



On the possibilistic approach to linear regression models involving uncertain, indeterminate or interval data



Michal Černý^{a,*}, Jaromír Antoch^b, Milan Hladík^{a,c}

^a Department of Econometrics, Faculty of Computer Science and Statistics, University of Economics, Prague, Winston Churchill Square 4, 13067 Prague, Czech Republic

^b Department of Probability and Mathematical Statistics, Faculty of Mathematics and Physics, Charles University, Prague, Sokolovská 83, 18675 Prague, Czech Republic

^c Department of Applied Mathematics, Faculty of Mathematics and Physics, Charles University, Prague, Malostranské náměstí 25, 11000 Prague, Czech Republic

ARTICLE INFO

Article history:

Received 14 September 2011

Received in revised form 29 March 2013

Accepted 28 April 2013

Available online 6 May 2013

Keywords:

Interval data

Uncertain data

Possibilistic regression

Computational complexity

ABSTRACT

We consider linear regression models where both input data (the observations of independent variables) and output data (the observations of the dependent variable) are affected by loss of information caused by uncertainty, indeterminacy, rounding or censoring. Instead of real-valued (crisp) data, only intervals are available. We study a possibilistic generalization of the least squares estimator, so called OLS-set for the interval model. Investigation of the OLS-set allows us to quantify whether the replacement of real-valued (crisp) data by interval values can have a significant impact on our knowledge of the value of the OLS estimator. We show that in the general case, very elementary questions about properties of the OLS-set are computationally intractable (assuming $P \neq NP$). We also focus on restricted versions of the general interval linear regression model to the crisp input case. Taking the advantage of the fact that in the crisp input – interval output model the OLS-set is a zonotope, we design both exact and approximate methods for its description. We also discuss special cases of the regression model, e.g. a model with repeated observations.

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1. Introduction

Consider the linear regression model

$$y = X\beta + \varepsilon, \quad (1)$$

where y denotes the vector of observations of the dependent variable, X denotes the design matrix of the regression model, β denotes the vector of unknown regression parameters and ε is the vector of disturbances. For the purposes of this paper, we do not need to make any special assumptions on probabilistic properties of ε . We just assume that for estimation of β a linear estimator can be used, i.e. an estimator of the form

$$\hat{\beta} = Qy, \quad (2)$$

where Q is a matrix. In particular we shall concentrate on the Ordinary Least Squares (OLS) estimator, which corresponds to the choice $Q = (X^T X)^{-1} X^T$ in (2). (As it is well-known, this estimator is a “good” estimator e.g. when the disturbances are independent, identically distributed, with zero mean and finite variance.) Nevertheless, the theory is also applicable for other linear

* Corresponding author.

E-mail addresses: cernym@vse.cz (M. Černý), antoch@karlin.mff.cuni.cz (J. Antoch), milan.hladik@vse.cz, hladik@kam.mff.cuni.cz (M. Hladík).

estimators, such as the Generalized Least Squares (GLS) estimator, which corresponds to the choice $Q = (X^T \Omega^{-1} X)^{-1} \Omega^{-1} X^T$ in (2), where Ω is either known or estimated covariance matrix of ε . Other examples include estimation methods which, at the beginning, exclude outliers and then apply OLS or GLS. These estimators are often used in analysis of contaminated data.

Throughout the paper, the symbol n stands for the number of observations and the symbol p stands for the number of regression parameters, as it is usual in statistics.

We shall treat X and y as constants representing observed values of the independent variables and the dependent variable, respectively. Then the tuple (X, y) is called *data* for the regression model (1).

1.1. Interval data in the linear regression model

We shall study the situation when the data (X, y) cannot be observed directly. Instead of y_i and X_{ij} , only intervals of the form $[\underline{y}_i, \bar{y}_i]$ and $[\underline{X}_{ij}, \bar{X}_{ij}]$ are available, where it is guaranteed that for all $i \in \{1, \dots, n\}$ and $j \in \{1, \dots, p\}$,

$$y_i \in [\underline{y}_i, \bar{y}_i] \quad \text{and} \quad X_{ij} \in [\underline{X}_{ij}, \bar{X}_{ij}],$$

where y_i denotes the i th element of y and X_{ij} denotes the (i, j) th element of X .

The replacement of real-valued (crisp) data by intervals is henceforth referred to as “censoring”. In some literature, this process is also called “trimming”, “uncertaintification” or “intervalization”.

1.2. Motivation

Inclusion of interval data in linear regression models is suitable for modeling variety of real-world problems. For example:

- The data (X, y) have been interval-censored. This is often the case of medical, epidemiologic or demographic data—only interval-censored data are published while the exact individual values are kept secret.
- Data are rounded. If we store data using data types of restricted precision, then instead of exact values we are only guaranteed that the true value is in an interval of width 2^{-d} where d is the number of bits of the data type for representation of the non-integer part. For example, if we store data as integers (i.e., $d = 0$), then we know only the interval $[\bar{y} - 0.5, \bar{y} + 0.5]$ instead of the exact value y , where \bar{y} is y rounded to the nearest integer. This application is important in the theory of reliable computing.
- The data are uncertain or unstable. For that reason it might be inappropriate to describe them in terms of fixed values (X, y) only.
- Categorical data may be sometimes interpreted as interval data; for example, credit rating grades can be understood as intervals of credit spreads over the risk-free yield curve.
- In econometric regression models, it is often the case that varying quantities are represented by their average or median values. For example, if the exchange rate for a period of 1 year should be included in the regression model, usually the average rate of that year is taken. However, it might be more appropriate to regard the exchange rate as an interval inside which the variable changes.
- Sometimes we use interval predictions as data in regression models. For example, consider a predictor of future inflation (an econometric model or a panel of experts, say), which is assumed to form inflation expectations. The predictions are interval. Then, another model—such as consumption model or capital expenditure model—uses the predicted inflation expectations as a regressor. Thus, the model has to be able to work with an interval regressor.

More applications of interval data in econometrics are found in [7]. Applications in information sciences can be found in [11]; see also applications in ergonomics [10], optimization and operational research [15,37,42,71], speech learning [45] and in pattern recognition [39,43].

A variety of methods for estimation of regression parameters in a regression with interval data has been developed; they are studied in statistics [8,22,36,41,44,49,55,76], where also robust regression methods have been proposed [32,50], in fuzzy theory [24,29,30,72–74] as well as in computer science [12,31,34]. An algebraic treatment of least squares methods for interval data has been considered in [5,18].

1.3. Crisp and interval numbers, vectors and matrices

We need to distinguish between real-valued data and interval data. In the context of this distinction, real-valued (or: numeric) data are called *crisp data*. Then, a *crisp number* is just a real number. Similarly, we say that a matrix/vector is *crisp* when we want to emphasize that all elements of the matrix/vector are real numbers (and not intervals). In general, the term “crisp” can be also understood as “non-interval”.

If two real matrices X_1, X_2 are of the same dimension, the relation $X_1 \leq X_2$ is understood componentwise.

Definition 1.

- (a) Let \underline{a} and \bar{a} be scalars such that $-\infty < \underline{a} \leq \bar{a} < \infty$. The *interval number* \mathbf{a} is the closed interval $[\underline{a}, \bar{a}]$.
 (b) Let $\underline{X} \leq \bar{X}$ be two $M \times N$ real matrices. The *interval matrix* $\mathbf{X} = [\underline{X}, \bar{X}]$ is the set

$$\{X \in \mathbb{R}^{M \times N} : \underline{X} \leq X \leq \bar{X}\}.$$

The *interval vector* $\mathbf{y} = [\underline{y}, \bar{y}]$ is a special case of the interval matrix with one column.

Interval numbers, vectors and matrices are typeset in boldface.

Arithmetic operations $+$ and \times with interval numbers $\mathbf{a} = [\underline{a}, \bar{a}]$ and $\mathbf{b} = [\underline{b}, \bar{b}]$ are defined in a natural way (see [1]):

$$\begin{aligned} \mathbf{a} + \mathbf{b} &= [\underline{a} + \underline{b}, \bar{a} + \bar{b}], \\ \mathbf{a} \cdot \mathbf{b} &= [\min\{\underline{a}\underline{b}, \underline{a}\bar{b}, \bar{a}\underline{b}, \bar{a}\bar{b}\}, \max\{\underline{a}\underline{b}, \underline{a}\bar{b}, \bar{a}\underline{b}, \bar{a}\bar{b}\}]. \end{aligned} \quad (3)$$

From the definition, the following lemma is obvious:

Lemma 2. *A finite sequence of sums and products of interval numbers is a bounded set.*

1.4. The possibilistic approach to linear regression models with interval data

To recall: we are in the situation that only intervals (\mathbf{X}, \mathbf{y}) are available instead of the exact values (X, y) and we know that $X \in \mathbf{X}$ and $y \in \mathbf{y}$. The replacement of real-valued data (X, y) by interval values (\mathbf{X}, \mathbf{y}) causes some loss of information. *The main aim of this text is to quantify how the loss of information caused by replacement of (X, y) by (\mathbf{X}, \mathbf{y}) (henceforth referred to as “censoring”)¹ influences our knowledge of the value of the OLS estimator $\hat{\beta}$.* In particular, our aim is to study tools which can help the analyst of data (\mathbf{X}, \mathbf{y}) to understand whether censoring of data can cause a “serious” uncertainty about $\hat{\beta}$.

The next definition generalizes of the notion of the estimator $\hat{\beta}$ for the case when the real-valued data (X, y) are replaced by intervals (\mathbf{X}, \mathbf{y}) in (1). The definition generalizes the notion of the OLS-set studied in [9].

Definition 3.

- (a) A tuple (\mathbf{X}, \mathbf{y}) , where \mathbf{X} is an $n \times p$ interval matrix and \mathbf{y} is an $n \times 1$ interval vector, is called *data of an interval regression model*, or just *interval model* for short.
 (b) The *OLS-set* of the interval model (\mathbf{X}, \mathbf{y}) is defined as

$$OLS(\mathbf{X}, \mathbf{y}) = \{\beta \in \mathbb{R}^p : (\exists X \in \mathbf{X})(\exists y \in \mathbf{y}) X^T X \beta = X^T y\}.$$

The motivation for the definition is straightforward. Our aim is to use OLS to obtain an estimate of the unknown vector of regression parameters β in the model (1). However, observations are censored, i.e., we only know intervals \mathbf{X} and \mathbf{y} that are guaranteed to contain the directly unobservable data (X, y) . Then, the set $OLS(\mathbf{X}, \mathbf{y})$ contains *all possible* values of OLS-estimates of β as X and y range over \mathbf{X} and \mathbf{y} , respectively. We say that $OLS(\mathbf{X}, \mathbf{y})$ is a *possibilistic* version of the notion of the OLS estimator.

The set $OLS(\mathbf{X}, \mathbf{y})$ captures the loss of information caused by censoring of the data included in the regression model. For a user of such a regression model, it is essential to understand whether the set $OLS(\mathbf{X}, \mathbf{y})$ is, in some sense, “large” or “small”; that is, whether the impact of the loss of information on our knowledge of the value of the OLS estimator may be considered to be serious or not. More generally, the user of (\mathbf{X}, \mathbf{y}) needs a suitable description of the set $OLS(\mathbf{X}, \mathbf{y})$. When $p = 2$ or $p = 3$, then the set can be visualized in the parameter space. However, in higher dimensions visualization is quite complicated. Hence we need methods for a suitable description of the set $OLS(\mathbf{X}, \mathbf{y})$; in particular, we would like to design computationally feasible methods. In Section 2 we shall show that this task is very hard from the computational point of view.

