Solving interval linear least squares problems by PPS-methods

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Abstract

In our work, we consider the linear least squares problem for $m \times n$ -systems of linear equations Ax = b, $m \ge n$, such that the matrix A and right-hand side vector b can vary within an interval $m \times n$ -matrix A and an interval m-vector b, respectively. We have to compute, as sharp as possible, an interval enclosure of the set of all least squares solutions to Ax = b for $A \in A$ and $b \in b$. Our article is devoted to the development of the so-called PPS-methods (based on partitioning of the parameter set) to solve the above problem.

We reduce the normal equation system, associated with the linear lest squares problem, to a special extended matrix form and produce a symmetric interval system of linear equations that is equivalent to the interval least squares problem under solution. To solve such symmetric system, we propose a new construction of PPS-methods, called ILSQ-PPS, which estimates the enclosure of the solution set with practical efficiency. To demonstrate the capabilities of the ILSQ-PPS method, we present a number of numerical tests and compare their results with those obtained by other methods.

Key words. Interval systems of linear equations, least squares problems, outer estimation of solution set, PPS-method.

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1 Introduction

The subject of our paper is the traditional linear least squares problem in which the input data are not precise and have interval uncertainty. We need to evaluate the variation in the solution of the linear least squares problem when its data changes in the prescribed intervals.

Let us be given an $m \times n$ -system of linear algebraic equations of the form

or, briefly,

$$Ax = b \tag{2}$$

with an $m \times n$ -matrix $A = (a_{ij}), m \ge n$, and a right-hand side *m*-vector $b = (b_i)$. This system of equations may or may not have the usual solution, but in our paper we will look for its least squares pseudo-solution that minimizes the Euclidean norm of its residual, that is,

$$||Ax - b||_2 = \left(\sum_{i=1}^m \left((Ax)_i - b_i\right)^2\right)^{1/2}$$

(see e.g. [6]). In practice, the matrix A and vector b are often imprecise, and we only know interval bounds \mathbf{a}_{ij} and \mathbf{b}_i for the respective coefficients and right-hand side components, such that $a_{ij} \in \mathbf{a}_{ij}$ and $b_i \in \mathbf{b}_i$. Therefore, instead of the above systems of linear equations, we get an interval linear system of the form

or, briefly,

$$\mathbf{A}x = \mathbf{b} \tag{4}$$

with interval $m \times n$ -matrix $\mathbf{A} = (\mathbf{a}_{ij})$ and interval *m*-vector $\mathbf{b} = (\mathbf{b}_i)$ in the right-hand side. Boldface letters in the above formulas and throughout this article denote intervals.

How do the least squares solutions for system (3)–(4) change when its coefficients and the right-hand sides vary within the intervals \boldsymbol{a}_{ij} and \boldsymbol{b}_i respectively? In other words, what will be the set of all such pseudo-solutions to system (1)–(2) for $A \in \boldsymbol{A}$ and $b \in \boldsymbol{b}$?

Formally, all such points that deliver the minimum to $||Ax - b||_2$ constitute the set

$$\Xi_{lsq}(\boldsymbol{A}, \boldsymbol{b}) = \left\{ \tilde{x} \in \mathbb{R}^n \mid (\exists A \in \boldsymbol{A}) (\exists b \in \boldsymbol{b}) (\tilde{x} \text{ minimizes } \|Ax - b\|_2) \right\},\tag{5}$$

which will be called *least squares solution set* to the interval linear system (3)–(4). Usually, this set can have a complex configuration, it can be bounded by curved surfaces, etc. As a rule, in practice we do not need to describe it completely and precisely, since this is difficult and not very convenient. Instead, it makes sense to find some approximate descriptions of the solution set $\Xi_{lsq}(\mathbf{A}, \mathbf{b})$, that is, some its estimates.

In the rest of our article, we are going to consider outer interval estimation of the least squares solution set $\Xi_{lsq}(\mathbf{A}, \mathbf{b})$, i. e., we solve the problem

given an interval linear equation system $Ax = b$, we have	
to compute, as narrow as possible, an interval box	(6)
that contains the least squares solution set $\Xi_{lsq}(\boldsymbol{A}, \boldsymbol{b})$.	

One should bear in mind that the other ways of estimating the solution set $\Xi_{lsq}(\mathbf{A}, \mathbf{b})$ are possible. For example, an inner interval box contained in the least squares solution set may be of interest in some practical problems. These may be the subject of further study, and we do not consider them in our article.

The problem (6) has, in fact, quite a long history. It was first formulated in explicit interval form by D.M. Gay in the paper [9], but its appearance should be dated back to the articles [5, 7, 12] and others.

1.1 Preliminaries and auxiliary results

In our work, intervals are bounded closed and connected subsets of the real axis \mathbb{R} , i.e. sets of the form $\boldsymbol{x} = \{x \in \mathbb{R} \mid a \leq x \leq b\}$. The numbers a and b are called *endpoints* or bounds of the interval \boldsymbol{x} , *lower* (left) and *upper* (right) respectively. Throughout the text, we adhere to the informal notation standard [15] and, as a consequence, denote intervals and other interval objects by boldface letters $(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \ldots, \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$, while non-interval (point) objects are not specifically marked. IR stands for the set of all real intervals, and

$$\mathbb{IR}^{n} = \{ (\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \dots, \boldsymbol{x}_{n})^{\top} \mid \boldsymbol{x}_{i} \in \mathbb{IR}, 1 \leq i \leq n \}$$

is the set of *n*-dimensional interval vectors, also called *boxes*. The interval matrix is a rectangular table of intervals, which is designated by $\mathbf{A} = (\mathbf{a}_{ij})$, meaning that the intersection of the *i*-th row and *j*-th column contains the element \mathbf{a}_{ij} . The set of all interval $m \times n$ -matrices is denoted as $\mathbb{IR}^{m \times n}$.

Also, we need the following notation:

 $\begin{array}{lll} \underline{x} \,, \, \overline{x} & - \text{lower and upper bound of the interval } x, \text{ respectively,} \\ \text{mid } x = \frac{1}{2} \left(\underline{x} + \overline{x} \right) & - \text{midpoint of the interval } x, \\ \text{rad } = \frac{1}{2} \left(\overline{x} - \underline{x} \right) & - \text{radius of the interval } x, \\ \text{wid } x = \overline{x} - \underline{x} & - \text{width of the interval } x, \\ |x| = \max\{ |\underline{x}|, |\overline{x}| \} & - \text{absolute value (magnitude) of the interval } x. \end{array}$

The above operations are applied to interval vectors and matrices componentwise and elementwise. For matrices $A = (a_{ij})$ and $\mathbf{A} = (\mathbf{a}_{ij})$ of identical dimensions, the relation $A \in \mathbf{A}$ means that $a_{ij} \in \mathbf{a}_{ij}$ for all matrix elements, and the same is understood for vectors. Also, "int \mathbf{a} " means interior of the interval \mathbf{a} , i.e., the interval without its endpoints.

The interval hull of a set $S \subset \mathbb{R}^n$ is defined as the least inclusive interval vector (box) that contains the set S. The interval hull is usually denoted as $\Box S$.

In this paper, we consider only interval linear systems of equations having full-rank matrices. Let us remind what this means.

An interval square matrix A is called a *nonsingular* (regular) matrix if all point matrices $A \in A$ are nonsingular (regular) [13, 16]. An interval square matrix A is called a *singular* matrix if it is not nonsingular, which is equivalent to the fact that A contains at least one singular point matrix. A generalization of the concept of non-singularity to rectangular (not necessarily square) matrices is the notion of a full rank matrix. The rank of the matrix is the maximum of its linearly independent rows or columns [13, 16]. A real $m \times n$ -matrix is called a *full-rank* matrix (or, has full rank) if its rank is equal to the minimum number among m and n (it cannot be greater). An interval matrix is called a *full-rank* matrix if it contains only full-rank point matrices. Otherwise, we say that this matrix has *incomplete rank*.

In the interval linear least squares problem (6), we require that the interval system under study should have a full rank to ensure that its least squares solution set is bounded. Several necessary and sufficient criteria of the full-rank matrices are presented in [24, 29], and further we will need some of them.

The first criterion is based on the concept of pseudo-inverse matrix (see [6, 33]). We remind that a pseudoinverse matrix (or Moore-Penrose inverse matrix) for a real $m \times n$ -matrix A is a real $n \times m$ -matrix A^+ such that AA^+ and A^+A are symmetric matrices and $AA^+A = A$, $A^+AA^+ = A^+$. If A is a full-rank matrix and $m \ge n$, then $A^+ = (A^\top A)^{-1}A^\top$:

Theorem 1 [24, 29] Let an interval $m \times n$ -matrix \mathbf{A} be such that $m \ge n$, the midpoint matrix mid \mathbf{A} be full-rank, and

$$\rho(|\operatorname{mid} \boldsymbol{A}|^+ \cdot \operatorname{rad} \boldsymbol{A}) < 1, \tag{7}$$

where $\rho(\cdot)$ means taking the spectral radius of the square matrix. Then **A** has full rank.

Note that the smaller the left-hand side of inequality (7) compared to 1, the larger the "full-rankness" of the matrix.

Theorem 2 [29] Let $\sigma_{\max}(A)$ and $\sigma_{\min}(A)$ denote the greatest and smallest singular values of the matrix A. If the inequality

$$\sigma_{\max}(\operatorname{rad} \boldsymbol{A}) < \sigma_{\min}(\operatorname{mid} \boldsymbol{A}) \tag{8}$$

is satisfied for the interval $m \times n$ matrix A, then it has full-rank.

In inequality (8), the difference between the right-hand side and left-hand side or ratio of these values may serve as a measure of the "full-rankness reserve" of the matrix, that is, how far the matrix is from the boundary of the set of full-rank matrices. The larger this difference or the ratio, the larger the reserve, the "better" the matrix is.

1.2 Interval least squares problems

Let Ax = b be an interval $m \times n$ -system of linear equations. The interval linear least squares problem (6) is an interval extension of the traditional linear least squares problem that was first solved by C.F. Gauss at the beginning of the XIX century. This solution is well-known, being a part of the standard university linear algebra courses. Given a system of linear equations Ax = b, the minimization of $||Ax - b||_2$ reduces to the solution of the so-called normal equations system $A^{T}Ax = A^{T}b$ (see e.g. [6, 31]).

Following this way in the interval context, when the matrix A and right-hand side b vary within the respective interval matrix A and interval vector b, we will have to "solve the interval normal system"

$$\boldsymbol{A}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^{\mathsf{T}}\boldsymbol{b},\tag{9}$$

i.e., to enclose the solution set

$$\Xi_{lsq}(\boldsymbol{A}, \boldsymbol{b}) = \left\{ \tilde{x} \in \mathbb{R}^n \mid (\exists A \in \boldsymbol{A}) (\exists b \in \boldsymbol{b}) (A^{\top} A \tilde{x} = A^{\top} b) \right\}.$$
(10)

But the formally written system (9), which arises in connection with the interval linear leastsquares problem, is not an ordinary interval system of equations with the matrix $\mathbf{A}^{\top}\mathbf{A}$ and the right-hand side $\mathbf{A}^{\top}\mathbf{b}$, as it is usually understood in interval analysis (see e.g. [1, 11, 18, 19, 20, 30]). The interval system (9) is a system of equations in which interval parameters are highly "dependent on each other" in the sense that we define below. We notice that the interval itself describes only the boundaries of possible values of a particular variable. Finer analysis often requires an indication of which variable can run through this interval, since the same interval can represent the values of completely different variables.

