(:,2)]';
ao=-ao/ao(3)
subplot(234); hold on;
plot(Po(1:j,1),Po(1:j,2),'r*');
plot([-Vo(1,1),Vo(1,1)]...
      ,[-Vo(2,1),Vo(2,1)],'b');
subplot(235);
plot(1:j, So(1,1)*Uo(:,1),'g*');
subplot(236); hold on;
plot(1:j,So(2,2)*Uo(:,2),'c*');
plot([0 j],[L L],'k',[0 j],[-L -L],'k');
pause;

%% Objective functional
h=2^(-4)
q=Inf %% 1 or 2 ... or Inf
min_c=Inf;
C=zeros((2/h+1)*(2/h+1));
A=zeros((2/h+1)*(2/h+1),3);
m=0;
%% the rectangle with a uniform grid
for a1=-1:h:1, for a2=-1:h:1,
    b=a1^2+a2^2;
    %% if the point (a1,a2) is in unit disk,
    if b<=1, a=[ a1; a2; sqrt(1-b)];
        for i=1, %% !! for i=1:2, !! a sphere
            m=m+1;
            A(m,:)=a;
            c=norm(F*a,q); C(m)=c;
            if min_c>c, min_c=c; mm=m; ma=a; end;
            a=[ a1; a2; -sqrt(1-b)];
        end;
    end;
end; end;

```

```

min_a=-ma'/ma(3) %190
subplot(121); %191
plot(1:m,A(1:m,3),'xy'); xlim([1 m]); %192
subplot(122); %193
plot(1:m,C(1:m),'xg'); xlim([1 m]); %194
pause; clf; %195
%196
%% Histograms of parameters %197
maxK=1; %198
for i=1:N-1, maxK=maxK*(M-i+1)/i; end; %199
K=25000; if K>maxK, K=maxK; end; %200
A=zeros(N,K); F_k=zeros(N-1,N); %201
for k=1:K, %%% casual realisations %202
    for i=1:N-1, F_k(i,:)=F(randi(M),:); end; %203
    [u,s,v]=svd(F_k); %204
    if v(N,N)<0, v(:,N)=-v(:,N); end %205
    A(:,k)=v(:,N); %206
end; %207
P=F*V; B=V'*A; %208
I=32; axi=cos(-pi:pi/I:0); %209
for n=1:N, subplot(1,N,n); %210
    H=hist(B(n,:),axi); %211
    plot(-1:2/I:1,H/K,'b',[-1 1],[1/I 1/I]... %212
        ,'-k','LineWidth',2); %213
    title(['\bfb_',int2str(n)]); %214
    xlim([-1 1]); ylim([0 1]); %215
end; %216
pause; clf; %217
%218
%% Projections onto guarantors %219
g_t=zeros(sx-4,st-2); %220
g_xx=zeros(sx-4,st-2); %221
G=zeros((sx-4)*(st-2),2); %222
m=0; %223
for i=3:sx-2, for j=2:st-1, %224
    g_t(i-2,j-1)=... %225
        (g(i,j+1)-g(i,j-1))/(t(j+1)-t(j-1)); %226
    g_xx(i-2,j-1)=... %227
        (g(i+2,j)-2*g(i,j)+g(i-2,j))... %228
        /((x(i+1)-x(i-1))^2); %229
    m=m+1; %230
    G(m,1)=g_t(i-2,j-1); %231
    G(m,2)=g_xx(i-2,j-1); %232
end; end; %233
[Qg,Tg]=qr(G(:,1:2)); %234
Pr=Qg'*F; proF=Qg(:,1:2)*Pr(1:2,:); %235
[Upro,Spro,Vpro]=svd(Pr(1:2,1:3),0); %236
a_pro=-Vpro(:,3)'/Vpro(3,3) %237
%% LSModel elements %238
subplot(2,3,1); plot(F(:,1),'m*'); %239
    xlim([1 M]);ylim([-2 2]); %240
subplot(2,3,2); plot(F(:,2),'m*'); %241
    xlim([1 M]);ylim([-2 2]); %242
subplot(2,3,3); plot(F(:,3),'m*'); %243
    xlim([1 M]);ylim([-2 2]); %244
%% their perpendiculars %245
subplot(4,3,7); %246
    plot([0 0 Pr(3:M,1)'],'b*'); %247
    xlim([1 M]);ylim([-1 1]); %248
subplot(4,3,8); %249
    plot([0 0 Pr(3:M,2)'],'b*'); %250
    xlim([1 M]);ylim([-1 1]); %251
subplot(4,3,9); %252
    plot([0 0 Pr(3:M,3)'],'b*'); %253
    xlim([1 M]);ylim([-1 1]); %254
%% and projections %255
subplot(4,3,10); plot(proF(:,1),'r*'); %256
    xlim([1 M]);ylim([-1 1]); %257
subplot(4,3,11); plot(proF(:,2),'r*'); %258
    xlim([1 M]);ylim([-1 1]); %259
subplot(4,3,12); plot(proF(:,3),'r*'); %260

```

```
xlim([1 M]);ylim([-1 1]);
%% END of Projections onto guarantors
```

```
%261
%%262
```

---

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