1.5. Two interpretations of the possibilistic approach

Possibilistic interpretation. If we do not assume any distribution on \mathbf{X} or \mathbf{y} , then the set $OLS(\mathbf{X}, \mathbf{y})$ contains all possible values of $\hat{\beta} = (X^T X)^{-1} X^T y$ as X ranges over \mathbf{X} and y ranges over \mathbf{y} . We also say that $OLS(\mathbf{X}, \mathbf{y})$ is a *covering* of $\hat{\beta}$.

The boundary of the set $OLS(\mathbf{X}, \mathbf{y})$ can be understood as the *worst-case impact* of interval censoring on our knowledge of the value of the estimator. The possibilistic approach then can be characterized as a tool for analysis of the worst case.

Probabilistic interpretation. If X and y are random variables such that the supports of the distributions of X and y are \mathbf{X} and \mathbf{y} , respectively, then $\hat{\beta} = (X^T X)^{-1} X^T y$ is a random variable satisfying $\Pr[\hat{\beta} \in OLS(\mathbf{X}, \mathbf{y})] = 1$. Then the covering $OLS(\mathbf{X}, \mathbf{y})$ can be regarded as a “region of 100% certainty about $\hat{\beta}$ ”.

¹ Though, for simplicity of presentation, we speak about “censoring”, it should be kept in mind that not only censoring, but also rounding, uncertainty, indeterminacy, instability or interval nature of data can be the reason for inclusion of intervals in the model.

In the theory of Sections 2–6, we do not treat (X, y) as random variables over (\mathbf{X}, \mathbf{y}) (though it is one of possible interpretations); hence we need no assumptions about their distribution. (The case when (X, y) are considered as random variables is studied in literature, see e.g. [68].)

1.6. Special cases of the interval regression model

An interval regression model $(\mathbf{X} = [\underline{X}, \overline{X}], \mathbf{y} = [\underline{y}, \overline{y}])$ is also called a *general model* or *interval input – interval output model*. Interesting special cases are (see [29,33]):

- (i) *crisp input – interval output model* is a model with $\underline{X} = \overline{X}$;
- (ii) *interval input – crisp output model* is a model with $\underline{y} = \overline{y}$;
- (iii) *crisp input – crisp output model* is a model with $\underline{X} = \overline{X}$ and $\underline{y} = \overline{y}$.

“Crisp input – crisp output” is just another name for the traditional model (1).

If \mathbf{X} is real-valued (crisp), i.e. if $\underline{X} = \overline{X} =: X$, then instead of $OLS(\mathbf{X}, \mathbf{y})$ we write $OLS(X, \mathbf{y})$. (And similarly in the case of \mathbf{y} crisp.)

1.7. The structure and contribution of the paper

Sections 2 and 6 are devoted to the OLS-set of the general model, its computational properties and approximation methods. In particular, we prove that very basic questions about the OLS set are computationally hard. In Section 3 we deal with a geometric characterization of the OLS-set of the crisp input – interval output model and prove several computational results. We also investigate special cases, such as models with repeated observations, where we can improve some results. In Section 4 we design and discuss methods for approximation of the OLS-set of the crisp input – interval output model and in Section 5 we propose a general meta-algorithm for construction of exact descriptions of the OLS-set of the crisp input – interval output model. Finally, in Section 6 we discuss several methods for computation of approximations (enclosures) of the OLS-set for the general interval input – interval output model.

2. The general model

Our aim is to find a description of the set $OLS(\mathbf{X}, \mathbf{y})$ given $\mathbf{X} = [\underline{X}, \overline{X}]$ and $\mathbf{y} = [\underline{y}, \overline{y}]$. Such a description may take a variety of forms—for example, we might try to find the smallest enclosing ellipse, to find the small enclosing box (i.e. interval vector) or to determine other characteristics of the set such as volume or diameter.

Theorem 4, which is the main result of this Section, shows that in general we cannot expect to be successful in a computationally feasible way. The point is that any reasonable description of $OLS(\mathbf{X}, \mathbf{y})$ must allow the user to decide whether the set is bounded or not. **Theorem 4** says that there is no polynomial-time method for this question (assuming $\mathbf{P} \neq \mathbf{NP}$).

Some complexity-theoretic notions. Before we state and prove **Theorem 4**, we briefly sketch some notions from complexity theory, which will be used throughout the paper. Details can be found e.g. in [3,56]. We assume that the following notions are well-known: \mathbf{P} , \mathbf{NP} , $co\text{-}\mathbf{NP}$, $\#P$, polynomial-time many-one reducibility, hardness and completeness for the classes \mathbf{NP} , $co\text{-}\mathbf{NP}$, $\#P$. (Recall that $\#P$ can be seen as a problem of computing the number of satisfying assignments of a given boolean formula.)

The symbol \mathbf{PF} stands for the class of total functions computable in Turing deterministic polynomial time.

2.1. The main result of Section 2

Theorem 4. Let $\underline{X}, \overline{X}, \underline{y}, \overline{y}$ be rational and denote $\mathbf{X} = [\underline{X}, \overline{X}]$ and $\mathbf{y} = [\underline{y}, \overline{y}]$. Deciding whether the set $OLS(\mathbf{X}, \mathbf{y})$ is bounded is a $co\text{-}\mathbf{NP}$ -hard problem.

Proof. Let \mathbf{X} be an $n \times p$ interval matrix. If there is $X \in \mathbf{X}$ with column rank $< p$, then for any y the set

$$\{\beta : X^T X \beta = X^T y\}$$

is an affine space of dimension at least one, and hence is unbounded.

Assume that for every $X \in \mathbf{X}$, the column rank of X is p . Then $(X^T X)^{-1}$ exists for each $X \in \mathbf{X}$. By Cramer’s Rule, we can write

$$((X^T X)^{-1})_{ij} = \pm \frac{\det(X^T X)^{[i,j]}}{\det(X^T X)}$$

where $A^{[i,j]}$ results from A by deleting the j th row and the i th column. By continuity of $\det(\cdot)$ on the compact set \mathbf{X} , the set

$$\{\det(X^T X) : X \in \mathbf{X}\}$$

is a closed interval which, by assumption, does not contain zero. It follows that the set

$$\left\{ \frac{1}{\det(X^T X)} : X \in \mathbf{X} \right\}$$

is a closed interval. Let us denote the interval $[\underline{d}, \bar{d}]$. Also the set

$$\{\det(X^T X)^{i|j} : X \in \mathbf{X}\}$$

is an interval of the form $[\underline{\delta}_{ij}, \bar{\delta}_{ij}]$. Hence we can write

$$\begin{aligned} \hat{\beta}_i &= \{(X^T X)^{-1} X^T y\}_i : X \in \mathbf{X}, y \in \mathbf{y}\} \\ &= \left\{ \sum_{j=1}^p \left[((X^T X)^{-1})_{ij} \cdot \sum_{k=1}^n X_{kj} \cdot y_k \right] : X \in \mathbf{X}, y \in \mathbf{y} \right\} \\ &\subseteq \sum_{j=1}^p \left[\pm [\underline{d}, \bar{d}] \cdot [\underline{\delta}_{ij}, \bar{\delta}_{ij}] \cdot \sum_{k=1}^n [\underline{X}_{kj}, \bar{X}_{kj}] \cdot [\underline{y}_k, \bar{y}_k] \right] \end{aligned}$$

and the last expression is a finite sequence of sums and products of intervals. By Lemma 2 it follows that it is a bounded set.

We have shown that the set $OLS(\mathbf{X}, \mathbf{y})$ is unbounded if and only if there is an $X \in \mathbf{X}$ such that the column rank of X is $< p$. In Section 3.19 of [63] it is shown that the latter problem is **NP**-hard. We have constructed a reduction from an **NP**-hard problem to the problem $C :=$ “is $OLS(\mathbf{X}, \mathbf{y})$ unbounded?”. It follows that the problem $co-C =$ “is $OLS(\mathbf{X}, \mathbf{y})$ bounded?” is **co-NP**-hard. \square

It follows that if we want to find a computationally feasible description of $OLS(\mathbf{X}, \mathbf{y})$ we must reformulate the problem. We can follow (at least) two ways:

- either to search for descriptions and/or approximations of $OLS(\mathbf{X}, \mathbf{y})$ which are guaranteed to be correct only under additional assumptions, or
- to consider special cases of the general model.

There is a variety of approaches to (a), see [1,25,27,28,35,52,63] and a comparison study [53]. Some of them will be discussed in Section 6.

In the next section we follow the way (b) and study the restriction to the crisp input – interval output model. Observe that this restriction is the only restriction among (i–iii) worth of further investigation. (Recall that the restrictions (i–iii) were defined in Section 1.6.) In the crisp input – crisp output model, the set $OLS(X, y)$ is trivial—it is either a single point or an affine space in the parameter space. And the restriction to the interval input – crisp output model is ruled out by the following observation.

Corollary 5 (to the proof of Theorem 4). Let \underline{X}, \bar{X} and y be rational and denote $\mathbf{X} = [\underline{X}, \bar{X}]$. Deciding whether the set $OLS(\mathbf{X}, y)$ is bounded is a **co-NP**-hard problem.

Proof. The reduction constructed in the proof of Theorem 4 remains valid also if \mathbf{y} is crisp. \square

Remark to Theorem 4. The hardness result of Theorem 4 does not guarantee decidability of the problem whether the set $OLS(\mathbf{X}, \mathbf{y})$ is unbounded. Let us show that the problem is decidable. (This fact is not obvious at the first sight.) We have seen that the set $OLS(\mathbf{X}, \mathbf{y})$ is unbounded iff there is a matrix $X \in \mathbf{X} = [\underline{X}, \bar{X}]$ which does not have full column rank. Assume that \underline{X} and \bar{X} are rational; then it is easy to see that if there is a matrix $X \in \mathbf{X}$ which does not have full column rank, then there is a rational matrix $X' \in \mathbf{X}$ which does not have full column rank. This observation proves that the problem is recursively enumerable—it suffices to enumerate all rational matrices $X \in \mathbf{X}$, using the fact that the set of all rational matrices $X \in \mathbf{X}$ is countable. (Notions of Recursion Theory can be found in [54].)

The assumption that \underline{X} and \bar{X} are rational implies that all entries of \underline{X} and \bar{X} can be multiplied by the common denominator of fractions occurring in \underline{X} and \bar{X} . It means that we can assume that \underline{X} and \bar{X} are integer matrices. The following holds: there is $X \in \mathbf{X}$ which does not have full column rank if and only if

$$(\exists X) [\underline{X} \leq X \leq \bar{X} \& \det X^T X = 0], \quad (4)$$

where X ranges over $\mathbb{R}^{n \times p}$. By the assumption of integrality of \underline{X} and \bar{X} , the expression (4) is a sentence in the language of arithmetic (see [23]) – indeed, $\det X^T X$ is a polynomial in X_{11}, \dots, X_{np} and thus can be expressed only with addition and multiplication.

Recall that the theory of Real Closed Fields (*RCF*) is a theory with arithmetical language which proves:

- basic properties of the theory of fields (in particular, closure under additive inversion and closure under multiplicative inversion for all nonzero elements);

- Bolzano’s Intermediate Value Theorem for all polynomials of one variable (with integer coefficients).