Definition 1 [27, 30] Let us say that interval quantity (interval parameter) is specified if there is a variable that can take values within a certain interval.

In formal mathematical language, an interval quantity is an ordered pair, which we will denote with special brackets $\lfloor a, a \rceil$, where a is a variable and **a** is an interval of its possible values, so that $a \in a$.

Definition 2 $[27, 30]^1$ The interval quantities $\lfloor z_1, z_1 \rceil$, $\lfloor z_2, z_2 \rceil$, ..., $\lfloor z_n, z_n \rceil$ will be called independent (untied), if the n-tuple of the corresponding variables (z_1, z_2, \ldots, z_n) takes any values from the direct Cartesian product of the intervals of their changes z_1, z_2, \ldots, z_n , i.e. from the interval box (z_1, z_2, \ldots, z_n) . Otherwise, the interval quantities are called dependent or tied.

For example, turning to the interval system (9), we can see that, in the interval matrix $C = A^{\top}A$ obtained by interval matrix multiplication, the elements are dependent (tied). The reason is that the set of all products "by representatives", i. e. $C = \{A^{\top}A \mid A \in A\}$, does not cover the interval box C, although the projections of the set C onto the coordinate axes coincide with the elements of C. In addition, the interval right-hand side in system (9) is dependent on the matrix, which also gives extra specificity to the problem.

The mutual ties and dependencies of variables is a very common phenomenon in the world around us, but the classical interval arithmetic and some other elementary tools of interval analysis are adapted to process only independent variables. The majority of interval methods for the solution of interval systems of equations (presented e.g. in [1, 11, 18, 19, 20, 30]) are designed for systems with independent interval parameters. As for the interval system (9), its interval parameters are highly dependent, and, hence, enclosing its solution set (10) is a very complex problem. Currently, there are few developed numerical methods for its solution, and they are of low efficiency.

We reformulate the "normal system" approach in the way that does not involve direct multiplication of matrices, thus avoiding the multiple occurrences of parameters in the expressions that form the equations system equivalent to minimization of $||Ax - b||_2$. This technique is also well known and is called reduction to an "extended system of equations".

The normal system $A^{\top}Ax = A^{\top}b$ is equivalent to the system of linear equations

$$A^{\top}(b - Ax) = 0.$$

Introducing the new variable y = b - Ax, we can rewrite the normal system as

$$\begin{cases} y + Ax = b, \\ A^{\mathsf{T}}y = 0. \end{cases}$$

In the matrix-vector form, if we take the unknown vector in aggregated form as $(y, x)^{\top}$, the above is equivalent to the equation

$$\begin{pmatrix} I & A \\ A^{\top} & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix},$$
(11)

¹Later, a similar definition of dependent intervals was given in [8].

where I is the identity $m \times m$ -matrix, 0 in the matrix is zero $n \times n$ -matrix, and 0 in the righthand side vector is the zero *n*-vector. System (11) is a symmetric square linear system of the size m + n.

To solve the interval linear least squares problem (6), we can intervalize system (11), which gives

$$\begin{pmatrix} I & \mathbf{A} \\ \mathbf{A}^{\top} & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 0 \end{pmatrix}.$$
 (12)

We need computing an enclosure of its solution set with respect to the variable x, that is, for the set

$$\left\{ x \in \mathbb{R}^n \mid \begin{pmatrix} I & A \\ A^\top & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix} \text{ for some } A \in \mathbf{A} \text{ and } b \in \mathbf{b} \right\}.$$
 (13)

System (12) is an symmetric interval system of linear equations, that is, a system of linear algebraic equations in which the elements of the matrix and right-hand side vector can vary within prescribed intervals, but in such a way that the resulting matrix is always symmetric. Such systems are the simplest representatives of the so-called interval systems of equations with dependent parameters (or "tied interval systems of equations"), but in symmetric interval linear systems, the dependence between the parameters has a fairly simple form that can be handled by existing numerical methods. In particular, the so-called PPS-methods (based on Partitioning of the Parameter Set and developed in [25, 27, 28]) can be applied for enclosing the solution set (13) for system (12). This is the main idea of our work.



Figure 1: The least squares solution set to the interval linear system (15).

There is another way to reduce the normal system $A^{\top}Ax = A^{\top}b$ to an extended linear system. If we denote y = Ax, then -y + Ax = 0, and the normal system can be rewritten as

$$\begin{pmatrix} -I & A \\ A^{\top} & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} 0 \\ A^{\top}b \end{pmatrix}.$$
 (14)

This method is not as good for our purposes as the previous one, since the matrix of system (14) is almost the same, but the product $A^{\top}b$ appears in the right-hand side. The latter means

that the right-hand side is dependent on the matrix of the system, and in the interval context this problem is more complex than (12).

We consider, as an example, the interval linear system

$$\begin{pmatrix} [-13, -11] & [-7, -5] \\ [-3, -1] & [1, 3] \\ [5, 7] & [11, 13] \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} [-1, 0] \\ [0, 1] \\ [-1, 1] \end{pmatrix}.$$
(15)

Its least squares solution set, constructed by Monte-Carlo simulation, is depicted in Fig. 1.

The solution sets of symmetric interval linear systems of equations are known to have a structure which is significantly different from that of the solution sets for usual interval linear systems with independent parameters. Thus, the solution sets of interval linear systems of equations are polyhedra, bounded by pieces of hyperplanes. The solution sets to symmetric interval linear systems of equations are bounded by pieces of hyperplanes and second-order (quadratic) algebraic surfaces [2, 18], being curvilinear in general. The least squares solution set (5) in full rank situation coincides with (10), and then, in its turn, with the solution set (13) to the symmetric interval linear system (12). As a consequence, if the interval matrix of the system has full rank, then the least squares solution sets have all the properties of the solution set for the symmetric case (which is seen from Fig. 1).

2 Theory

The problem we set in the first section will be solved with the help of the so-called PPS-methods proposed and developed in the works [25, 27, 28]. These methods are based on adaptive splitting (subdivision) of the interval parameters of the equations system into smaller subintervals and solving the resulting subsystems (also called *descendant systems*). Since the results produced by interval methods are more accurate for narrower interval data, the subdivision process leads to increasingly accurate estimates of the solution to the problem. Overall, PPS-methods can be considered as an extension of the well-known interval methods of global optimization, based on the adaptive "branch-and-bound" strategy, to the case of estimating solution sets of interval systems of equations, when the objective function is specified implicitly. We will see that in the next section.

The key point in the organization of PPS-methods is a way of splitting (subdividing) the interval elements of the equation system into subintervals. If the interval parameters of the system of linear algebraic equations are independent of each other in the sense of Definition 2, then the following statement is true:

Theorem 3 (Beeck-Nickel theorem) Let Ax = b be an interval system of linear algebraic equations with a regular matrix $A \in \mathbb{IR}^{n \times n}$, and let $\Xi(A, b)$ denote its united solution set, that is,

$$\Xi(\mathbf{A}, \mathbf{b}) = \big\{ x \in \mathbb{R}^n \mid (\exists A \in \mathbf{A}) (\exists b \in \mathbf{b}) (Ax = b) \big\}.$$

For any index $\nu \in \{1, 2, ..., n\}$, the exact coordinate estimates of the points from the solution set, i. e., the extreme values $\min\{x_{\nu} \mid x \in \Xi(\mathbf{A}, \mathbf{b})\}$ and $\max\{x_{\nu} \mid x \in \Xi(\mathbf{A}, \mathbf{b})\}$, are attained at the solutions to the "corner" systems of equations Ax = b, such that the matrix A and vector b are made up of endpoints of the interval elements of \mathbf{A} and \mathbf{b} respectively.

By virtue of the Beeck-Nickel theorem, PPS-methods can be organized so that the interval elements in the equations system are divided into their endpoints, that is, in the most advantageous way in which the interval parameters sequentially disappear (see the detailed derivation of this fact in [25, 28]). This greatly simplifies the implementation of PPS-methods and makes them very efficient in solving interval linear systems of moderate dimensions. But if the interval parameters of the equation system are dependent on each other, then the "endpoint splitting" of the intervals is no longer adequate, and we must split the parameter intervals into parts with non-zero widths, while maintaining the dependence between the parameters. Then the efficiency of PPS-algorithms becomes not so high as for the case of independent interval data.

For the problem considered in our work, when the symmetric interval system of linear equations is solved and the components of the right-hand side are independent of each other and of the matrix, we can apply a "mixed" subdivision strategy. Namely, the interval elements of the matrix will be split up into subintervals of nonzero width, whereas the components of the interval vector in the right side will be split up into their endpoints. Clearly, the "mixed" subdivision strategy is more effective than total subdivision of all interval elements of the system to their halves.

The theoretical basis for the "mixed" subdivision is the following result:

Theorem 4 Let a symmetric interval system of linear equations Ax = b be given with regular symmetric interval matrix $A = A^{\top} \in \mathbb{IR}^{n \times n}$ and right-hand side $b \in \mathbb{IR}^n$ such that its interval components are independent from each other and from the matrix A, and let Ξ_{sym} denote its united solution set, that is,

$$\Xi_{sym} = \left\{ x \in \mathbb{R}^n \mid (\exists A \in \mathbf{A}) (\exists b \in \mathbf{b}) (A = A^\top \& Ax = b) \right\}.$$

Then, for any $\nu \in \{1, 2, ..., n\}$, the exact component-wise estimates of the points from the united solution set Ξ_{sym} , i.e. $\min \{x_{\nu} \mid x \in \Xi_{sym}\}$ and $\max \{x_{\nu} \mid x \in \Xi_{sym}\}$, are attained at the point linear systems $\tilde{A}x = \tilde{b}$ for which the right-hand side vectors \tilde{b} are constructed of the endpoints of components of the interval vector \boldsymbol{b} .

Proof. Using Cramer's rule (see e.g. [13, 16, 31]), we can give expressions for each component of the solution to a system of linear algebraic equations Ax = b with $A \in \mathbf{A}$ and $b \in \mathbf{b}$:

$$x_{\nu} = \frac{\det \left(A_{:1}, \dots, A_{:,\nu-1}, b, A_{:,\nu+1}, \dots, A_{:n}\right)}{\det A}, \quad \nu = 1, 2, \dots, n,$$

where the numerator is the determinant of a matrix obtained from A by replacing its ν -th column $A_{:\nu}$ with the vector-column of the right-hand side b. Now, we are able to answer the question: how x_{ν} depends on the elements b_i of the right-hand side b?