By Tarski’s Theorem [75], the theory RCF is complete. And \mathbb{R} is a model of RCF. It follows that there is an algorithmic procedure which decides whether the sentence (4) is true (in \mathbb{R})—it suffices to enumerate all proofs of RCF (using the fact that RCF is recursively axiomatizable) and wait until a proof of (4) or its negation appears. This proves decidability.

More can be found in [60–62,64].

3. Characterization of the set $OLS(X, \mathbf{y})$ in the crisp input – interval output model

In this section we assume that X is a crisp matrix with full column rank.

The aim of this section is twofold:

- we shall show a geometric characterization of the set $OLS(X, \mathbf{y})$;
- we shall show that though there are natural descriptions of the set $OLS(X, \mathbf{y})$, in general they cannot be computed in polynomial time.

Hence, from the computational point of view, the situation is (in some sense) as disappointing as in the general case. However, the reason is quite different, as we shall see in Theorem 10.

The negative complexity result gives a good motivation for finding approximations and for inspection of special cases. We will

- show interval and ellipsoidal approximations of the set $OLS(X, \mathbf{y})$;
- show that natural descriptions of the set $OLS(X, \mathbf{y})$ are polynomial-time constructible if we restrict ourselves to a fixed p (i.e., to a class of regression models with a fixed number of parameters).

3.1. Geometric characterization of the set $OLS(X, \mathbf{y})$

First we need to review some notions from geometry of convex polyhedra; for further reading see [77]. The next definition formalizes the Minkowski sum. In geometry literature the sum is usually defined more generally. The following simpler definition is sufficient for our purposes.

Definition 6. The *Minkowski sum* of a set $A \subseteq \mathbb{R}^k$ and a vector $g \in \mathbb{R}^k$ is the set

$$A \dot{+} g = \{a + \lambda g : a \in A, \lambda \in [0, 1]\}.$$

It is easily seen that for a convex set A , it holds

$$A \dot{+} g = \text{conv}(A \cup \{a + g : a \in A\}),$$

where *conv* denotes the convex hull.

Definition 7.

(a) The *zonotope* generated by $g_1, \dots, g_N \in \mathbb{R}^k$ with shift $s \in \mathbb{R}^k$ is the set

$$\mathcal{Z}(s; g_1, \dots, g_N) = (\dots((\{s\} \dot{+} g_1) \dot{+} g_2) \dot{+} \dots \dot{+} g_N).$$

The vectors g_1, \dots, g_N are called *generators*.

(b) The *dimension* of the zonotope $\mathcal{Z} = \mathcal{Z}(s; g_1, \dots, g_N)$, denoted $\text{dim}(\mathcal{Z})$, is the dimension of the linear space generated by g_1, \dots, g_N .

Instead of $(\dots((\{s\} \dot{+} g_1) \dot{+} g_2) \dot{+} \dots \dot{+} g_N)$ we shall write $\{s\} \dot{+} g_1 \dot{+} g_2 \dot{+} \dots \dot{+} g_N$ only.

It is easily seen that a zonotope is a convex polyhedron; see Fig. 1.

The following geometric characterization of the set $OLS(X, \mathbf{y})$ was derived in [9]; see also [21,69].

Theorem 8. Let $X \in \mathbb{R}^{n \times p}$ be a matrix of full column rank and $\mathbf{y} = [\underline{y}, \bar{y}]$ an $n \times 1$ interval vector. Then

$$OLS(X, \mathbf{y}) = \mathcal{Z}(Q\mathbf{y}; Q_1(\bar{y}_1 - \underline{y}_1), \dots, Q_n(\bar{y}_n - \underline{y}_n)),$$

where $Q = (X^T X)^{-1} X^T$ and Q_i is the i th column of Q . \square

There is an interesting geometric characterization of zonotopes. Namely, a set $\mathcal{Z} \subseteq \mathbb{R}^k$ is a zonotope if and only if there exists a number m , a matrix $Q \in \mathbb{R}^{k \times m}$ and an interval m -dimensional vector \mathbf{y} (called *m-dimensional cube*) such that $\mathcal{Z} = \{Q\mathbf{y} : \mathbf{y} \in \mathbf{y}\}$. The interesting case is $m > k$. In that case we can say that zonotopes are images of “high-dimensional” cubes

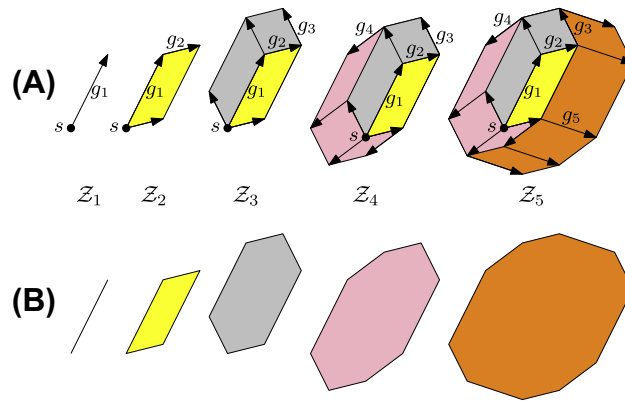


Fig. 1. A sequence of zonotopes $Z_1 = Z(s; g_1)$, $Z_2 = Z(s; g_1, g_2)$, \dots , $Z_5 = Z(s; g_1, g_2, g_3, g_4, g_5)$, called *evolution* of the zonotope $Z(s; g_1, g_2, g_3, g_4, g_5)$. (A) with generators Depicted and (B) the same zonotopes plotted simply as polytopes (without generators depicted).

in “low-dimensional” spaces under linear mappings, see Fig. 2. In our setting, the set $OLS(X, \mathbf{y})$ is an image of the cube \mathbf{y} under the mapping determined by the matrix $Q = (X^T X)^{-1} X^T$. (Recall that in standard crisp input – crisp output regression, this corresponds to the fact that the OLS-estimator $\hat{\beta}$ is the image of the output vector \mathbf{y} under the same mapping.)

In the next lemma we summarize basic symmetry properties of the zonotope $OLS(X, \mathbf{y})$. In fact, the symmetry properties hold for any zonotope.

Lemma 9.

- (a) The set $OLS(X, \mathbf{y})$ is centrally symmetric.
- (b) The center of $OLS(X, \mathbf{y})$ is $c := Q\mathbf{y} + \frac{1}{2} \sum_{i=1}^n Q_i(\bar{y}_i - \underline{y}_i)$.
- (c) Every face of the zonotope $OLS(X, \mathbf{y})$ is a zonotope; in particular, every face is centrally symmetric.
- (d) The point v is a vertex of $OLS(X, \mathbf{y})$ if and only if $c - 2v$ is a vertex.

Proof. The symmetry properties follow from the observation that Minkowski sum preserves central symmetry (i.e. if A is centrally symmetric, then $A+g$ is centrally symmetric). \square

3.2. Descriptions of the set $OLS(X, \mathbf{y})$

In order the user can understand what the set $OLS(X, \mathbf{y})$ looks like, she/he can use any standard description applicable for convex polyhedra. In particular, three descriptions come to mind:

- (a) description of the zonotope $OLS(X, \mathbf{y})$ by the shift vector and the set of generators;
- (b) description of the zonotope $OLS(X, \mathbf{y})$ by the enumeration of vertices;

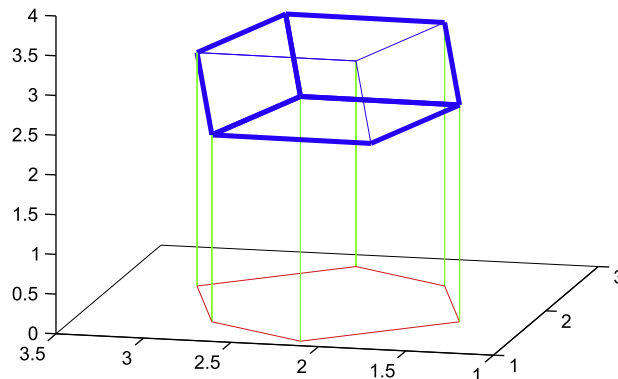


Fig. 2. A zonotope as an image of a higher-dimensional cube [9].

(c) description of the zonotope $OLS(X, \mathbf{y})$ by the enumeration of facets. Each facet of a polyhedron can be identified with a supporting halfspace (or hyperplane), i.e. with an inequality of the form $a^T x \leq \gamma$. Hence, construction of a facet description amounts to constructing a matrix A and a vector c such that $OLS(X, \mathbf{y}) = \{x \in \mathbb{R}^p: Ax \leq c\}$.

The description (a) has been given by the **Theorem 8**: we have

$$s = Q\underline{y}, \quad g_i = Q_i(\bar{y}_i - \underline{y}_i) \quad \text{for } i = 1, \dots, n. \tag{5}$$

The descriptions (b and c) will be investigated in Sections 3.3, 3.4 and 3.5. Algorithms for their construction will be studied in Section 5.

3.3. A negative complexity result

It is an interesting question whether there are efficient algorithms which can construct the enumerations (b and c) given X , \underline{y} and \bar{y} . We give an argument that the answer is negative. The answer follows from the simple fact that zonotopes can have too many vertices and facets. Let $V(\mathcal{Z})$ and $F(\mathcal{Z})$ denote the number of vertices and facets of a zonotope \mathcal{Z} , respectively.

Theorem 10. [77] *For a zonotope $\mathcal{Z} \subseteq \mathbb{R}^p$ with n generators it holds*

$$V(\mathcal{Z}) \leq 2 \sum_{k=0}^{p-1} \binom{n-1}{k} \quad \text{and} \quad F(\mathcal{Z}) \leq 2 \binom{n}{p-1}.$$

Moreover, the bounds cannot be improved: for each n and p there are p -dimensional zonotopes \mathcal{Z}_V and \mathcal{Z}_F with n generators such that $V(\mathcal{Z}_V)$ and $F(\mathcal{Z}_F)$ attain the bounds. \square

The numbers $V(\mathcal{Z})$ and $F(\mathcal{Z})$ cannot be bounded by a polynomial in n and p ; hence, the functions enumerating vertices and facets are not in **PF** for the simple reason that their output cannot be bounded by a polynomial in the size of the input. By the next lemma we know that this negative result also holds for zonotopes which are OLS-sets of crisp input – interval output regression models.

Lemma 11. *For every p -dimensional zonotope \mathcal{Z} with n generators, there exists a regression model (X, \mathbf{y}) with p regression parameters and n observations such that $V(OLS(X, \mathbf{y})) = V(\mathcal{Z})$ and $F(OLS(X, \mathbf{y})) = F(\mathcal{Z})$.*

Proof. Let g_1, \dots, g_n be the generators of \mathcal{Z} . Consider the matrix $G \in \mathbb{R}^{p \times n}$ with columns g_1, \dots, g_n and the n -dimensional vector \mathbf{z} with $z_i := [0, 1]$ for $i = 1, \dots, n$.

First we observe that the zonotope

$$\mathcal{Z}' := \{Gz : z \in \mathbf{z}\}$$

is, up to a shift, the same zonotope as $\mathcal{Z} = \mathcal{Z}(s; g_1, \dots, g_n)$:

$$\begin{aligned} \{Gz : z \in \mathbf{z}\} &= \{g_1 z_1 + g_2 z_2 + \dots + g_n z_n : \\ &\quad z_1 \in [0, 1], z_2 \in [0, 1], \dots, z_n \in [0, 1]\} \\ &= \{0\} + g_1 + g_2 + \dots + g_n \\ &= \mathcal{Z}(0; g_1, \dots, g_n). \end{aligned}$$

By the assumption that \mathcal{Z} has dimension p , we know that G has full row rank, and hence GG^T is regular.

Consider the model (X, \mathbf{y}) with $X := G^T$ and $\mathbf{y} := \mathbf{z}$. Then

$$OLS(X, \mathbf{y}) = \{(X^T X)^{-1} X^T \mathbf{y} : \mathbf{y} \in \mathbf{y}\} = \{(GG^T)^{-1} Gz : z \in \mathbf{z}\}.$$

The last expression shows that the zonotope $OLS(X, \mathbf{y})$ is an image of the zonotope \mathcal{Z}' under the regular linear mapping $\xi \mapsto (GG^T)^{-1} \xi$. Regular linear mappings preserve the number of facets and vertices of polyhedra; hence $V(OLS(X, \mathbf{y})) = V(\mathcal{Z})$ and $F(OLS(X, \mathbf{y})) = F(\mathcal{Z})$. \square

3.4. A positive complexity result

Theorem 10 has an interesting corollary if we treat the number p as a fixed constant (i.e. if we restrict ourselves to a class of regression models with a fixed number of regression parameters).

Corollary 12 9. *If p is fixed then*

$$V(OLS(X, \mathbf{y})) \leq O(n^{p-1}) \quad \text{and} \quad F(OLS(X, \mathbf{y})) \leq O(n^{p-1}). \quad \square$$

Corollary 12 implies that the number of vertices and the number of facets is polynomial in n (provided that p is fixed). In Section 5 we show a general method for enumeration of vertices and facets. The assumption that p is fixed implies that the method of Section 5 runs in polynomial time under that assumption.

3.5. Regression models with repeated observations

Let p be fixed. The statement of Corollary 12 can be easily strengthened to the form

$$V(OLS(X, \mathbf{y})) \leq O(n^{\dim(OLS(X, \mathbf{y})) - 1}),$$

$$F(OLS(X, \mathbf{y})) \leq O(n^{\dim(OLS(X, \mathbf{y})) - 1}),$$

where \dim refers to Definition 7b. In statistical applications, this reduction usually does not help since we have $\dim(OLS(X, \mathbf{y})) < p$ only rarely. This could happen, for example, if a great majority of observations are crisp, i.e. if the cardinality of $\{i \in \{1, \dots, n\} : \underline{y}_i < \bar{y}_i\}$ is smaller than p .

However, there are important special cases where another significant reduction can be reached. The reduction is based on the following lemma, the proof of which is straightforward.

Lemma 13 (reduction lemma). *Let $\mathcal{Z} := \mathcal{Z}(s; \mathbf{g}_1, \mathbf{g}_2, \dots, \mathbf{g}_n)$ and for some i and $j, i < j$ it holds $\mathbf{g}_j = \alpha \mathbf{g}_i$, where $\alpha \in \mathbb{R}$. Then*

$$\mathcal{Z} = \begin{cases} \mathcal{Z}(s; \mathbf{g}_1, \dots, \mathbf{g}_{i-1}, \mathbf{g}_i + \mathbf{g}_j, \mathbf{g}_{i+1}, \dots, \mathbf{g}_{j-1}, \mathbf{g}_{j+1}, \dots, \mathbf{g}_n) & \text{if } \alpha \geq 0, \\ \mathcal{Z}(s + \mathbf{g}_j; \mathbf{g}_1, \dots, \mathbf{g}_{i-1}, \mathbf{g}_i - \mathbf{g}_j, \mathbf{g}_{i+1}, \dots, \mathbf{g}_{j-1}, \mathbf{g}_{j+1}, \dots, \mathbf{g}_n) & \text{if } \alpha < 0. \end{cases} \quad \square$$

The generator \mathbf{g}_j is called *redundant*. The process of removal of redundant generators may be iterated until all are removed; then we obtain a certain shift s' and a reduced set of generators $\mathbf{g}'_1, \dots, \mathbf{g}'_{n'}$ with $n' \leq n$ defining the same zonotope. Later, the following notation will be useful:

$$red(s; \mathbf{g}_1, \dots, \mathbf{g}_n) := (s', \mathbf{g}'_1, \dots, \mathbf{g}'_{n'}). \tag{6}$$

We can reformulate Theorem 10 and Corollary 12 in the following way.

Corollary 14. *Let \sim be an equivalence on rows of X : $X_i \sim X_j$ iff X_i is a multiple of X_j . Let v be the number of equivalence classes of \sim . Then,*

$$V(OLS(X, \mathbf{y})) \leq 2 \sum_{k=0}^{p-1} \binom{v-1}{k} \quad \text{and} \quad F(OLS(X, \mathbf{y})) \leq 2 \binom{v}{p-1}.$$

In particular, if p is fixed, then $V(OLS(X, \mathbf{y})) \leq O(v^{p-1})$ and $F(OLS(X, \mathbf{y})) \leq O(v^{p-1})$.

Proof. If X_i is a multiple of X_j , then $Q_i(\bar{y}_i - \underline{y}_i)$ is a multiple of $Q_j(\bar{y}_j - \underline{y}_j)$ and we may apply Lemma 13. \square

If the absolute term is involved in the regression model (i.e., X contains all-one column), then $X_i \sim X_j$ iff $X_i = X_j$. So, rather than saying that the combinatorial complexity of the zonotope $OLS(X, \mathbf{y})$ depends on the number of observations, it is more appropriate to say that *the complexity depends on the number of distinct design points* (i.e. distinct rows of X). Regression models with $v \ll n$, called *models with repeated observations*, are very important in practice.

3.6. Algorithmic properties of $OLS(X, \mathbf{y})$

The following theorem summarizes some complexity-theoretic facts about the set $OLS(X, \mathbf{y})$, which will be useful in the next sections. In the proof we use the well-known fact that linear programming is a polynomial-time solvable problem, see [70].

Definition and Theorem 15. Whenever we write $X, \underline{y}, \bar{y}$ and β , we assume that they are rational.

- (a) We say that β is *admissible* for (X, \mathbf{y}) if $\beta \in OLS(X, \mathbf{y})$. The question “is β admissible?” is in **P**.
- (b) We say that β is *extremal* for (X, \mathbf{y}) if β is on the boundary of $OLS(X, \mathbf{y})$. The question “is β extremal?” is in **P**.
- (c) The question “is β a vertex of $OLS(X, \mathbf{y})$?” is in **P**.

Proof. As observed in [9], admissibility is decidable via the linear program

$$\max 0^T \mathbf{y} : \beta = Q\mathbf{y}, \underline{y} \leq \mathbf{y} \leq \bar{y}. \tag{7}$$

To prove (b) assume that the center of $OLS(X, \mathbf{y})$ is 0 (by Lemma 9b, the zonotope $OLS(X, \mathbf{y})$ can be shifted). Then β is extremal iff the optimal value of the linear program

$$\max w : w\beta = Q\mathbf{y}, \underline{\mathbf{y}} \leq \mathbf{y} \leq \bar{\mathbf{y}}$$

is $w = 1$.

In the proof of (c) we may assume that all generators $\mathbf{g}_i := Q_i(\bar{\mathbf{y}}_i - \underline{\mathbf{y}}_i)$ are nonzero. Observe that β is not a vertex iff there exists a generator \mathbf{g}_i such that β can be shifted both in the direction \mathbf{g}_i and in the direction $-\mathbf{g}_i$. So, β is a vertex iff for each $i = 1, \dots, n$ it holds that the linear program

$$\max w : \beta + w\mathbf{g}_i = Q\mathbf{y}, \beta - w\mathbf{g}_i = Q\mathbf{z}, \underline{\mathbf{y}} \leq \mathbf{y} \leq \bar{\mathbf{y}}, \underline{\mathbf{z}} \leq \mathbf{z} \leq \bar{\mathbf{z}}$$

has the optimal value $w = 0$. \square

3.7. A linear combination of regression parameters

Assume that a nonzero vector c of parameters is given. Sometimes we need to estimate the linear combination $c^T\beta$ of regression parameters.

An example of the choice of c is $c^T = (1, 0, \dots, 0)$. In this case we want to estimate the first regression parameter. This choice is interesting, for example, in the model $y = \beta_1 x^2 + \beta_2 x + \beta_3 + \varepsilon$; if we can estimate β_1 with high precision, then we can (reliably) decide whether it is zero or not. In other words, we can test whether the model is linear in x or not.

This is just a short motivation, why the linear combination $c^T\hat{\beta}$ is important in classical statistics. Here we address the question how our knowledge of the value $c^T\hat{\beta}$ can be affected by censoring.

By Lemma 9(b) we can assume that the center of $OLS(X, \mathbf{y})$ is 0 . Then we can solve the linear program

$$\max w : w\mathbf{c} = Q\mathbf{y}, \underline{\mathbf{y}} \leq \mathbf{y} \leq \bar{\mathbf{y}}.$$

If w^* is the optimal value, then $\chi_c := w^* \|c\|$, where $\|\cdot\|$ is the L_2 -norm, is the radius of $OLS(X, \mathbf{y})$ in the direction c . Then χ_c measures how censoring can affect our knowledge of the value $c^T\hat{\beta}$ in the worst case. If the value χ_c is small, then we can say that *the loss of information caused by censoring effect is negligible*. (Often it is the case that for some choices of c the value χ_c is small while for other choices of c the value χ_c is large.) The interval $[-\chi_c, \chi_c]$ can be called as *covering of $c^T\hat{\beta}$* or “region of 100% certainty” about the value $c^T\hat{\beta}$.

4. Approximations of the set $OLS(X, \mathbf{y})$ in the crisp input – interval output model

A complete vertex description and a complete facet description of the zonotope $OLS(X, \mathbf{y})$ is available using the methods described in Section 5. In many cases this description is not friendly for a user—for example, in a model with $p = 4$ regression parameters and $n = 100$ observations, the enumeration of vertices or facets can fill up a thick book. This is just one reason justifying that it is suitable to consider some user-friendly approximations of the set $OLS(X, \mathbf{y})$. Another reason is that the methods of Section 5 do not run in polynomial time.

Let Q denote the matrix $(X^T X)^{-1} X^T$.

4.1. Interval approximation

As observed in [9], by (3) we obtain that for any $b \in OLS(X, \mathbf{y})$ and any $i = 1, \dots, p$,

$$\underbrace{\sum_{j=1}^n \min\{Q_{ij}\underline{\mathbf{y}}_j, Q_{ij}\bar{\mathbf{y}}_j\}}_{=: \underline{b}_i} \leq b_i \leq \underbrace{\sum_{j=1}^n \max\{Q_{ij}\underline{\mathbf{y}}_j, Q_{ij}\bar{\mathbf{y}}_j\}}_{=: \bar{b}_i}. \tag{8}$$

Moreover, the cube $[\underline{b}, \bar{b}]$ is the smallest cube containing $OLS(X, \mathbf{y})$. This bound is easily computable.

4.2. Ellipsoidal approximations

Combinatorially complex polyhedra are often approximated with ellipses: an ellipse is a convex set which is quite flexible to approximate the shape of the polyhedron and it is sufficiently simple to be described.

An ellipse \mathcal{E} is described by a center point s and a positive definite matrix E such that

$$\mathcal{E} = \{x \in \mathbb{R}^p : (x - s)^T E^{-1} (x - s) \leq 1\}.$$

We do not know a polynomial-time algorithm for construction of the *best* (i.e., the smallest with respect to volume) circumscribing ellipse for the set $OLS(X, \mathbf{y})$. It is an intriguing research problem; however, we expect a hardness result on this computational problem rather than a polynomial-time algorithm.