From the properties of the determinant, we can conclude that, for any i = 1, 2, ..., n,

$$x_{\nu} = x_{\nu}(b_i) = \frac{\xi b_i + \eta}{\det A},\tag{16}$$

where ξ, η do not depend on b_i . These relations are valid for all values of the remaining components of the right-hand side b and all elements of the matrix A within the respective intervals. Now, the statement of the theorem follows from the monotonicity of the linear functions $x_{\nu}(b), \nu = 1, 2, ..., n$, of the arguments b_i determined by (16).

3 The simplest PPS-algorithm

3.1 A short overview of PPS-methods

If the system of linear algebraic equations Ax = b has a regular $n \times n$ -matrix $A = (a_{ij})$, then its solution x^* is known to be

$$x^* = A^{-1}b,$$

and its k-th components is $(A^{-1}b)_k$. For an interval linear system Ax = b with a regular interval $n \times n$ -matrix A, the united solution set

$$\Xi(\mathbf{A}, \mathbf{b}) = \{ x \in \mathbb{R}^n \mid (\exists A \in \mathbf{A}) (\exists b \in \mathbf{b}) (Ax = b) \}$$

can be equivalently represented as

$$\Xi(\boldsymbol{A},\boldsymbol{b}) = \bigcup_{A \in \boldsymbol{A}, \, b \in \boldsymbol{b}} A^{-1}b$$

Therefore, for any fixed index $\nu \in \{1, 2, \ldots, n\}$,

$$\min\left\{x_{\nu} \mid x \in \Xi(\boldsymbol{A}, \boldsymbol{b})\right\} = \min_{A \in \boldsymbol{A}, b \in \boldsymbol{b}} \left(A^{-1}b\right)_{\nu},$$

which means that our problem reduces to a global optimization problem

find min
$$\phi(A, b)$$
 over the interval box $\mathbf{A} \times \mathbf{b}$ (17)

for the objective function $\phi(A, b) := (A^{-1}b)_{\nu}$. To solve it, we can apply the well-known and developed interval global optimization methods, based on adaptive subdivision of the domain of the objective function (see e.g. [11, 22, 30]). A prerequisite for the application of these methods is the constructive estimation of the ranges of values of the objective function ϕ over interval boxes, or at least available estimates of this ranges from below (in the case of minimization problems).

The latter can be done using existing interval methods that compute interval enclosures for the united solution sets to interval linear systems, see [1, 11, 18, 19, 20, 30]. If, for any interval linear system Qx = r, we know an enclosure X for its solution set, $X \supseteq \Xi(Q, r)$, produced by an interval method, then

$$\underline{\boldsymbol{X}}_{\nu} \leq \min_{\boldsymbol{A} \in \boldsymbol{Q}, \, b \in \boldsymbol{r}} \phi(\boldsymbol{A}, b),$$

and the discrepancy between the left-hand and right-hand sides of the above inequality vanishes with decreasing widths of Q and r for most interval methods. Thus, the basic prerequisite for the application of interval global optimization methods to (17) is fulfilled, which results in PPS-methods [25, 28]. The facts that the objective function ϕ is specified implicitly in the optimization problem to be solved, and the estimates of its range of values are performed not in the usual way, through the solution of auxiliary interval linear systems, are secondary and should not be confusing.

In PPS-methods, we organize the adaptive subdivision of the initial interval linear system into systems with narrower interval elements and then sequentially solve them, computing increasingly accurate estimates for min $\{x_{\nu} \mid x \in \Xi(\mathbf{A}, \mathbf{b})\}$ from below (see details in [25, 28]). An important feature of PPS-methods is their ability to adapt to the problem being solved. In particular, the PPS-method can be terminated early, if we have exhausted the computing resources or the time allotted for solving the problem. As a result, an answer will still be obtained, i.e. we will get the desired lower estimate for min $\{x_{\nu} \mid x \in \Xi(\mathbf{A}, \mathbf{b})\}$.

3.2 PPS-methods for symmetric interval systems

3.2.1 A general idea

How can one adapt the computational scheme of PPS-methods for the case when the interval parameters of the equations system are dependent from each other in the sense of Definition 2?

If these dependencies can be described, for example, as additional inequalities or equalities on parameter values, then we should include these new conditions in the statement of the optimization problem (17). Then the objective function will not change, but its domain of definition, on which we search for the minimum, can change very significantly. It will not be the box $\mathbf{A} \times \mathbf{b}$ any longer, it should be its subset or even a set of smaller dimension than $\mathbf{A} \times \mathbf{b}$.

If the specific form of dependencies between the interval parameters of the system is known, then, to solve the problem, we can use the interval technique of constrained optimization, which is presented, for example, in the book [11]. But in some simple cases, processing additional restrictions on interval parameters can be performed very simply. Such a case is the symmetric interval system of linear equations Ax = b, in which $A = (a_{ij})$, $A^{\top} = A$ and point values a_{ij} , a_{ji} are taken from the respective intervals a_{ij} and a_{ji} so that $a_{ij} = a_{ji}$. Then the interval parameters a_{ij} and a_{ji} become identical, and we can, in fact, reduce the dimension of the domain of the objective function in (17): the total number of interval parameters, associated with the matrix, becomes just n(n + 1)/2 instead of n^2 .

In terms of subdivision procedure, the main ideas of our modification of the original PPSmethods are simple and natural, and they have been formulated in [27, 30]:

- instead of splitting the elements of the interval linear system to their endpoints, we will subdivide the interval parameters of the system into subintervals of nonzero widths, their union being equal to the initial interval;
- we subdivide the interval system so that the resulting systems ("descendant systems") conform to the dependencies (constraints) imposed on interval parameters of the system.

In particular, if a symmetric interval system of linear equations is considered, then, in a single partitioning act, we should simultaneously split two intervals symmetric with respect to the main diagonal of the matrix, so that the resulting interval subsystems again have symmetric interval matrices.

Let us give a rigorous exposition of the informal ideas expressed above. We introduce the following notation:

- *Encl* is a fixed numerical method for outer interval estimation (enclosing) of the symmetric solution sets for interval linear systems (we will call it *basic method*);
- $Encl(\boldsymbol{Q}, \boldsymbol{r})$ is an interval vector produced by the method Encl when applied to the interval linear system $\boldsymbol{Q}x = \boldsymbol{r}$, i.e., $Encl(\boldsymbol{Q}, \boldsymbol{r}) \in \mathbb{IR}^n$ being an interval box that encloses the symmetric solution set $\Xi_{sym}(\boldsymbol{Q}, \boldsymbol{r})$ for the system $\boldsymbol{Q}x = \boldsymbol{r}$,

$$Encl(\boldsymbol{Q},\boldsymbol{r}) \supseteq \Xi_{sym}(\boldsymbol{Q},\boldsymbol{r});$$

 $\Upsilon(\mathbf{Q}, \mathbf{r})$ is the lower endpoint of the ν -th component (for a given $\nu \in \{1, 2, ..., n\}$) of the enclosure for the solution set $\Xi_{sum}(\mathbf{Q}, \mathbf{r})$ produced by the method *Encl*, i.e.

$$\Upsilon(\boldsymbol{Q}, \boldsymbol{r}) := \underline{\left(\operatorname{Encl}(\boldsymbol{Q}, \boldsymbol{r})\right)_{\nu}}.$$
(18)

Since $\Xi_{sym}(\mathbf{A}, \mathbf{b}) \subseteq \Xi(\mathbf{A}, \mathbf{b})$, then traditional and well-developed methods of outer interval estimation of the solution set can be taken as basic methods, for example, those described e.g. in [1, 11, 19, 20, 30]. This means that the algorithm for estimating the solution sets to interval systems with dependencies (ties) between interval parameters is constructed from simple methods for the solution of interval systems with independent data.

Two natural requirements that we impose on the basic method *Encl* are as follows:

the estimate $\Upsilon(\boldsymbol{Q}, \boldsymbol{r})$ is inclusion monotonic with respect to the matrix \boldsymbol{Q} and vector \boldsymbol{r} , i. e., for any $\boldsymbol{Q}', \boldsymbol{Q}'' \in \mathbb{IR}^{n \times n}$ and $\boldsymbol{r}', \boldsymbol{r}'' \in \mathbb{IR}^n$, the inclusions $\boldsymbol{Q}' \subseteq \boldsymbol{Q}''$ and $\boldsymbol{r}' \subseteq \boldsymbol{r}''$ imply $\Upsilon(\boldsymbol{Q}', \boldsymbol{r}') \geq \Upsilon(\boldsymbol{Q}'', \boldsymbol{r}'')$ (C1)

and

the estimate
$$\Upsilon(\boldsymbol{Q}, \boldsymbol{r})$$
 is exact for point linear algebraic systems,
i.e. $\Upsilon(\boldsymbol{Q}, r) = (Q^{-1}r)_{\nu}$ for every $Q \in \mathbb{R}^{n \times n}$ and $r \in \mathbb{R}^{n}$. (C2)

If the basic method Encl is a natural interval extension of a point (non-interval) method (such as the interval Gauss method for linear systems), or, more generally, the result of the basic method Encl is obtained using only interval arithmetic operations, then property (C1) is obviously satisfied due to the inclusion monotonicity of interval arithmetic. Otherwise, if noninterval operations are encountered in the algorithm of the basic method, then property (C1) may be violated. We assign to program developers to check whether a particular basic method satisfies property (C1).

We have

$$\min\{x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{A}, \boldsymbol{b})\} = (\tilde{A}^{-1}\tilde{b})_{\mu}$$

for a certain symmetric point matrix $\tilde{A} = (\tilde{a}_{ij}) \in \mathbb{R}^{n \times n}$ and a point vector $\tilde{b} = (\tilde{b}_i) \in \mathbb{R}^n$ made up of representatives of the elements of the matrix A and vector b. Then, according to the very definition of the estimate Υ ,

$$\Upsilon(\tilde{A}, \tilde{b}) \leq \left(\tilde{A}^{-1}\tilde{b}\right)_{\nu}$$

3.2.2 Subdivision of the interval matrix of the system

Suppose that, for a certain pair of the indices $k, l \in \{1, 2, ..., n\}$, the elements a_{kl} and a_{lk} in the matrix A, symmetric with respect to the main diagonal, have non-zero width. Let

- A' be the matrix obtained from A by replacing the elements a_{kl} and a_{lk} with $[\underline{a}_{kl}, \operatorname{mid} a_{lk}]$,
- A'' be the matrix obtained from A by replacing the elements a_{kl} and a_{lk} with [mid $a_{kl}, \overline{a}_{kl}$],
- \hat{A}' be the matrix obtained from \hat{A} by replacing the elements \tilde{a}_{kl} and \tilde{a}_{lk} with $[\underline{a}_{kl}, \text{mid } a_{kl}]$,
- $\tilde{\boldsymbol{A}}''$ be the matrix obtained from \tilde{A} by replacing the elements \tilde{a}_{kl} and \tilde{a}_{lk} with [mid $\boldsymbol{a}_{kl}, \overline{\boldsymbol{a}}_{kl}$].