The following ellipse $\mathcal{E} = (E, s)$, studied in [9], can be seen as a weaker form:

$$s = \frac{1}{2} Q(\bar{\mathbf{y}} + \mathbf{y}),$$

$$E = Q \cdot \text{diag}\left(\frac{n}{4}(\bar{y}_1 - \underline{y}_1)^2, \dots, \frac{n}{4}(\bar{y}_n - \underline{y}_n)^2\right) \cdot Q^T, \tag{9}$$

where $\text{diag}(\xi_1, \dots, \xi_n)$ denotes the diagonal matrix with diagonal entries ξ_1, \dots, ξ_n . This is the ellipse which is the image of the smallest ellipse circumscribing \mathbf{y} in \mathbb{R}^n under the mapping $\xi \mapsto Q\xi$. This proves $OLS(X, \mathbf{y}) \subseteq \mathcal{E}$.

However, the ellipse (9) is highly redundant if $p \ll n$. Thus, in high dimensions (i.e., with n large), other methods for ellipsoidal approximation are more suitable. They will be investigated in the next section.

The paper [9] also contains an example on the tightness of approximations (8) and (9).

A comment on the relation between interval and ellipsoidal approximations. In general, ellipsoidal approximations give slightly different information than the interval approximation given by (8). The interval $[\underline{b}_i, \bar{b}_i]$ given by (8) provides a tight bound for the value $\hat{\beta}_i$ individually. Notwithstanding, the box $\mathbf{b} = [\underline{b}_1, \bar{b}_1] \times \dots \times [\underline{b}_p, \bar{b}_p]$ may overestimate the zonotope $OLS(X, \mathbf{y})$ significantly. Such a situation is depicted in Fig. 3. We can see that $[\underline{b}_1, \bar{b}_1]$ is the tightest interval covering $\hat{\beta}_1$. And, independently, we can see that $[\underline{b}_2, \bar{b}_2]$ is the tightest interval covering $\hat{\beta}_2$. The ellipsoidal approximation gives additional information: it shows us, for example, that it cannot happen that $\hat{\beta}_1 = \underline{b}_1$ and $\hat{\beta}_2 = \bar{b}_2$ simultaneously.

In some sense, the situation is similar to the construction of confidence regions in classical (probabilistic) linear regression: either we can construct the confidence interval for each individual regression parameter separately, or we can construct the confidence ellipsoid for all regression parameters simultaneously.

4.3. Approximation of $OLS(X, \mathbf{y})$ by (a form of) the Löwner–John ellipse

If \mathcal{E} is an ellipse (E, s) , then $\alpha \cdot \mathcal{E}$ is the ellipse $(\alpha^2 E, s)$, i.e. an ellipse blown-up by a factor α .

Definition 16. Let $P \subseteq \mathbb{R}^p$ and $\varepsilon > 0$.

- (a) Any ellipse \mathcal{E} satisfying $\frac{1}{p} \cdot \mathcal{E} \subseteq P \subseteq \mathcal{E}$ is called *Löwner–John ellipse* for P . Any ellipse \mathcal{E} satisfying $\frac{1}{p} \cdot \mathcal{E} \subseteq P \subseteq (1 + \varepsilon) \cdot \mathcal{E}$ is called *ε -approximate Löwner–John ellipse* for P .
- (b) Any ellipse \mathcal{E} satisfying $\frac{1}{\sqrt{p}} \cdot \mathcal{E} \subseteq P \subseteq \mathcal{E}$ is called *Jordan ellipse* for P . Any ellipse \mathcal{E} satisfying $\frac{1}{\sqrt{p}} \cdot \mathcal{E} \subseteq P \subseteq (1 + \varepsilon) \cdot \mathcal{E}$ is called *ε -approximate Jordan ellipse* for P .

The following theorems, known as Löwner–John Theorem and Jordan Theorem, respectively, are basic results in polyhedral geometry (see [20,70]):

- (i) any full-dimensional bounded convex set $P \subseteq \mathbb{R}^p$ has a Löwner–John ellipse;
- (ii) any full-dimensional bounded centrally symmetric convex set $P \subseteq \mathbb{R}^p$ has a Jordan ellipse.

Moreover, the factors $\frac{1}{p}$ and $\frac{1}{\sqrt{p}}$ in Definition 16 cannot be improved in general unless the statements (i and ii) are violated.

The Löwner–John and Jordan ellipses have the advantage that they provide us with both a lower and an upper bound on the boundary of P . When $P = OLS(X, \mathbf{y})$, we get an interesting approximation of $OLS(X, \mathbf{y})$.

If the set $OLS(X, \mathbf{y})$ is full-dimensional, it has a Jordan ellipse—we know that zonotopes are centrally symmetric. Of course, we would like to describe an *algorithmic method* for finding the ellipse. Unfortunately, proofs of both theorems (i and ii) are nonconstructive.

Algorithms for construction of Löwner–John ellipses and Jordan ellipses are studied in computational geometry. In particular, the following theorem was proved by Goffin [19]; see also [6,20,70]. It is known as a constructive form of the Löwner–John Theorem for polyhedra.

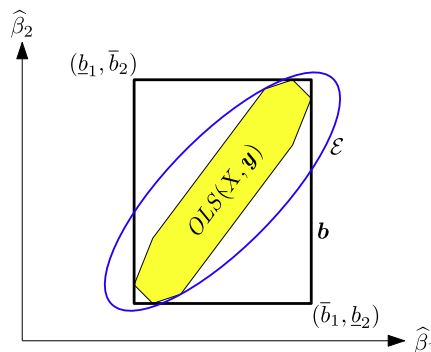


Fig. 3. Interval and ellipsoidal approximations of $OLS(X, \mathbf{y})$.

- (i) Let $\varepsilon > 0$ be fixed. Given rational A and b such that the polyhedron $P := \{x \in \mathbb{R}^p: Ax \leq b\}$ is full-dimensional and bounded, its ε -approximate Löwner–John ellipse can be found in polynomial time.

The method is known as Goffin's Algorithm and it is based on Khachiyan's Ellipsoid Method. The method can be adapted for central-symmetric polyhedra (see [6,20]). Then, Goffin's Theorem can be stated in the following way. It is known as a constructive form of the Jordan Theorem for polyhedra.

- (ii) Let $\varepsilon > 0$ be fixed. Given rational A and b such that the polyhedron $P := \{x \in \mathbb{R}^p: Ax \leq b\}$ is full-dimensional, bounded and centrally symmetric, its ε -approximate Jordan ellipse can be found in polynomial time.

At the first sight it seems that the form (ii) of Goffin's Theorem could be used for a polynomial-time construction of the Jordan ellipse for $OLS(X, \mathbf{y})$. But there is a serious obstacle: the algorithm requires the facet description $Ax \leq b$ of the set $OLS(X, \mathbf{y})$. From Section 3.3 we know that in general, computation of A and b , when generators g_1, \dots, g_n are given, is not a polynomial-time procedure.

From Section 3.4 we know that it is a polynomial time procedure under the assumption that the dimension p is fixed. Indeed, the facet description can be found using the methods of Section 5. This observation together with Goffin's Theorem (ii) imply the following interesting statement:

Corollary 17. *Let $\varepsilon > 0$. Let the dimension p be fixed. There is a polynomial-time algorithm which computes the ε -approximate Jordan ellipse for $OLS(X, \mathbf{y})$.*

If the dimension is not fixed, we can prove only a weaker result [6].

Theorem 18 6. *Let $\varepsilon > 0$ be fixed. There is a polynomial-time algorithm which computes the ε -approximate Löwner–John ellipse for $OLS(X, \mathbf{y})$.*

Problem. It is an intriguing research problem whether Theorem 18 can be reformulated with the Jordan ellipse instead of the Löwner–John ellipse. (Or at least with an ellipse \mathcal{E} satisfying $p^{-\gamma} \cdot \mathcal{E} \subseteq OLS(X, \mathbf{y}) \subseteq (1 + \varepsilon) \cdot \mathcal{E}$ with some $\gamma \in (\frac{1}{2}, 1)$.)

By [6], the problem is tightly interconnected with the following question. Assume that $OLS(X, \mathbf{y})$ is centered at zero (by Lemma 9(b), this assumption is without loss of generality). Let $K_\gamma := \{x: \|x\| \leq \gamma\}$ be a ball with radius γ . Let T be the problem “given rational $X, \underline{y}, \bar{y}$ and $\gamma > 0$, decide whether $K_\gamma \subseteq OLS(X, \mathbf{y})$ ”. The following holds: if $T \in \mathbf{P}$, in Theorem 18 the Löwner–John ellipse can be replaced by the Jordan ellipse. On the other hand, if $T \notin \mathbf{P}$, this fact seems to be a serious obstacle for the Goffin's method which probably rules out the method from the attempts to improve Theorem 18.

At the moment we cannot prove $T \in \mathbf{P}$. We conjecture that the problem T is *co-NP*-complete.

4.4. Approximation of volume of $OLS(X, \mathbf{y})$

Volume of $OLS(X, \mathbf{y})$ is a natural measure of its size, i.e. a natural measure of “uncertainty” about the value of the OLS-estimator. In Section 5 we shall present an algorithm for exact computation of volume of $OLS(X, \mathbf{y})$. However, that algorithms requires (in general) high computation resources: no polynomial-time algorithm (polynomial in n and p) is known, and probably none exists, since the problem is known to be $\#\mathbf{P}$ -complete [14].

Theorem 15a combined with (8) suggests a simple procedure for Monte-Carlo approximation of volume:

1. using (8), generate a random point $b \in [\underline{b}, \bar{b}]$;
2. using Theorem 15a, test whether it is admissible.

The ratio of the admissible points to the total number of repetitions of 1. –2. converges to the ratio of the volume of $OLS(X, \mathbf{y})$ to the volume of the box $[\underline{b}, \bar{b}]$. This procedure is interesting in particular in high dimensions. However, more interesting algorithms for the problem are known; in particular, see the randomized algorithm in [13].

5. The Reduction-and-Reconstruction-Recursion (“RRR”) Algorithm

In this section we are still dealing with the crisp input – interval output model, i.e. $\underline{X} = \bar{X} =: X$. From the previous sections we know that in this case, the set $OLS(X, \mathbf{y})$ is a zonotope. Here we introduce a meta-algorithm that can be used for answering several questions about $OLS(X, \mathbf{y})$. In particular, we get an algorithm for

- (a) enumeration of vertices of $OLS(X, \mathbf{y})$,
- (b) enumeration of facets of $OLS(X, \mathbf{y})$ (i.e. finding a description of $OLS(X, \mathbf{y})$ in terms of linear inequalities in \mathbb{R}^p),
- (c) computation of volume of $OLS(X, \mathbf{y})$.

Recall that an approximate algorithm for estimation of volume has been presented in Section 4.4.

Algorithms for zonotopes are discussed in [4,16].

Given a family a_1, \dots, a_k of vectors, $\mathcal{L}(a_1, \dots, a_k)$ denotes the linear space spanned by a_1, \dots, a_k .