Interval system of linear algebraic equations $\mathbf{A}' x = \mathbf{b}$ and $\mathbf{A}'' x = \mathbf{b}$, obtained from the original system by dissecting, to their halves, pairs of interval elements symmetric with respect to the main diagonal, will be called *descendant systems* of $\mathbf{A}x = \mathbf{b}$.

Inasmuch as

$$ilde{oldsymbol{A}}' \subseteq oldsymbol{A}' \subseteq oldsymbol{A}'' \subseteq oldsymbol{A}'' \subseteq oldsymbol{A}'' \subseteq oldsymbol{A}$$

and $\tilde{b} \subseteq \boldsymbol{b}$, then condition (C1) has, as a consequence, the inequalities

$$\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leq \Upsilon(\boldsymbol{A}', \boldsymbol{b}) \leq \Upsilon(\tilde{\boldsymbol{A}}', \tilde{b})$$

and

$$\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leq \Upsilon(\boldsymbol{A}'', \boldsymbol{b}) \leq \Upsilon(\tilde{\boldsymbol{A}}'', \tilde{b}).$$

Consequently, by taking the minimums from the corresponding parts of the inequalities, we get

$$\Upsilon(\boldsymbol{A},\boldsymbol{b}) \le \min\{\Upsilon(\boldsymbol{A}',\boldsymbol{b}),\Upsilon(\boldsymbol{A}'',\boldsymbol{b})\} \le \min\{\Upsilon(\tilde{\boldsymbol{A}}',\tilde{b}),\Upsilon(\tilde{\boldsymbol{A}}'',\tilde{b})\}.$$
(19)

In addition, since the matrix \tilde{A} is necessarily contained either in \tilde{A}' or in \tilde{A}'' , then at least one of the inequalities

$$\Upsilon(\tilde{\boldsymbol{A}}',\tilde{b}) \leq \Upsilon(\tilde{A},\tilde{b}) \qquad \text{ or } \qquad \Upsilon(\tilde{\boldsymbol{A}}'',\tilde{b}) \leq \Upsilon(\tilde{A},\tilde{b})$$

is fulfilled. Taking the minimum of the left-hand sides of these inequalities, we get

$$\min\{\Upsilon(\tilde{\boldsymbol{A}}',\tilde{b}),\Upsilon(\tilde{\boldsymbol{A}}'',\tilde{b})\} \leq \Upsilon(\tilde{A},\tilde{b}) \leq (\tilde{A}^{-1}\tilde{b})_{\nu} = \min\{x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{A},\boldsymbol{b})\}.$$
 (20)

Comparison of inequalities (19) and (20) leads to the relation

$$\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leq \min \{ \Upsilon(\boldsymbol{A}', \boldsymbol{b}), \Upsilon(\boldsymbol{A}'', \boldsymbol{b}) \} \leq \min \{ x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{A}, \boldsymbol{b}) \},$$

and, hence, to the following practical prescription: solving two interval "descendant systems" $\mathbf{A}'x = \mathbf{b}$ and $\mathbf{A}''x = \mathbf{b}$, in which \mathbf{A}' and \mathbf{A}'' are obtained by dividing an interval element in the matrix \mathbf{A} to its halves, we generally come to a more accurate lower bound for the desired value min{ $x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})$ }, in the form of min{ $\Upsilon(\mathbf{A}', \mathbf{b}), \Upsilon(\mathbf{A}'', \mathbf{b})$ }.

The same effect is achieved by splitting the right-hand side vector \boldsymbol{b} in some interval component \boldsymbol{b}_i into subintervals $[\underline{\boldsymbol{b}}_i, \operatorname{mid} \boldsymbol{b}_i]$ and $[\operatorname{mid} \boldsymbol{b}_i, \overline{\boldsymbol{b}}_i]$, which can be justified by calculations that are completely similar to (19)–(20). However, we can perform the subdivision of the right-hand side vector much more efficiently, based on the result of Theorem 4.

3.2.3 Subdivision of the right-hand side vector

Suppose that, for a certain index $k \in \{1, 2, ..., n\}$, the component \boldsymbol{b}_k in the vector \boldsymbol{b} has non-zero width. Let

b' be the vector obtained from b by replacing the component b_k with \underline{b}_k ,

 \boldsymbol{b}'' be the vector obtained from \boldsymbol{b} by replacing the component \boldsymbol{b}_k with $\overline{\boldsymbol{b}}_k$,

 $\tilde{\boldsymbol{b}}'$ be the vector obtained from \tilde{b} by replacing the component \tilde{b}_k with $\underline{\boldsymbol{b}}_k$,

 $\tilde{\boldsymbol{b}}''$ be the vector obtained from \tilde{b} by replacing the component \tilde{b}_k with $\overline{\boldsymbol{b}}_k$.

Inasmuch as

$$ilde{m{b}}' \subseteq m{b}' \subseteq m{b}, \qquad \qquad ilde{m{b}}'' \subseteq m{b}'' \subseteq m{b}$$

and $\tilde{A} \subseteq \mathbf{A}$, then condition (C1) has, as a consequence, the inequalities

$$\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leq \Upsilon(\boldsymbol{A}, \boldsymbol{b}') \leq \Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}')$$

and

$$\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leq \Upsilon(\boldsymbol{A}, \boldsymbol{b}'') \leq \Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}'').$$

Consequently, by taking the minimums from the corresponding parts of the inequalities, we get

$$\Upsilon(\boldsymbol{A},\boldsymbol{b}) \leq \min\left\{\Upsilon(\boldsymbol{A},\boldsymbol{b}'),\Upsilon(\boldsymbol{A},\boldsymbol{b}'')\right\} \leq \min\left\{\Upsilon(\tilde{A},\tilde{\boldsymbol{b}}'),\Upsilon(\tilde{A},\tilde{\boldsymbol{b}}'')\right\}.$$
(21)

In addition, since the vector \tilde{b} is necessarily contained either in \tilde{b}' or in \tilde{b}'' , then at least one of the inequalities

$$\Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}') \leq \Upsilon(\tilde{A}, \tilde{b})$$
 or $\Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}'') \leq \Upsilon(\tilde{A}, \tilde{b})$

is fulfilled. Taking the minimum of the left-hand sides of these inequalities, we get

$$\min\{\Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}'), \Upsilon(\tilde{A}, \tilde{\boldsymbol{b}}'')\} \le \Upsilon(\tilde{A}, \tilde{b}) \le (\tilde{A}^{-1}\tilde{b})_{\nu} = \min\{x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{A}, \boldsymbol{b})\}.$$
(22)

Comparison of inequalities (21) and (22) leads to the relation

$$\Upsilon(\boldsymbol{A},\boldsymbol{b}) \leq \min\{\,\Upsilon(\boldsymbol{A},\boldsymbol{b}'),\,\Upsilon(\boldsymbol{A},\boldsymbol{b}'')\,\} \leq \min\{\,x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{A},\boldsymbol{b})\,\},\,$$

and, hence, to the following practical prescription: solving two interval "descendant systems" $\mathbf{A}x = \mathbf{b}'$ and $\mathbf{A}x = \mathbf{b}''$, in which \mathbf{b}' and \mathbf{b}'' are obtained by dividing an interval component in the right-hand side vector \mathbf{b} to its endpoints, we generally come to a more accurate lower bound for the desired value min{ $x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})$ }, in the form of min{ $\Upsilon(\mathbf{A}, \mathbf{b}'), \Upsilon(\mathbf{A}, \mathbf{b}'')$ }.

From now on, for consistency, we agree to denote descendants systems, obtained from Ax = b by halving two symmetric interval elements in the matrix A or by splitting to endpoints one interval element in b, through A'x = b' and A''x = b''.

3.2.4 An overall algorithm

The procedure improving the estimate for $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}$ by splitting the elements of the interval system (12) can be repeated with respect to the descendant systems $\mathbf{A}'x = \mathbf{b}'$ and $\mathbf{A}''x = \mathbf{b}''$. Then we can split again the descendants of $\mathbf{A}'x = \mathbf{b}'$ and $\mathbf{A}''x = \mathbf{b}''$ and further improve the estimate, and so on. We will formalize this process of successive improving the lower bound for $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}$ in the way implemented in the well-known "branch-and-bound" method of combinatorial optimization [21] and how it was adapted for interval methods of global optimization (see, for example, books [11, 22]):

first, we organize all the interval systems Qx = r that result from splitting the original interval system Ax = b, together with their estimates $\Upsilon(Q, r)$, in the form of records (structures) that will be stored in a special working list \mathcal{L} ;

Table 1: The simplest PPS-method for symmetric interval systems

Input

A symmetric interval linear system Ax = b.

A number $\nu \in \{1, 2, ..., n\}$ of the component to be estimated.

A method *Encl* that computes the estimate Υ according to the rule (18). A constant $\epsilon > 0$.

Output

An estimate Z from below for $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}.$

Algorithm

assign $\boldsymbol{Q} \leftarrow \boldsymbol{A}$ and $\boldsymbol{r} \leftarrow \boldsymbol{b}$;

compute the estimate $v \leftarrow \Upsilon(\boldsymbol{Q}, \boldsymbol{r});$

initialize the working list $\mathcal{L} \leftarrow \{ (\boldsymbol{Q}, \boldsymbol{r}, \upsilon) \};$

DO WHILE ((maximum width of the elements from Q and r) $\leq \epsilon$)

in the matrix $\boldsymbol{Q} = (\boldsymbol{q}_{ij})$ and vector $\boldsymbol{r} = (\boldsymbol{r}_i)$, we choose the interval element \boldsymbol{s} having the maximum width;

generate the interval descendant systems Q'x = r' and Q''x = r'':

$$\begin{split} \text{if } \boldsymbol{s} &= \boldsymbol{q}_{kl} \text{ for some } k,l \in \{1,2,\ldots,n\}, \text{ then assign} \\ \boldsymbol{q}'_{ij} \leftarrow \boldsymbol{q}''_{ij} \leftarrow \boldsymbol{q}_{ij} \text{ for } (i,j) \neq (k,l) \text{ or } (i,j) \neq (l,k), \\ \boldsymbol{q}'_{lk} \leftarrow \boldsymbol{q}'_{kl} \leftarrow [\ \underline{\boldsymbol{q}}_{kl}, \text{mid } \boldsymbol{q}_{kl}], \ \boldsymbol{q}''_{lk} \leftarrow \boldsymbol{q}''_{kl} \leftarrow [\ \text{mid } \boldsymbol{q}_{kl}, \overline{\boldsymbol{q}}_{kl}], \\ \boldsymbol{r}' \leftarrow \boldsymbol{r}'' \leftarrow \boldsymbol{r}; \end{split}$$

if $\boldsymbol{s} = \boldsymbol{r}_k$ for some $k \in \{1, 2, ..., n\}$, then assign $\boldsymbol{Q}' \leftarrow \boldsymbol{Q}'' \leftarrow \boldsymbol{Q}, \ \boldsymbol{r}'_k \leftarrow \underline{\boldsymbol{r}}_k, \ \boldsymbol{r}''_k \leftarrow \overline{\boldsymbol{r}}_k,$ $\boldsymbol{r}'_i \leftarrow \boldsymbol{r}''_i \leftarrow \boldsymbol{r}_i \text{ for } i \neq k;$

compute the estimates $v' \leftarrow \Upsilon(\mathbf{Q}', \mathbf{r}')$ and $v'' \leftarrow \Upsilon(\mathbf{Q}'', \mathbf{r}'')$;

delete the late leading record $(\boldsymbol{Q}, \boldsymbol{r}, \upsilon)$ from the working list \mathcal{L} ;

put the records $(\mathbf{Q}', \mathbf{r}', v')$ and $(\mathbf{Q}'', \mathbf{r}'', v')$ into the working list \mathcal{L} , keeping its ordering with respect to the third field;

denote the first record of the list by $(\boldsymbol{Q}, \boldsymbol{r}, v)$;

END DO

 $Z \leftarrow v;$

- second, we split such interval system Qx = r from the list \mathcal{L} that provides the smallest current estimate of $\Upsilon(Q, r)$ for the value min{ $x_{\nu} \mid x \in \Xi_{sym}(A, b)$ };
- third, in the interval system chosen from the list \mathcal{L} for splitting, we subdivide the element with the maximum width.