Remark 1. Given a sequence of generators g_1, \dots, g_n of a zonotope $\mathcal{Z} \subseteq \mathbb{R}^p$, we can easily determine $D := \dim(\mathcal{Z})$ by evaluation of the dimension of $\mathcal{L}(g_1, \dots, g_n)$. *Volume* is understood as volume in the D -dimensional space $\mathcal{L}(g_1, \dots, g_n)$, since \mathcal{Z} is full-dimensional in that space (while it is of zero volume in \mathbb{R}^p if $D < p$).

The Reduction-and-Reconstruction-Recursion (RRR) Algorithm is a meta-algorithm which uses routines *BasicCase* and *Combine*. Particular choices of these routines will be specified later.

Observe that for any permutation π of $\{1, \dots, n\}$, $\mathcal{Z}(s, g_1, \dots, g_n) = \mathcal{Z}(s, g_{\pi(1)}, \dots, g_{\pi(n)})$. We may assume that whenever we work with a sequence g_1, \dots, g_n of generators of a zonotope \mathcal{Z} , the vectors $g_1, \dots, g_{\dim(\mathcal{Z})}$ are linearly independent. Say that the output of the procedure *red* defined by (6) meets this requirement. Let $\mathcal{P}_v(u)$ denote the orthogonal projection of the vector u into the space $\{\xi: v^T \xi = 0\}$.

```

{1} function RRR( $\tilde{s}; \tilde{g}_1, \dots, \tilde{g}_n$ )
{2}   ( $s, g_1, \dots, g_n := \text{red}(\tilde{s}; \tilde{g}_1, \dots, \tilde{g}_n)$ )
{3}   if  $g_1, \dots, g_n$  are linearly independent then
{4}     OUTPUT := BasicCase( $s; g_1, \dots, g_n$ )
{5}   else
{6}     DATA1 := RRR( $s; g_1, g_2, \dots, g_{n-1}$ )
{7}     DATA2 := RRR( $\mathcal{P}_{g_n}(s); \mathcal{P}_{g_n}(g_1), \mathcal{P}_{g_n}(g_2), \dots, \mathcal{P}_{g_n}(g_{n-1})$ )
{8}     OUTPUT := Combine( $s; g_1, \dots, g_n; \text{DATA}_1, \text{DATA}_2$ )
{9}   end.

```

The steps {6} and {7} are computed recursively.

Observe that by {2} it holds that in the collection g_1, \dots, g_n there is no pair of parallel generators. This observation is important for the correctness of Application 2.

5.1. Application 1—volume computation

Let us define

$$\text{Combine}(s; g_1, \dots, g_n; \alpha_1, \alpha_2) = \alpha_1 + \alpha_2 \|g_n\|,$$

where $\|\cdot\|$ denotes the L_2 -norm, and

```

function BasicCase( $s; g_1, \dots, g_n \in \mathbb{R}^k$ )
  let  $H$  be the matrix with columns  $g_1, \dots, g_n$ 
  OUTPUT :=  $\sqrt{\det H^T H}$ 
end.

```

In the basic case, by the instruction {3} of RRR we know that the generators g_1, \dots, g_n are linearly independent. Hence, the zonotope is an n -dimensional parallelogram in \mathbb{R}^k (it may be $k > n$) and its volume is thus $\sqrt{\det H^T H}$.

By symmetry of zonotopes, adding a new generator g_n to the zonotope $\mathcal{Z}(s; g_1, \dots, g_{n-1})$ increases its volume α_1 by the volume of the prism with base $\mathcal{Z}(\mathcal{P}_{g_n}(s); \mathcal{P}_{g_n}(g_1), \dots, \mathcal{P}_{g_n}(g_{n-1}))$ and height $\|g_n\|$. (See also the evolution process of Fig. 1.) From the recursion, α_2 is the area of the base.

5.2. Application 2—enumeration of vertices

In the Basic Case, the zonotope is a parallelogram:

$$\text{BasicCase}(s; g_1, \dots, g_n) := \left\{ s + \sum_{i=1}^n c_i g_i : c_i \in \{0, 1\}^n \right\}.$$

We shall describe the function *Combine*($s; g_1, \dots, g_n; \text{VertexSet}_1, \text{VertexSet}_2$) with reference to Fig. 4. From the recursion, *VertexSet*₁ is the set of vertices of the zonotope $\mathcal{Z}_1 := \mathcal{Z}(s; g_1, \dots, g_{n-1})$ and *VertexSet*₂ the set of vertices of a zonotope \mathcal{Z}_2 , which is the projection of \mathcal{Z}_1 on the hyperplane $\{\xi: g_n^T \xi = 0\}$.

We say that a vertex $v \in \text{VertexSet}_1$ is *utmost* if $\mathcal{P}_{g_n}(v) \in \text{VertexSet}_2$. Otherwise it is *inner*. Consider the decomposition *VertexSet*₁ = $U \cup I$, where U are utmost vertices and I are inner vertices.

Now we process the utmost vertices: we set *OUTPUT*₁ := $\{u, u + g_n : u \in U\}$.

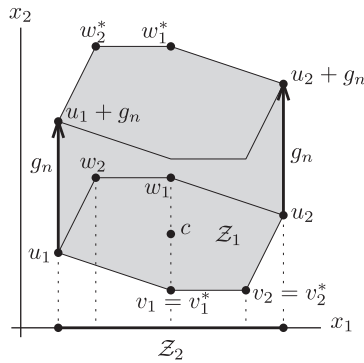


Fig. 4. Enumeration of vertices. The zonotope $Z := Z(s; g_1, \dots, g_n)$ is shaded. From the recursion, the vertex description $U \cup I$ of Z_1 is available, where $U = \{u_1, u_2\}$ and $I = \{(v_1, w_1), (v_2, w_2)\}$. The center of Z_1 is denoted c . The vertices u_1, u_2 are utmost; they can be detected with the knowledge of the vertex description of Z_2 which is also available from recursion. The vertex description of Z is $u_1, u_1 + g_n, u_2, u_2 + g_n, v_1, w_1, v_2, w_2$.

By central symmetry of the zonotope Z_1 , the set I of inner vertices can be seen as a set of centrally symmetric pairs $(v_i, w_i), \dots (v_\ell, w_\ell)$. For each pair (v_i, w_i) , we get the transformed pair (v_i^*, w_i^*) in the way that one of the vertices is preserved and the other is shifted by the generator g_n ; in Fig. 4 we have, for example, $v_i^* = v_i$ and $w_i^* = w_i + g_n$ for $i = 1, 2$. Then we set $OUTPUT_2 := \{v_i^*, w_i^* : i = 1, \dots, \ell\}$. The final output of the procedure Combine is $OUTPUT_1 \cup OUTPUT_2$.

5.3. Application 3—enumeration of facets

The procedure *BasicCase*($s; g_1, \dots, g_n \in \mathbb{R}^k$) finds the facet description of the parallelogram generated by g_1, \dots, g_n . Let g_{n+1}, \dots, g_k be any basis of $\mathcal{L}(g_1, \dots, g_n)^\perp$ and let G be the matrix with columns g_1, \dots, g_k . Then, the facet description is

$$\left\{ x : \begin{array}{l} -e_i^T G^{-1}(x - s) \leq 0, \quad e_i^T G^{-1}(x - s) \leq 1, \quad i = 1, \dots, n; \\ -e_i^T G^{-1}(x - s) \leq 0, \quad e_i^T G^{-1}(x - s) \leq 0, \quad i = n + 1, \dots, k \end{array} \right\},$$

where e_i is the i th column of the unit matrix.

We shall describe the function *Combine*($s; g_1, \dots, g_n \in \mathbb{R}^k; Facets_1, Facets_2$) with reference to Fig. 5. From the recursion, $Facets_1$ is the set of facets of the zonotope $Z_1 := Z(s; g_1, \dots, g_{n-1})$ and $Facets_2$ is the set of facets of the zonotope Z_2 , which is the projection of Z_1 on the hyperplane $\{\xi : g_n^T \xi = 0\}$. For simplicity say that g_n is parallel with e_k (which can be achieved by rotation). Then, the set $Facets_2$ contains inequalities $x_k \leq 0$ and $x_k \geq 0$. These inequalities are disregarded; the remaining ones are copied to $OUTPUT_1$.

By symmetry of Z_1 , the inequalities in $Facets_1$ can be seen as pairs $(J_i, K_i) := (a_i^T x \geq b_i, a_i^T x \leq b'_i)$, $i = 1, \dots, \ell$. Each pair (J_i, K_i) is transformed to a pair (J_i^*, K_i^*) in the way that one inequality is preserved and the other is shifted by the generator g_n . In Fig. 5, we have $J_i^* = J_i$ and $K_i^* = [a_i^T(x - g_n) \leq b'_i]$ for $i = 1, 2, 3$. We set $OUTPUT_2 = \{J_i^*, K_i^* : i = 1, \dots, \ell\}$. The final output of the procedure *Combine* is $OUTPUT_1 \cup OUTPUT_2$.

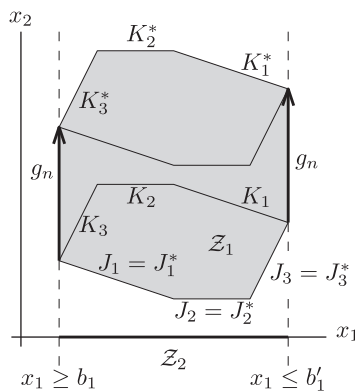


Fig. 5. Enumeration of facets. The zonotope $Z := Z(s; g_1, \dots, g_n)$ is shaded. From the recursion, the facet description $x_1 \geq b_1, x_1 \leq b'_1, x_2 \geq 0, x_2 \leq 0$ of Z_2 and the facet description $(J_1, K_1), (J_2, K_2), (J_3, K_3)$ of Z_1 is available. The facet description of Z is $x_1 \geq b_1, x_1 \leq b'_1, (J_1^*, K_1^*), (J_2^*, K_2^*), (J_3^*, K_3^*)$.

6. Approximations of $OLS(\mathbf{X}, \mathbf{y})$ in the general case

As we know from [Theorem 4](#), in the general case (\mathbf{X}, \mathbf{y}) the situation is much more difficult than in the crisp input case. Therefore we cannot expect general results. However, the *co-NP*-hardness result does not rule out that good approximations of $OLS(\mathbf{X}, \mathbf{y})$ could be found in particular cases. As the general case is very important in practice, in this section we review applicable methods for interval approximation of $OLS(\mathbf{X}, \mathbf{y})$. Those methods, which—to our knowledge—provide the tightest approximations, are illustrated by three examples. The examples should provide a basic insight showing what results could be expected. However, the main message of the examples is that—even in very simple cases—the known methods for the general case can hardly be considered as satisfactory. The examples could also serve as an impulse for further research.

To our knowledge, known methods for the general case (\mathbf{X}, \mathbf{y}) are based on finding enclosures for general systems of linear equations with interval coefficients of the form $\mathbf{A}\mathbf{x} = \mathbf{c}$, taking no advantage of the fact that here we solving the particular system

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}, \quad \mathbf{X} \in \mathbf{X}, \quad \mathbf{y} \in \mathbf{y}. \quad (10)$$

Though there exist experimental studies, showing practical performance of various methods, we are not aware of a study focused on their behavior when processing the special system (10). Moreover, at the moment we do not know how to utilize the specific dependency problem, described in [Section 6.1](#), in a better way than by relaxation or using general purpose methods. This is an interesting problem for further research which undoubtedly deserves attention.

For the sake of completeness, we also give a short overview of available software.