So, in the process of executing the algorithm, we will maintain a list \mathcal{L} , consisting of triples of the form

$$(\boldsymbol{Q}, \boldsymbol{r}, \Upsilon(\boldsymbol{Q}, \boldsymbol{r})),$$
 (23)

where \boldsymbol{Q} is an interval $n \times n$ -matrix, $\boldsymbol{Q} \subseteq \boldsymbol{A}$,

 \boldsymbol{r} is an interval *n*-vector, $\boldsymbol{r} \subseteq \boldsymbol{b}$.

In addition, the records that form \mathcal{L} will be ordered in ascending order of the values of the estimate $\Upsilon(\mathbf{Q}, \mathbf{r})$, and the first record of the list, as well as the corresponding interval system $\mathbf{Q}x = \mathbf{r}$ and the estimate $\Upsilon(\mathbf{Q}, \mathbf{r})$ (record #1 in the list) will be called *leading* at the current step. The complete pseudocode of the resulting new algorithm, which we call PPS-method (meaning <u>Partitioning Parameter Set</u>), is presented in Table 1 (where " \leftarrow " denotes the assignment operator). It differs from the PPS-methods presented in [25, 28] by the process of generating interval descendant systems from the leading interval system and the termination criterion.

How close the result of the algorithm and the desired $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}$ will be to each other depends, on the one hand, on the numerical method by which we compute the estimate $\Upsilon(\mathbf{Q}, \mathbf{r})$, i. e., on the basic method chosen for solving the descendant systems. On the other hand, this depends on the sensitivity of the solution to the point systems that form the last leading system (that can be evaluated during the execution of the algorithm). In particular, in order for the value calculated by the algorithm to tend to $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}$) for $\epsilon \to 0$, it is necessary and sufficient to fulfill condition (C2). If, in the original interval system, the total width of interval elements is "large" compared to ϵ , then, as a rule, the simplest PPS-method will not work until the end, and therefore it is more expedient to consider it as an iterative refinement procedure.

4 Modification of PPS-methods for symmetric systems

The simplest algorithm we considered in the previous section computes a solution to our problem, but in reality it may take too much time and memory to find estimates for the symmetric solution set in real-life problems. In order to make the algorithm more practical, we have to supplement it with additional improvements that increase its overall efficacy.

4.1 Monotonicity test

Let us be given a system of linear algebraic equations Qx = r with a symmetric matrix $Q = (q_{ij})$, $Q^{\top} = Q$, and a right-hand side vector $r = (r_i)$. Suppose that the elements of the matrix Qand r vary within some intervals and the matrix Q remains symmetric in this variation. We can say then that a symmetric interval linear system Qx = r is defined. Recall a fact from calculus: the solution vector of a system of linear algebraic equations with a nonsingular matrix is a smooth (continuously differentiable) function of the elements of this and of the components of the right-hand side vector. The same is true for systems of linear equations with symmetric matrices. Consequently, we can investigate the monotonicity of the individual components of the solution, i.e. their increase or decrease relative to certain arguments, using standard tools of differential calculus. Assume that we know interval enclosures of the derivatives

$$\frac{\partial x_{\nu}(Q,r)}{\partial q_{ij}}$$
 and $\frac{\partial x_{\nu}(Q,r)}{\partial r_i}$

of the ν -th component of the solution x(Q, r) to the point symmetric system Qx = r with respect to the *ij*-th entry of the matrix Q and *i*-th element of the vector r. We will denote these interval enclosures by

$$rac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial q_{ij}}$$
 and $rac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial r_{i}}$

respectively. Now, if we take a symmetric interval $n \times n$ -matrix $\tilde{Q} = (\tilde{q}_{ij})$ and an interval n-vector $\tilde{r} = (\tilde{r}_i)$ with their elements in the form

$$\tilde{\boldsymbol{q}}_{ij} = \begin{cases} \left[\underline{\boldsymbol{q}}_{ij}, \underline{\boldsymbol{q}}_{ij}\right] & \text{for} & \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial q_{ij}} \ge 0, \\\\ \left[\overline{\boldsymbol{q}}_{ij}, \overline{\boldsymbol{q}}_{ij}\right] & \text{for} & \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial q_{ij}} \le 0, \\\\ \boldsymbol{q}_{ij} & \text{for} & \text{int} \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial q_{ij}} \ni 0 \end{cases}$$
(24)

and

$$\tilde{\boldsymbol{r}}_{i} = \begin{cases} [\underline{\boldsymbol{r}}_{i}, \underline{\boldsymbol{r}}_{i}] & \text{for} & \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial r_{i}} \geq 0, \\ \\ [\overline{\boldsymbol{r}}_{i}, \overline{\boldsymbol{r}}_{i}] & \text{for} & \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial r_{i}} \leq 0, \\ \\ \boldsymbol{r}_{i} & \text{for} & \text{int} \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial r_{i}} \geq 0, \end{cases}$$
(25)

then, obviously,

$$\min\{x_{\nu} \mid x \in \Xi_{sym}(\tilde{\boldsymbol{Q}}, \tilde{\boldsymbol{r}})\} = \min\{x_{\nu} \mid x \in \Xi_{sym}(\boldsymbol{Q}, \boldsymbol{r})\}$$
(26)

due to monotonicity reasons.

Then, since the number of interval elements (with nonzero widths) in \tilde{Q} and \tilde{r} may be substantially less than that in Q and r, reducing the interval system Qx = r to $\tilde{Q}x = \tilde{r}$ generally simplifies the computation of the desired min $\{x_{\nu} \mid x \in \Xi_{sym}(Q, r)\}$.

Earlier in the interval analysis, a number of numerical schemes have already used derivatives of the solution of system of linear algebraic equations with respect to matrix elements and righthand sides (see, e. g. [1]). Below, we derive formulas for these derivatives taking into account the symmetric form of the matrix of the equation system.

Let l and k be some fixed indices such that $1 \le k \le l \le n$. We rewrite the system of linear equations Qx = r in the expanded form

$$\sum_{j=1}^{n} q_{ij} x_j = r_i , \quad i = 1, 2, \dots, n,$$
(27)

and differentiate it with respect to q_{kl} . Since

$$\frac{\partial}{\partial q_{kl}}(q_{ij}x_j) = \frac{\partial q_{ij}}{\partial q_{kl}}x_j + q_{ij}\frac{\partial x_j}{\partial q_{kl}},$$

where

$$\frac{\partial q_{ij}}{\partial q_{kl}} = \begin{cases} 0, & \text{if } (i,j) \neq (k,l), \\ 1, & \text{if } (i,j) = (k,l), \end{cases}$$

we get from (27)

$$\begin{cases} \sum_{j=1}^{n} q_{ij} \frac{\partial x_j}{\partial q_{kl}} = 0, & \text{if } i \neq k \text{ and } i \neq l, \\ \sum_{j=1}^{n} q_{ij} \frac{\partial x_j}{\partial q_{kl}} + x_l = 0, & \text{if } i = k, \\ \sum_{j=1}^{n} q_{ij} \frac{\partial x_j}{\partial q_{kl}} + x_k = 0, & \text{if } i = l. \end{cases}$$

Therefore, if

$$\frac{\partial x}{\partial q_{kl}} = \left(\frac{\partial x_1}{\partial q_{kl}}, \dots, \frac{\partial x_n}{\partial q_{kl}}\right)^\top,$$

then

$$Q \cdot \frac{\partial x}{\partial q_{kl}} = (0, \dots, 0, -x_l, 0, \dots, 0, -x_k, 0, \dots, 0)^\top$$

where $(-x_l)$ is in the k-th position of the vector, and $(-x_k)$ is in the l-th position. Hence,

$$\frac{\partial x}{\partial q_{kl}} = Q^{-1} \cdot (0, \dots, 0, -x_l, 0, \dots, 0, -x_k, 0, \dots, 0)^\top.$$

If $Y = (y_{ij})$ is the inverse matrix for Q, then the derivatives of the solution to the symmetric system of linear equation Qx = r with respect to the elements of the matrix are given by the formulas

$$\frac{\partial x}{\partial q_{kl}} = -y_{\nu k} x_l - y_{\nu l} x_k.$$

Differentiating of equalities (27) with respect to r_k results in simpler relations

$$\begin{cases} \sum_{j=1}^{n} q_{ij} \frac{\partial x_j}{\partial r_k} = 0, & \text{if } i \neq k, \\ \sum_{j=1}^{n} q_{ij} \frac{\partial x_j}{\partial r_k} + x_l = 1, & \text{if } i = k. \end{cases}$$

Therefore, if

$$\frac{\partial x}{\partial r_k} = \left(\frac{\partial x_1}{\partial r_k}, \dots, \frac{\partial x_n}{\partial r_k}\right)^\top,$$

then

$$Q \cdot \frac{\partial x}{\partial r_k} = (0, \dots, 0, 1, 0, \dots, 0)^\top,$$

where 1 is in the k-th position of the vector. Hence,

$$\frac{\partial x}{\partial r_k} = Q^{-1} \cdot (0, \dots, 0, 1, 0, \dots, 0)^\top.$$

If $Y = (y_{ij})$ is, as before, the inverse matrix for Q, then the derivatives of the solution of the symmetric system of linear equations Qx = r with respect to the components of the right-hand side vector are given by the formulas

$$\frac{\partial x_{\nu}}{\partial r_k} = y_{\nu k}.$$

Finally, let $\mathbf{Y} = (\mathbf{y}_{ij})$ be the inverse interval matrix for \mathbf{Q} , i.e., an interval enclosure for the set of inverse matrices from \mathbf{Q} ,

$$\boldsymbol{Y} \supseteq \{Q^{-1} \mid Q \in \boldsymbol{Q}\},\$$

and \boldsymbol{x}_k and \boldsymbol{x}_l be components of an interval vector \boldsymbol{x} such that $\boldsymbol{x} \supseteq \Xi_{sym}(\boldsymbol{Q}, \boldsymbol{r})$. Then we can take the following interval enclosures of the derivatives:

$$\frac{\partial x_{\nu}(\boldsymbol{Q},\boldsymbol{r})}{\partial q_{kl}} = -\boldsymbol{y}_{\nu k}\boldsymbol{x}_{l} - \boldsymbol{y}_{\nu l}\boldsymbol{x}_{k}, \qquad \frac{\partial \boldsymbol{x}_{\nu}(\boldsymbol{Q},\boldsymbol{r})}{\partial r_{k}} = -\boldsymbol{y}_{\nu k}.$$
(28)

To use the above results effectively, we will need to have some (rough) outer estimate \boldsymbol{x} for the solution set and outer estimates for the elements of the inverse interval matrix dirung the execution of the algorithm. This complicates the algorithm a bit, but does not pose a big problem.