This Section might serve for practical purposes as a guidance for selection of a particular method and software. However, it is also interesting from a theoretical point of view: it shows the main drawbacks and bottlenecks of currently available methods and thus can be understood as a motivation for research in the field.

Given an interval matrix $\mathbf{Z} = [\underline{\mathbf{Z}}, \overline{\mathbf{Z}}]$, the matrix

$$\mathbf{Z}^c = \frac{1}{2}(\underline{\mathbf{Z}} + \overline{\mathbf{Z}})$$

is called *center matrix* and the matrix

$$\mathbf{Z}^A = \frac{1}{2}(\overline{\mathbf{Z}} - \underline{\mathbf{Z}})$$

is called *radius matrix*.

Recall also that interval addition and multiplication has been defined by (3). We shall also need the division of interval numbers $\mathbf{a} = [\underline{a}, \overline{a}]$ and $\mathbf{b} = [\underline{b}, \overline{b}]$, which is defined as

$$\frac{\mathbf{a}}{\mathbf{b}} = \begin{cases} [\min\{\underline{a} \div \underline{b}, \underline{a} \div \overline{b}, \overline{a} \div \underline{b}, \overline{a} \div \overline{b}\}, \max\{\underline{a} \div \underline{b}, \underline{a} \div \overline{b}, \overline{a} \div \underline{b}, \overline{a} \div \overline{b}\}] & \text{if } 0 \notin \mathbf{b}, \\ \text{undefined} & \text{otherwise,} \end{cases}$$

where the relation \div stands for the traditional crisp division.

A lot of effort has been devoted to finding tight interval enclosures of solution sets of interval equations. Given an interval matrix \mathbf{A} and an interval vector \mathbf{c} , the *enclosure of the solution set* is a box $\boldsymbol{\beta} = [\underline{\boldsymbol{\beta}}, \overline{\boldsymbol{\beta}}]$, which is as small as possible, satisfying $\boldsymbol{\beta} \supseteq \{\xi: \mathbf{A}\xi = \mathbf{c}, \mathbf{A} \in \mathbf{A}, \mathbf{c} \in \mathbf{c}\}$.

6.1. Relaxation

The basic approach to find an interval enclosure is by relaxation. Consider an interval system of equations

$$\mathbf{Z}\boldsymbol{\beta} = \mathbf{z}, \quad (11)$$

where the results of products $\mathbf{Z} := \mathbf{X}^T \mathbf{X}$ and $\mathbf{z} := \mathbf{X}^T \mathbf{y}$ are calculated using interval arithmetic. The interval system (11) covers all equation systems from (10) and typically some more. This redundancy, which is called *overestimation* in interval algebra, is caused by the so called *dependency problem*, which occurs when an interval quantity appears several times in the description of the interval system (in our case it is \mathbf{X}). Dependencies are hard to deal with, and often they are relaxed. Any enclosure of the solution set of (11) serves as an enclosure of $OLS(\mathbf{X}, \mathbf{y})$, too.

It is known that determining the interval hull (i.e., the optimal enclosure, or, exact bounds of the solution set) is an *NP*-hard problem. However, there are many methods for calculating quite sharp bounds in short time [52,63,65]. Some of them employ the basic form (11), however, often a preconditioning is used to improve the performance. Preconditioning means premultiplication of the system (11) by a crisp matrix; usually an inverse of \mathbf{Z}^c (or its numerically computed approximation) is used, where \mathbf{Z}^c is the center matrix of \mathbf{Z} . Even though it leads to further overestimation of the solution set, surprisingly the resulting enclosures are usually tighter.

First we mention three direct methods and then two iterative ones. Further, more general methods capable of dealing with dependencies are introduced, and finally other possible approaches are commented.

6.2. Interval Gaussian elimination

Implementing Gaussian elimination with interval arithmetic leads to the Interval Gaussian elimination. It works well in special cases (e.g. when the interval matrix is diagonally dominant or M -matrix), but it almost always causes high overestimation.

6.3. Hansen–Bliék–Rohn’s bounds

One of the best direct methods is the Hansen–Bliék–Rohn’s formula [53,63] which works as follows. Precondition the system (11) by the inverse of Z^c and denote the resulting interval system by $A\beta = r$. Suppose that $\underline{A}^{-1} \geq 0$ and denote $\beta^* := \underline{A}^{-1}(|r^c| + r^\Delta)$. Then the enclosing box $\beta = [\underline{\beta}, \overline{\beta}]$ is of the form

$$\begin{aligned} \overline{\beta}_i &:= \max \left\{ \beta_i^* + (\underline{A}^{-1})_{ii}(r^c - |r^c|)_i, \frac{1}{2(\underline{A}^{-1})_{ii} - 1} (\beta_i^* + (\underline{A}^{-1})_{ii}(r^c - |r^c|)_i) \right\}, \\ \underline{\beta}_i &:= \min \left\{ -\beta_i^* + (\underline{A}^{-1})_{ii}(r^c + |r^c|)_i, \frac{1}{2(\underline{A}^{-1})_{ii} - 1} (-\beta_i^* + (\underline{A}^{-1})_{ii}(r^c + |r^c|)_i) \right\}. \end{aligned}$$

Notice that the assumption $\underline{A}^{-1} \geq 0$ is not very restrictive. Indeed, it is frequently used as a sufficient condition for regularity of interval matrices (or its equivalent form $\rho(A^d) < 1$, where $\rho(\cdot)$ stands for the spectral radius). It was proved that the Hansen–Bliék–Rohn method calculates exact bounds for the solution set of the preconditioned system $A\beta = r$, and so it gives a very tight enclosure to (11).

6.4. Jansson’s algorithm

There is an algorithm that computes the optimal bounds. The solution set of (11) represents a finite union of convex polyhedra. When restricting on any orthant, it becomes a convex polyhedron the bounds of which can be exactly determined by solving $2p$ linear programs. Thus, the interval hull is computable by inspecting all of the 2^p orthants. This tremendous number can be reduced by the method of Jansson [35]. The method is based on the observation that the solution set is compact and connected provided Z is regular, and it is unbounded (moreover, each topologically connected component is unbounded) in case Z is not regular. Thus, the Jansson’s algorithm concentrates on just one connected component and goes through all orthants it intersects. Even though it may be exponential in the worst case, it often inspects only a fraction of all orthants.

6.5. Krawczyk’s method

A popular and efficient Krawczyk’s method [48,52] is an iterative method based on the preconditioning of (11) by a point matrix Y , usually $Y \approx (Z^c)^{-1}$. Let an initial enclosure β^0 be given. Then we iteratively calculate a nested sequence of enclosures β^k , $k = 0, 1, \dots$, where the iteration step is

$$\begin{array}{l} \{1\} \quad \beta' := Yz + (I - YZ)\beta^k \\ \{2\} \quad \beta^{k+1} := \beta' \cap \beta^k. \end{array}$$

Convergence and the approximation order is discussed deeply in [52].

6.6. Interval Gauss–Seidel’s iteration

It is a straightforward extension of the Gauss–Seidel’s iteration method for intervals [48,52]. Once an initial enclosure β^0 to the solution set is known, a nested sequence of enclosures β^k , $k = 0, 1, \dots$ is calculated. One iteration is

$$\begin{array}{l} \{1\} \quad \mathbf{for } i = 1, \dots, p \mathbf{ do} \\ \{2\} \quad \beta_i := \left(z_i - \sum_{j < i} Z_{ij} \beta_j^{k+1} - \sum_{j > i} Z_{ij} \beta_j^k \right) / Z_{ii} \\ \{3\} \quad \beta_i^{k+1} := \beta_i' \cap \beta_i^k \\ \{4\} \quad \mathbf{end do.} \end{array}$$

For special matrices (e.g. M -matrices), convergence to the interval hull is guaranteed. Applied to a preconditioned system, Gauss–Seidel’s iteration yields tighter intervals than Krawczyk’s method.

6.7. Parametric approach

Due to the relaxation of (10) and (11), the resulting enclosure β is overestimated. To reduce the overestimation, we can consider (10) to be a nonlinear parametric interval system of equations. That is, each matrix and right-hand side entry is considered as a nonlinear function of interval parameters. Several methods for such systems are available [59,40], however, their usage for high-dimensional problems (with respect to n and/or p) is questionable.

Since the constraint matrix in (10) is symmetric positive definite, we can consider a partial relaxation, too. That is, we relax the correlations between the interval parameters and keep only the symmetry and positive definiteness. For such interval systems, various approaches are known. The interval Cholesky's method [2] naturally extends Cholesky's method for interval data. Unfortunately, its efficiency is quite low, despite some pivot tightening improvements [17]. Since the symmetry condition is linear, we can utilize any solver for (more general) linear parametric interval systems. As numerical results in [26] indicate, this approach leads to quite tight bounds.

6.8. Software

Interval arithmetic is implemented in many programming languages. INTLAB [67] is a powerful MATLAB toolbox comprising not only the basic interval arithmetic, but also some useful interval functions. For instance, `verifylss` is a Krawczyk iteration-based function for interval linear systems of equations. VERSOFT [66] is a collection of verification and interval software written in INTLAB/ MATLAB. For interval linear systems, it contains e.g. `verenclinhull`, a function for computing the Hansen–Bliiek–Rohn's bounds, and `verintervalhull` for calculating the interval hull. The parametric solver by Popova [57] can handle interval systems with dependencies; the readers can experiment using the free webComputing service [58].

6.9. Other approaches

Another way to solve the problem is to rewrite it in the form

$$\begin{pmatrix} 0_p & \mathbf{X}^T \\ \mathbf{X} & I_n \end{pmatrix} \begin{pmatrix} \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{y} \end{pmatrix}. \quad (12)$$

Again, a relaxation leads to an ordinary interval linear system of equations, and we can employ the above mentioned solvers. Because the dependence structure in (12) is simpler than in (11) (it is just a condition on symmetry), it is easily shown that the resulting interval box β will be tighter.

Proposition 19. *The solution set of (12) is contained in the solution set of (11).*

Proof. Let us consider any instance of the system (12)

$$\begin{pmatrix} 0_p & \mathbf{X}^T \\ \mathbf{X}' & I_n \end{pmatrix} \begin{pmatrix} \beta \\ \gamma \end{pmatrix} = \begin{pmatrix} 0 \\ \mathbf{y} \end{pmatrix},$$

where $\mathbf{X}, \mathbf{X}' \in \mathbf{X}$ and $\mathbf{y} \in \mathbf{y}$. Then $\gamma = \mathbf{y} - \mathbf{X}'\beta$, and by substituting $\mathbf{X}'^T(\mathbf{y} - \mathbf{X}'\beta) = 0$. Hence $\mathbf{X}'^T\mathbf{X}'\beta = \mathbf{X}'^T\mathbf{y}$. Since $\mathbf{X}'^T\mathbf{X}' \in \mathbf{X}'^T\mathbf{X} = \mathbf{Z}$ and $\mathbf{X}'^T\mathbf{y} \in \mathbf{X}'^T\mathbf{y} = \mathbf{z}$, we have an instance of the system (11). \square

More details can be found in [51,38, pp. 109–120].

The drawback of this approach is that the system may be very large provided the number of observations is large. So it may be time-consuming to calculate sharp enough enclosures.

The constraint matrix in (12) is symmetric, so we can again utilize any method for symmetric interval systems to obtain more accurate enclosures.

An alternative approach to solve the problem is based on the adaptation of the QR factorization for interval data [18], e.g. using interval Householder's method [5,46]. Another method is described in [47].