Now, instead of triples $(\boldsymbol{Q}, \boldsymbol{r}, \upsilon)$, the working list \mathcal{L} of the algorithm will consist of records of the form

$$(\boldsymbol{Q}, \boldsymbol{r}, \upsilon, \boldsymbol{x}, \boldsymbol{Y}),$$

where Q, r are the interval matrix and right-hand side vector

of the interval linear "descendant systems" obtained

from the subdivision of the original system Ax = b,

- v is an estimate for min $\{x_{\nu} \mid x \in \Xi(Q, r)\}$ from below,
- \boldsymbol{x} is an enclosure of the solution set,

Y is an enclosure of the inverse interval matrix for Q.

4.2 Improving the subdivision process

The PPS-method we have constructed to solve our problem is an essentially iterative algorithm that provides the exact answer as the limit of a sequence. But it has a substantial distinction from the traditional iterative methods (considered e.g. in computational linear algebra) in that the complete convergence, when the error of the approximate solution becomes sufficiently small, requires so many steps that usually it is never carried out in practice when solving real problems. This is caused by the intractability of our problem, which requires a special organization of the algorithm to obtain the best possible results.

Suppose that $\mathcal{E}(N)$ is the error in estimating the solution set at the Nth iteration of an algorithm implementing the PPS-method. Fig. 2 shows a collection of graphs of $\mathcal{E}(N)$, where different graphs correspond to different subdivision strategies.² The error function \mathcal{E}^* has a higher decrease rate than the other error functions on the number of steps that are actually available to us (it is marked with a vertical dashed line in Fig. 2).

The last point is especially important since in practice we work within a relatively small starting area of a large set of steps necessary for the complete convergence of the algorithm. The actual error we have achieved with this or that version of the PPS-algorithm will depend

²The graphs at Fig. 2, of course, are idealized and depict the functions $\mathcal{E}(N)$ as smooth, whereas in reality they have a discrete "stepwise" character.



Figure 2: Error functions $\mathcal{E}(N)$ for various subdivision strategies in PPS-methods.

on the behavior of the error function $\mathcal{E}(N)$. According to the algorithm properties, all the functions $\mathcal{E}(N)$ are descending, but the more steep is the function decrease the better accuracy of the result we get with the PPS-algorithm in a finite number of its steps.

To generate subsystems, the main PPS-method selects, in each iteration, an interval element with the largest width from the interval system. The choice of the widest element is motivated by the well-known convergence result for interval global optimization algorithms based on "branch-and-bound" strategy (see [22, 26]), which are the nearest "relatives" of the PPS-methods. But sometimes the strategy of selecting the widest element is not optimal in the sense that it does not provide the fastest convergence to the solution for "not very large" values of N, which we can practically reach.

Therefore, we need a better subdivision strategy for the subsystems, which would provide at each step a faster improvement in the estimate for $\min\{x_{\nu} \mid x \in \Xi(\mathbf{Q}, \mathbf{r})\}$. One of the useful ideas that can help in this is the use of information about the speed of change of the objective function depending on changes of parameters of the system, i.e. information about its derivatives with respect to these parameters. For PPS-methods, this technique has been successfully applied in [25, 28] for interval linear systems with independent parameters.

In the following, we extend this strategy to symmetric interval linear systems. Let us consider two linear equations systems

$$\check{Q}x = r$$
 and $\hat{Q}x = r$

with the symmetric regular matrices $\check{Q} = (\check{q}_{ij})$ and $\hat{Q} = (\hat{q}_{ij})$ such that they differ only in the (k, l)-th and (l, k)-th entries, i. e. $\check{q}_{kl} = \check{q}_{lk} \neq \hat{q}_{kl} = \hat{q}_{lk}$ and the rest of the entries in \check{Q} and \hat{Q} coincide with each other. The Lagrange mean-value theorem implies that the difference between the ν -th components of the solutions to these systems can be represented as follows:

$$(\check{Q}^{-1}r)_{\nu} - (\hat{Q}^{-1}r)_{\nu} = \frac{\partial x_{\nu}(\check{Q}, r)}{\partial q_{kl}} \cdot \left(\check{q}_{kl} - \hat{q}_{kl}\right)$$
(29)

for some matrix $\tilde{Q} \in \Box\{\check{Q}, \hat{Q}\}$. Strictly speaking, \tilde{Q} belongs to the straight line segment that connects the matrices \check{Q} and \hat{Q} , but this is not so important.

Similarly, if the vectors $\check{r} = (\check{r}_i)$ and $\hat{r} = (\hat{r}_i)$ differ only in the k-th component and $\check{r}_k < \hat{r}_k$,

then it follows from the Lagrange mean-value theorem that

$$(Q^{-1}\check{r})_{\nu} - (Q^{-1}\hat{r})_{\nu} = \frac{\partial x_{\nu}(Q,\tilde{r})}{\partial r_k} \cdot \left(\check{r}_k - \hat{r}_k\right)$$
(30)

for some vector $\tilde{r} \in \Box\{\check{r}, \hat{r}\}.$

Now, let the symmetric interval matrices $\hat{\boldsymbol{Q}}$ and $\hat{\boldsymbol{Q}}$ be obtained from the interval matrix $\boldsymbol{Q} = (\boldsymbol{q}_{ij})$ by subdividing its elements \boldsymbol{q}_{kl} and \boldsymbol{q}_{lk} into the subintervals $\check{\boldsymbol{q}}_{kl} = \check{\boldsymbol{q}}_{lk} = [\underline{\boldsymbol{q}}_{kl}, \text{mid } \boldsymbol{q}_{kl}],$ $\hat{\boldsymbol{q}}_{kl} = \hat{\boldsymbol{q}}_{lk} = [\text{mid } \boldsymbol{q}_{kl}, \overline{\boldsymbol{q}}_{kl}].$ According these subsystems, we have the solutions set min $\{x_{\nu} \mid x \in \Xi(\check{\boldsymbol{Q}}, \boldsymbol{r})\}$ and min $\{x_{\nu} \mid x \in \Xi(\hat{\boldsymbol{Q}}, \boldsymbol{r})\}$ with the same right vector \boldsymbol{r} . Therefore, by the continuity of these quantities, it follows from (29) that

$$\min\{x_{\nu} \mid x \in \Xi(\hat{\boldsymbol{Q}}, \boldsymbol{r})\} - \min\{x_{\nu} \mid x \in \Xi(\check{\boldsymbol{Q}}, \boldsymbol{r})\} = \frac{\partial x_{\nu}(\dot{\boldsymbol{Q}}, \acute{\boldsymbol{r}})}{\partial q_{kl}} \cdot \operatorname{wid} \boldsymbol{q}_{kl}$$
(31)

for some matrix $\acute{Q} \in \boldsymbol{Q}$ and vector $\acute{r} \in \boldsymbol{r}$.

Similarly, let $\check{\boldsymbol{r}}$ and $\hat{\boldsymbol{r}}$ be the interval vectors obtained from the interval vector \boldsymbol{r} by subdividing its k-th component into the endpoints $\underline{\boldsymbol{r}}_k$ and $\overline{\boldsymbol{r}}_k$, that is, $\check{\boldsymbol{r}}_k = \underline{\boldsymbol{r}}_k$, $\hat{\boldsymbol{r}}_k = \overline{\boldsymbol{r}}_k$. We have again

$$\min\{x_{\nu} \mid x \in \Xi(\boldsymbol{Q}, \hat{\boldsymbol{r}})\} - \min\{x_{\nu} \mid x \in \Xi(\boldsymbol{Q}, \check{\boldsymbol{r}})\} = \frac{\partial x_{\nu}(Q, \check{\boldsymbol{r}})}{\partial r_{k}} \cdot \operatorname{wid} \boldsymbol{r}_{k}$$
(32)

for some matrix $\hat{Q} \in \mathbf{Q}$ and vector $\hat{r} \in \mathbf{r}$. Hence, the value of the product of the width of an interval element from either \mathbf{Q} or \mathbf{r} by the absolute value of the interval extension of the corresponding derivative may serve, in a sense, as a local measure of how the subdivision of the element affects min $\{x_{\nu} \mid x \in \Xi(\mathbf{Q}, \mathbf{r})\}$ and the size of the solution set. Therefore, in order to reduce the size of the solution set $\Xi(\mathbf{Q}, \mathbf{r})$ to the maximum extent, we need to subdivide such elements for which the quantities (31) or (32) have the maximum value.

Overall, to increase the convergence rate of the PPS-method, we recommend to subdivide the leading symmetric interval systems along the elements on which the maximum of the values

$$\left|\frac{\partial x_{\nu}(\boldsymbol{Q},\boldsymbol{r})}{\partial q_{ij}}\right| \cdot \operatorname{wid} \boldsymbol{q}_{ij}, \qquad \left|\frac{\partial x_{\nu}(\boldsymbol{Q},\boldsymbol{r})}{\partial r_{i}}\right| \cdot \operatorname{wid} \boldsymbol{r}_{i}$$
(33)

i, j = 1, 2, ..., n, is attained, that is, along the element providing the maximal product of width by the derivative estimate. Note that in order for the system to remain symmetric, after determining the subdivided element, its symmetric element should also be subdivided, if this element is selected in the matrix of the system.

4.3 Cleaning the working list

During the execution of PPS-methods, the size of the working lists that they generate may become large. Processing such lists is laborious and can take much time, which slows down the overall speed of the algorithm. At the same time, some subsystems of the original interval system that the working list stores never becomes leading records and thus will not effect the execution of the algorithm. We will call such subsystems, as well as the corresponding records, *unpromising*.

To improve the overall efficiency of the algorithm, it makes sense to design and implement a special procedure that reduces the size of the working list \mathcal{L} by detecting the unpromising records and deleting them from \mathcal{L} . This can be done through using the upper estimate of the sought-for minimum, as described for interval global optimization methods in [10, 11] and other works. In the context of PPS-methods, that was developed in [25, 27, 28]. If ω is an upper bound of the minimum, then any subsystem Qx = r, such that

$$\Upsilon(\boldsymbol{Q}, \boldsymbol{r}) > \omega, \tag{34}$$

cannot become the leading subsystem, and deleting it from the working list \mathcal{L} in no way affects the results of the algorithm.