6.10. Examples

Example 20. Let

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ [0,2] & 2 & 3 & 4 & 5 \end{pmatrix}^T,$$

$$\mathbf{y} = (1 \ 1 \ 1 \ 1 \ 1)^T.$$

Table 1
Different enclosures in Example 20.

	Via system (11)	Via system (12)
verifylss	([-1.2858, 3.2858], [-0.7143, 0.7143])	(1, 0)
verenclinhull	([0.3043, 3.2858], [-0.7143, 0.7143])	(1, 0)
Parametric method [26]	([0.3043, 3.2858], [-0.7143, 0.7143])	(1, 0)
verintervalhull	([0.3043, 3.2858], [-0.7143, 0.2174])	(1, 0)

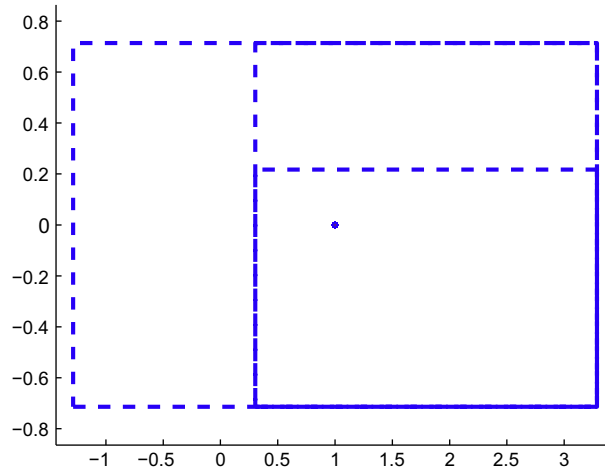


Fig. 6. Example 20 (Table 1). The dashed rectangles correspond to (11), computed by `verifylss`, `verenclinhull` and `verintervalhull`. By (12), we get the true point (1,0).

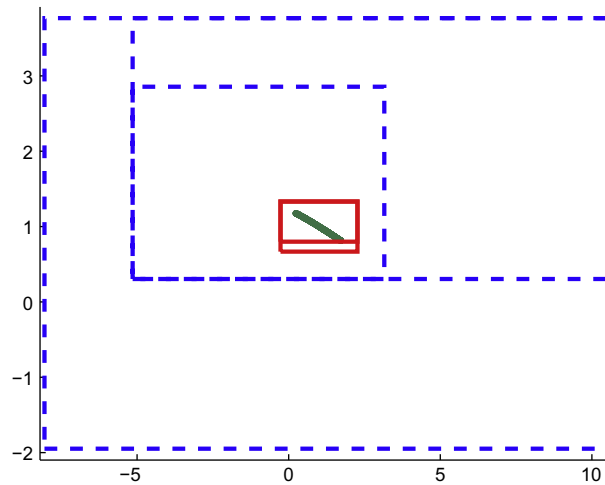


Fig. 7. Example 20, the modified case (Table 2). The dashed rectangles correspond to (11), computed by `verifylss`, `verenclinhull` and `verintervalhull`. The solid rectangles correspond to (12), computed by `verifylss` (the same as `verenclinhull`) and `verintervalhull`.

Obviously, the solution set consists of one point (1,0). The results of different approaches are displayed in Table 1 and illustrated in Fig. 6.

In Figs. 6–8, the dashed rectangles correspond to the enclosures resulting from the system (11), whereas the solid rectangles correspond to (12). Inside the rectangles, the true solution set (computed numerically) is plotted.

Example 20—a modified case. Now let us change the vector \mathbf{y} to

$$\mathbf{y}' = (2 \ 3 \ 4 \ 5 \ 6)^T.$$

The results are displayed in Table 2 and in Fig. 7.

Table 2
Different enclosures in Example 20, the modified case.

verifylss	Via system (11)
verenclinhull	([-8.0520, 10.5975], [-1.9481, 3.7663])
Parametric method [26]	([-5.1429, 10.5975], [0.3030, 3.7663])
verintervalhull	([-5.1429, 7.6884], [0.3030, 2.8572])
	([-5.1429, 3.1516], [0.3030, 2.8572])
	Via system (12)
verifylss	([-0.2667, 2.2667], [0.6666, 1.3334])
verenclinhull	([-0.2667, 2.2667], [0.6666, 1.3334])
Parametric method [26]	([-0.2667, 2.2667], [0.7999, 1.3334])
verintervalhull	([-0.1740, 1.7298], [0.8108, 1.3044])

Example 21. Let X, y be given with

$$\begin{aligned} \underline{X} &= \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -2.5 & -1.5 & -0.5 & 0.5 & 1.5 & 2.5 & 3.5 & 4.5 & 5.5 & 6.5 & 7.5 \end{pmatrix}^T, \\ \bar{X} &= \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1.5 & -0.5 & 0.5 & 1.5 & 2.5 & 3.5 & 4.5 & 5.5 & 6.5 & 7.5 & 8.5 \end{pmatrix}^T, \\ \underline{y} &= (1.5 \ 2.5 \ 3.5 \ 4.5 \ 5.5 \ 6.5 \ 7.5 \ 8.5 \ 9.5 \ 10.5 \ 11.5)^T, \\ \bar{y} &= (2.5 \ 3.5 \ 4.5 \ 5.5 \ 6.5 \ 7.5 \ 8.5 \ 9.5 \ 10.5 \ 11.5 \ 12.5)^T. \end{aligned}$$

The calculated enclosures are shown in Table 3 and illustrated in Fig. 8.

Example 22. Consider an example from [5]:

$$\mathbf{X} = \begin{pmatrix} [0.1, 0.3] & [0.9, 1.1] \\ [8.9, 9.1] & [0.4, 0.6] \\ [0.9, 1.1] & [6.9, 7.1] \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} [0.8, 1.2] \\ [-0.2, 0.2] \\ [1.8, 2.2] \end{pmatrix}.$$

Table 4 displays enclosures calculated by various methods; in the last line, there is the enclosure from [5] computed by the interval Householder's method.

6.11. Summary

We reviewed diverse methods for computation of interval enclosures of $OLS(X, y)$ in the general case. More numerical experiments would be needed to decide about efficiency of the presented methods, but some observations can be done now.

The system (12) yields provably tighter enclosures than (11), so provided the number of observations is mild, then it is a suitable method.

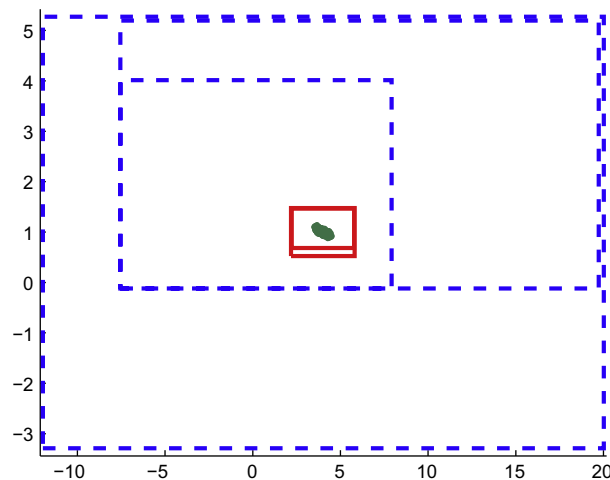


Fig. 8. Example 21. The dashed rectangles correspond to (11), computed by `verifylss`, `verenclinhull` and `verintervalhull`. The solid rectangles correspond to (12), computed by `verifylss` and the parametric method [26].

Table 3
Different enclosures in Example 21.

verifylss	Via system (11)
verenclinhull	([-11.9723, 20.0256], [-3.2903, 5.2725])
Parametric method [26]	([-7.5467, 19.7341], [-0.1201, 5.1945])
verintervalhull	([-7.5467, 16.2139], [-0.1201, 4.2770])
	([-7.5467, 7.9201], [-0.1201, 4.0134])
	Via system (12)
verifylss	([2.1858, 5.8142], [0.5234, 1.4766])
verenclinhull	([2.1858, 5.8142], [0.5234, 1.4766])
Parametric method [26]	([2.2206, 5.7794], [0.6820, 1.4661])
verintervalhull	([-∞, ∞], [-∞, ∞])

Table 4
Different enclosures in Example 22.

verifylss	via system (11)
verenclinhull	([-0.0644, 0.0324], [0.2364, 0.3693])
Parametric method [26]	([-0.0643, 0.0312], [0.2418, 0.3692])
verintervalhull	([-0.0643, 0.0312], [0.2418, 0.3692])
	([-0.0643, 0.0276], [0.2432, 0.3692])
	Via system (12)
verifylss	([-0.0471, 0.0145], [0.2569, 0.3477])
verenclinhull	([-0.0470, 0.0139], [0.2587, 0.3475])
Parametric method [26]	([-0.0469, 0.0139], [0.2587, 0.3462])
verintervalhull	([-0.0468, 0.0127], [0.2606, 0.3473])
Interval householder method [5]	([-0.0558, 0.0232], [0.2579, 0.3485])

In general, methods for solving symmetric interval linear systems can be sorted as follows:

- verifylss,
- verenclinhull,
- parametric method [26],
- verintervalhull.

The list is sorted from the computationally cheapest to the most expensive, but the same order is for the sorting from the least tight to the most tight resulting enclosures. Thus, it is the question for the decision maker to choose between the running time and tightness.

7. Conclusion

We have studied several properties of the set $OLS(\mathbf{X}, \mathbf{y})$ in the interval input – interval output model. It turned out that even very elementary questions about the set $OLS(\mathbf{X}, \mathbf{y})$ are computationally intractable. This negative result motivates a study on special cases, where we can hope that the situation is better.

We devoted our effort to the practically important case, when the input data X are crisp. Then, the set $OLS(\mathbf{X}, \mathbf{y})$ has better geometric and algorithmic properties. In particular, various descriptions of the set $OLS(\mathbf{X}, \mathbf{y})$ can be constructed efficiently, provided the number of regression parameters is low compared to the number of observations (which is a typical case in data analysis). Formally, we stated the results in the form that if the number of regression parameters is fixed, then many tasks can be solved in polynomial time. We also dealt with some special regression models, such as models with repeated observations, where we can achieve further speedup.

Finally we turned our attention back to the general case of interval input – interval output models from a practical point of view. For practical purposes, a variety of methods for finding interval enclosures for the set $OLS(\mathbf{X}, \mathbf{y})$ are available. Nevertheless, we have constructed some elementary examples showing that the methods can provide highly redundant (and hence practically useless) results. The main drawback is that the methods lean on relaxation as described in Section 6.1. We expect that the special form of dependence, either in the system (11) or in the system (12), could be further analyzed and utilized for improvement of the known enclosure methods. Moreover, not only interval enclosures, but also other types of enclosures (such as ellipsoidal enclosures) could be successful.

We also expect that ongoing research will bring further improvements. It might be possible to improve Theorem 18 as discussed in Section 4.3. We also expect that further applications of the RRR metaalgorithm of Section 5 could be found, in particular in polyhedral geometry.

We also think that methods of Sections 4 and 5 are suitable for implementation in software for analysis of interval data.

Acknowledgments

The work of the first author was supported by Grant No. P402/12/G097 of the Czech Science Foundation. The work of the second author was supported by Grant No. P201/09/0755 of the Czech Science Foundation. The work of the third author was supported by Grants No. P403/12/1947 and P402-13-10660S of the Czech Science Foundation.

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