Removing such unpromising records from the working list will be called its *cleaning*. It reduces the size of the working list and lessens the amount of memory used, which facilitates faster execution of the algorithm.

In the interval global optimization algorithms, the upper estimate ω is usually taken as the minimum of values of the objective function at various points from the domain of definition. In our situation, we have to compute, apart from the interval enclosures of the solution sets to subsystems, point solutions to some point systems within the interval subsystems. Solving the midpoint systems is, probably, the best choice from the general consideration, if we do not have any additional information about the location of the minimum. So, at each step of the algorithm, in addition to estimating min{ $x_{\nu} \mid x \in \Xi$ } for each partitioned systems Q'x = r' and Q''x = r'', we will compute solutions to the point systems

$$(\operatorname{mid} \mathbf{Q}') x' = \operatorname{mid} \mathbf{r}', \qquad (\operatorname{mid} \mathbf{Q}'') x'' = \operatorname{mid} \mathbf{r}''. \tag{35}$$

Then we assign

$$\omega \leftarrow \min\{x'_{\nu}, x''_{\nu}, \omega\},\$$

i.e. the new upper estimate is taken as the minimum of the previous value of ω and two newly computed values x'_{ν} and x''_{ν} . Then the upper estimate ω can be used in two ways.

First, we can test all newly generated subsystems by the inequality (34) before inserting them into the working list \mathcal{L} . If a subsystem satisfies inequality (34), then we "forget" about it, that is, do not put it into the working list.

Second, we can specially arrange looking through the working list \mathcal{L} and checking inequality (34), which was called "cleaning the working list". This procedure is time consuming, and it makes sense to do it not at every step of the algorithm, but after several steps, when the unpromising records accumulate. Yet another option is to fix a positive integer number M and make cleaning of the working list \mathcal{L} at every M-th step of the algorithm in which the change of the upper estimate ω occurred.

4.4 An overall algorithm

The pseudo-code in Table 2 below summarizes the modifications of the PPS-methods, developed in the preceding subsections, for outer estimation of the solution set sets to symmetric interval linear systems.

On input, it requires the same information as the simplest PPS-algorithm from Table 1:

- a symmetric interval linear system Ax = b,
- a number $\nu \in \{1, 2, \dots, n\}$ of the component to be estimated,
- a method Encl that computes the estimate Υ according to the rule (18),
- a precision constant $\epsilon > 0$.

Table 2: The modified PPS-method for symmetric interval systems

assign $\boldsymbol{Q} \leftarrow \boldsymbol{A}$ and $\boldsymbol{r} \leftarrow \boldsymbol{b}$;

compute the estimate $v \leftarrow \Upsilon(\boldsymbol{Q}, \boldsymbol{r});$

initialize the working list $\mathcal{L} \leftarrow \{ (\boldsymbol{Q}, \boldsymbol{r}, \upsilon, \boldsymbol{Y}, \boldsymbol{x}) \};$

DO WHILE ((maximum width of the elements from Q and r) $\leq \epsilon$)

using formulas (28), we compute interval enclosures for

$$rac{\partial x_{
u}(oldsymbol{Q},oldsymbol{r})}{\partial q_{ij}} \hspace{1cm} ext{and} \hspace{1cm} rac{\partial x_{
u}(oldsymbol{Q},oldsymbol{r})}{\partial r_i}$$

that correspond to interval elements q_{ij} and r_i with nonzero width;

"squeeze", according to (24)–(25), elements from Q and r for which the monotonicity of x_{ν} with respect to q_{ij} and r_i was revealed;

in the matrix $Q = (q_{ij})$ and vector $r = (r_i)$, we choose the interval element s which corresponds to the maximum product

$$\left| \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial q_{ij}} \right| \cdot \text{wid } \boldsymbol{q}_{ij}, \left| \frac{\partial x_{\nu}(\boldsymbol{Q}, \boldsymbol{r})}{\partial r_i} \right| \cdot \text{wid } \boldsymbol{r}_i, \quad i, j \in \{1, 2, \dots, n\};$$

generate the interval descendant systems Q'x = r' and Q''x = r'':

$$\begin{split} \text{if } \boldsymbol{s} &= \boldsymbol{q}_{kl} \text{ for some } k, l \in \{1, 2, \dots, n\}, \text{ then assign} \\ \boldsymbol{q}'_{ij} \leftarrow \boldsymbol{q}''_{ij} \leftarrow \boldsymbol{q}_{ij} \text{ for } (i, j) \neq (k, l) \text{ or } (i, j) \neq (l, k), \\ \boldsymbol{q}'_{lk} \leftarrow \boldsymbol{q}'_{kl} \leftarrow [\ \underline{\boldsymbol{q}}_{kl}, \text{mid } \boldsymbol{q}_{kl}], \ \boldsymbol{q}''_{lk} \leftarrow \boldsymbol{q}''_{kl} \leftarrow [\ \text{mid } \boldsymbol{q}_{kl}, \overline{\boldsymbol{q}}_{kl}], \\ \boldsymbol{r}' \leftarrow \boldsymbol{r}'' \leftarrow \boldsymbol{r}; \end{split}$$

if $\boldsymbol{s} = \boldsymbol{r}_k$ for some $k \in \{1, 2, \dots, n\}$, then assign

$$Q' \leftarrow Q'' \leftarrow Q, \ r'_k \leftarrow \underline{r}_k, \ r''_k \leftarrow \overline{r}_k, \ r''_k \leftarrow \overline{r}_k, \ r''_k \leftarrow \overline{r}_k,$$

 $r'_i \leftarrow r''_i \leftarrow r_i \text{ for } i \neq k;$

compute the estimates $v' \leftarrow \Upsilon(\mathbf{Q}', \mathbf{r}')$ and $v'' \leftarrow \Upsilon(\mathbf{Q}'', \mathbf{r}'')$;

compute interval enclosures for the "inverse interval matrices" $\mathbf{Y}' \supseteq (\mathbf{Q}')^{-1}$ and $\mathbf{Y}' \supseteq (\mathbf{Q}')^{-1}$;

compute the estimates $\Upsilon(\operatorname{mid} \mathbf{Q}', \operatorname{mid} \mathbf{r}')$ and $\Upsilon(\operatorname{mid} \mathbf{Q}'', \operatorname{mid} \mathbf{r}'')$, assign $\mu \leftarrow \min{\{\Upsilon(\operatorname{mid} \mathbf{Q}', \operatorname{mid} \mathbf{r}'), \Upsilon(\operatorname{mid} \mathbf{Q}'', \operatorname{mid} \mathbf{r}'')\}};$

delete the late leading record (Q, r, v, Y, x) from the list \mathcal{L} ;

if $v' \leq \omega$, then put the record (Q', r', v', Y', x')

into the list ${\mathcal L}$ keeping its ordering with respect to the third field;

if $v'' \leq \omega$, then put the record $(\boldsymbol{Q}'', \boldsymbol{r}'', v'', \boldsymbol{Y}'', \boldsymbol{x}'')$

into the list \mathcal{L} keeping its ordering with respect to the third field;

if $\omega > \mu$, then assign $\omega \leftarrow \mu$ and clean the working list \mathcal{L} : deleting from it all such records $(\boldsymbol{Q}, \boldsymbol{r}, \upsilon, \boldsymbol{Y}, \boldsymbol{x})$, that $\upsilon > \omega$;

denote the first record of the working list \mathcal{L} by $(\boldsymbol{Q}, \boldsymbol{r}, \boldsymbol{v}, \boldsymbol{Y}, \boldsymbol{x})$;

END DO

 $Z \leftarrow v;$

On output, we get an estimate Z from below for $\min\{x_{\nu} \mid x \in \Xi_{sym}(\mathbf{A}, \mathbf{b})\}$.

The worklist \mathcal{L} of the algorithm from Table 2 consists of five-membered records of the form

$$(\boldsymbol{Q}, \boldsymbol{r}, \Upsilon(\boldsymbol{Q}, \boldsymbol{r}), \boldsymbol{Y}, \boldsymbol{x}),$$

and the meaning and purpose of the individual members of this five was explained in the previous subsections (see, in particular, $\S4.1$). To get started with this algorithm, we need

- find preliminary rough enclosures for the united solution sets of the initial interval system and the "inverse interval matrix", i.e., compute $x \supseteq \Xi(A, b)$ and $Y \supseteq A^{-1}$,
- put $\Upsilon(\boldsymbol{A}, \boldsymbol{b}) \leftarrow \underline{\boldsymbol{x}}$ and $\omega \leftarrow +\infty$,
- initialize the working list \mathcal{L} with the record $(\mathbf{A}, \mathbf{b}, \underline{\mathbf{x}}, \mathbf{Y}, \mathbf{x})$.

To sum up, the algorithm described in Table 2 and applied to the auxiliary symmetric interval linear system (12) in order to solve the interval linear least-squares problem (6) for the system $\mathbf{A}x = \mathbf{b}$ will be called *ILSQ-PPS method*.

5 Numerical tests

In this section, we present results demonstrating the work of the ILSQ-PPS algorithm in a number of test problems. The ILSQ-PPS method was implemented using the interval package under Octave [14] on a laptop computer with Intel[®] Core i5-3337U CPU at 1.8 GHz and 6 GB RAM.

Example 1 Let us consider an interval 3×2 -system

$$\begin{pmatrix} [0,10] & 2\\ -1 & 3\\ 3 & -2 \end{pmatrix} \begin{pmatrix} x_1\\ x_2 \end{pmatrix} = \begin{pmatrix} 10\\ -20\\ 0 \end{pmatrix}$$
(36)

with only one interval element in the position (1, 1).

Its least squares solution set can be constructed analytically, if we reformulate the system in a parametric form as

$$\begin{pmatrix} t & 2 \\ -1 & 3 \\ 3 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 10 \\ -20 \\ 0 \end{pmatrix},$$

where $t \in [0, 10]$. Its normal linear system is

$$\begin{pmatrix} t^2 + 10 & 2t - 9\\ 2t - 9 & 17 \end{pmatrix} \begin{pmatrix} x_1\\ x_2 \end{pmatrix} = \begin{pmatrix} 10t + 20\\ -40 \end{pmatrix}.$$
 (37)

Therefore, according to Cramer's rule, we can express the components of the solution vector x(t) to (37):

$$x_1(t) = \frac{250t - 20}{13t^2 + 36t + 89}, \qquad \qquad x_2(t) = \frac{-60t^2 + 50t - 220}{13t^2 + 36t + 89}. \tag{38}$$

The graph of this parametric line is depicted in Fig. 3, and it coincides with the pictures of this solution set obtained in other ways. Now, if we implement ILSQ-PPS method for system (36), this yields the enclosure

$$\begin{pmatrix} [-0.2247, 2.3314] \\ [-3.2704, -1.6230] \end{pmatrix}$$

which is an optimal outer estimation for Fig. 3.

ł

Example 2 We consider a 6×2 -system Ax = b from [9] where

$$\mathbf{A} = \begin{pmatrix} [0.75, 1.25] & 1\\ [1.75, 2.25] & 1\\ [4.75, 5.25] & 1\\ [5.75, 6.25] & 1\\ [8.75, 9.25] & 1\\ [9.75, 10.25] & 1 \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} [2.25, 2.75]\\ [1.25, 1.75]\\ [3.25, 3.75]\\ [4.25, 4.75]\\ [7.25, 7.75]\\ [6.25, 6.75] \end{pmatrix}.$$
(39)

This system is obtained by "uniform intervalization" from the point linear least-squares problem with the following data:

$$A = \begin{pmatrix} 1 & 1 \\ 2 & 1 \\ 5 & 1 \\ 6 & 1 \\ 9 & 1 \\ 10 & 1 \end{pmatrix}, \qquad b = \begin{pmatrix} 2.5 \\ 1.5 \\ 3.5 \\ 4.5 \\ 7.5 \\ 6.5 \end{pmatrix}.$$
(40)

In the article [9], D. Gay presents a computational approach for estimation of the set of least squares solution (10). The essence of his approach is the use of the first order approximation of the solution to the problem (similar to the simplest sensitivity analysis) combined with the monotonicity examination. At the final stage, a set of endpoints within the interval matrix and



Figure 3: The least squares solution set to the interval linear system (36).

right-hand side is taken to produce the extreme values of the solution, thus constructing the lower and upper bounds of the enclosure.

The result of the above approach applied to system (39) in [9] is the following enclosure

$$\begin{pmatrix} [0.47, 0.736] \\ [0.205, 1.829] \end{pmatrix}$$

while the result of our method is more narrow estimate for the solution set of (39):

$$\begin{pmatrix} [0.5056, 0.7118] \\ [0.3363, 1.6503] \end{pmatrix}$$

Example 3 Let us consider a 3×2 -system Ax = b proposed by A.H. Bentbib in [4], such that

$$\boldsymbol{A} = \begin{pmatrix} [0.1, 0.3] & [0.9, 1.1] \\ [8.9, 9.1] & [0.4, 0.6] \\ [0.9, 1.1] & [6.9, 7.1] \end{pmatrix}, \qquad \boldsymbol{b} = \begin{pmatrix} [0.8, 1.2] \\ [-0.2, 0.2] \\ [1.8, 2.2] \end{pmatrix}, \qquad (41)$$

and compare the result obtained in [4] with that produced by ILSQ-PPS method. For the solution of the interval linear least squares problem, the article [4] develops an interval extension of QR-factorization based on Householder transformations, and the technique gives, for system (41), the interval box

$$\begin{pmatrix} [-0.0558, 0.0232] \\ [0.2560, 0.3486] \end{pmatrix}.$$

$$(42)$$

It is the best one among several results produced by various possible approaches to the interval linear least squares problem compared in [4]. With our ILSQ-PPS method, we obtain the box

$$\begin{pmatrix} [-0.0465, 0.0126] \\ [0.2616, 0.3454] \end{pmatrix}$$

that has a smaller width as compared to the Bentbib's result (42).

Next, let us replace, in system (41), the right-hand side \boldsymbol{b} with the vector

$$m{b}' = egin{pmatrix} [0.8, 1.2] \ [0.3, 0.7] \ [6.8, 7.2] \end{pmatrix}.$$

We thus obtain an interval system from the article [23], where J. Rohn considers a generalization, to overdetermined interval linear systems of equations, of the Hansen-Blick-Rohn method for enclosing the united solution sets. The united solution set for the interval system of equations is always included in the set of the least squares solutions (see [29]), and this is why we can compare the results obtained by our ILSQ-PPS method with those presented in [23]. The Rohn's method gives

$$\begin{pmatrix} [-0.0372, 0.0372] \\ [0.9471, 1.0548] \end{pmatrix},$$
(43)

while the result of ILSQ-PPS method is

$$\begin{pmatrix} [-0.0375, 0.0363] \\ [0.9467, 1.0543] \end{pmatrix}$$

We can see that the upper endpoints of both components have been improved in the above box, although the least squares solution set is usually wider than the united solution set, which is enclosed by (43).

Example 4 Consider an interval 3×2 -system of linear algebraic equations

$$\begin{pmatrix} \begin{bmatrix} 0,2 \end{bmatrix} & 2\\ -1 & \begin{bmatrix} 3,5 \end{bmatrix}\\ 5 & -2 \end{pmatrix} \begin{pmatrix} x_1\\ x_2 \end{pmatrix} = \begin{pmatrix} -3\\ 5\\ 7 \end{pmatrix}$$
(44)

with only 2 interval elements in its matrix.



Figure 4: The least squares solution set to the interval linear system (44).

The graph of the solution set to this system, depicted at Fig. 4, has curvilinear boundaries, which is not specific for the solution sets to interval linear systems with independent interval parameters. Again, ILSQ-PPS method gives

$$\begin{pmatrix} [0.8461, 1.6858] \\ [0.1538, 0.9889] \end{pmatrix},$$

which is an optimal enclosure of the least squares solution set for this system.

In the following two examples, to illustrate some of the features and performance of the ILSQ-PPS method, we provide a short statistic.

Example 5 Let us investigate the interval linear 3×2 -system (15) presented in Section 1:

$$\begin{pmatrix} [-13, -11] & [-7, -5] \\ [-3, -1] & [1, 3] \\ [5, 7] & [11, 13] \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} [-1, 0] \\ [0, 1] \\ [-1, 1] \end{pmatrix}.$$

The matrix A of the system satisfies inequalities (7) and (8) from Theorem 1 and 2, since

$$\rho(|\operatorname{mid} \boldsymbol{A}|^+ \cdot \operatorname{rad} \boldsymbol{A}) = 0.3636 < 1, \tag{45}$$

$$\frac{\sigma_{\min}(\text{mid } \mathbf{A})}{\sigma_{\max}(\text{rad } \mathbf{A})} = \frac{6.6332}{2.4495} \simeq 2.7080.$$
(46)

Using ILSQ-PPS method, we obtain the box

$$\begin{pmatrix} [-0.1460, 0.2222] \\ [-0.2222, 0.1998] \end{pmatrix}$$

which is the interval hull of the set of least squares solutions to the system considered. Table 3 shows some performance indicators of the ILSQ-PPS method, and the value of each indicator is displayed for both the lower and upper bounds of the components of the solution set.

		•		-	
Parameters	$ $ x_1		$oldsymbol{x}_2$		
	lower	upper	lower	upper	
Time	36.23	8.24	8.92	60.96	
Iter	132	27	29	225	
Error	$5.5 \cdot 10^{-6}$	$1.02 \cdot 10^{-15}$	$9.99 \cdot 10^{-16}$	$8.88\cdot10^{-16}$	

Table 3: The characteristics of the ILSQ-PPS method for Example 5

In Table 3, "Time" is the execution time, in seconds, of the ILSQ-PPS method, for the lower and upper bounds of each component of the solution set. "Iter" is the number of iterations for the same bounds and "Error" shows the difference between upper estimate and $\Upsilon(\mathbf{Q}, \mathbf{r})$ in the last iteration for each component of the solution set.

Finally, we present an example of a "moderate size" system.

Example 6 We take the Toft interval linear system, considered in the articles [17, 32], and add it to an overdetermined rectangular system that has the interval $m \times n$ -matrix (m > n) of the form

$$\boldsymbol{A} = \begin{pmatrix} \left[1-r,1+r\right] & 0 & \dots & 0 & \left[1-r,1+r\right] \\ 0 & \left[1-r,1+r\right] & \ddots & \vdots & \left[2-r,2+r\right] \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & \dots & 0 & \left[1-r,1+r\right] & \left[n-1-r,n-1+r\right] \\ \left[1-r,1+r\right] & \left[2-r,2+r\right] & \dots & \left[n-1-r,n-1+r\right] & \left[n-r,n+r\right] \\ \hline \\ \hline \left[\theta-s,\theta+s\right] & 0 & 0 & \dots & 0 \\ & \left[0,s\right] & \left[\theta-s,\theta+s\right] & 0 & \dots & 0 \\ & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ & & \left[0,s\right] & \dots & \left[0,s\right] & \left[\theta-s,\theta+s\right] & 0 \end{pmatrix} \end{pmatrix}$$
(47)

and the right-hand side m-vector

$$\boldsymbol{b} = \begin{pmatrix} [1 - R, 1 + R] \\ [1 - R, 1 + R] \\ \vdots \\ [1 - R, 1 + R] \end{pmatrix},$$

where r, s, θ and R are positive real numbers.

Table 4: The characteristics of the ILSQ-PPS method for Example 6							
Parameters	$ $ x_1		$oldsymbol{x}_{6}$		$oldsymbol{x}_{12}$		
	lower	upper	lower	upper	lower	upper	
Estimate	0.2200	0.3547	-0.1450	0.6649	0.1000	0.1661	
Time	27.02	31.87	34.31	275.39	17.60	19.91	
Iter	10	12	13	95	7	8	
Error	$6.0 \cdot 10^{-6}$	$9.0\cdot10^{-6}$	$1.4\cdot 10^{-14}$	$1.1\cdot 10^{-5}$	$6.7\cdot 10^{-6}$	$1.7\cdot 10^{-14}$	

Table 4 shows the results of the test runs for the 15×12 -system (47) corresponding to r = 0.1, s = 0.05, $\theta = 4$, and R = 0.2. For brevity, we present in Table 4 the performance of the ILSQ-PPS method for Example 6 with respect to only 3 selected components out of 12. The components 12 and 6 turn out to be the most complex for the solution, and the ILSQ-PPS method computed them most slowly.

In Example 6, the inequalities (7) and (8) are satisfied for A as follows:

$$\rho(|\operatorname{mid} \mathbf{A}|^{+} \cdot \operatorname{rad} \mathbf{A}) = 0.1964 < 1,$$

$$\frac{\sigma_{\min}(\operatorname{mid} \mathbf{A})}{\sigma_{\max}(\operatorname{rad} \mathbf{A})} = \frac{1}{0.4326} \simeq 2.3114.$$
(48)

In this case, inequalities (48) and Table 4 also show that criteria (7) and (8) influence the performance of the ILSQ-PPS method. The smaller the spectral radius $\rho(|\text{mid } A|^+ \cdot \text{rad } A)$ and the larger the difference between $\sigma_{\min}(\text{mid } A)$ and $\sigma_{\max}(\text{rad } A)$, the easier the problem for numerical solution by ILSQ-PPS method.

6 Conclusion

The paper presents a computational method for outer estimation of the least squares solution sets of interval systems of linear algebraic equations with a full-rank matrix. It is a further development of parameter partitioning methods (PPS-methods), adapted to the specifics of the linear least-squares problem.

The efficiency of the constructed method can be increased if the basic methods are not general-purpose methods designed for general interval linear systems with independent coefficients at unknowns, but specialized methods for symmetric interval linear systems, i.e. taking into account the symmetry of point matrices in the given interval matrix. Such is, for example, interval-affine Gauss method [3]. But this is the subject of further research.

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