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On Methodological Foundations of Interval Analysis of Empirical Dependencies

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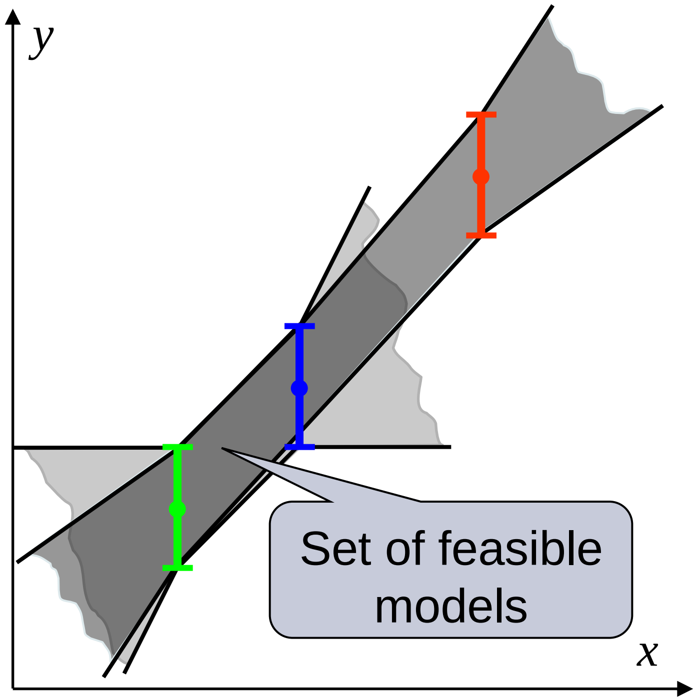
Outline

- Linear regression under interval error
- Validity of prior assumptions
- Revealing data inconsistency
- Basic principles and general scheme of empirical dependencies building
- Conclusions

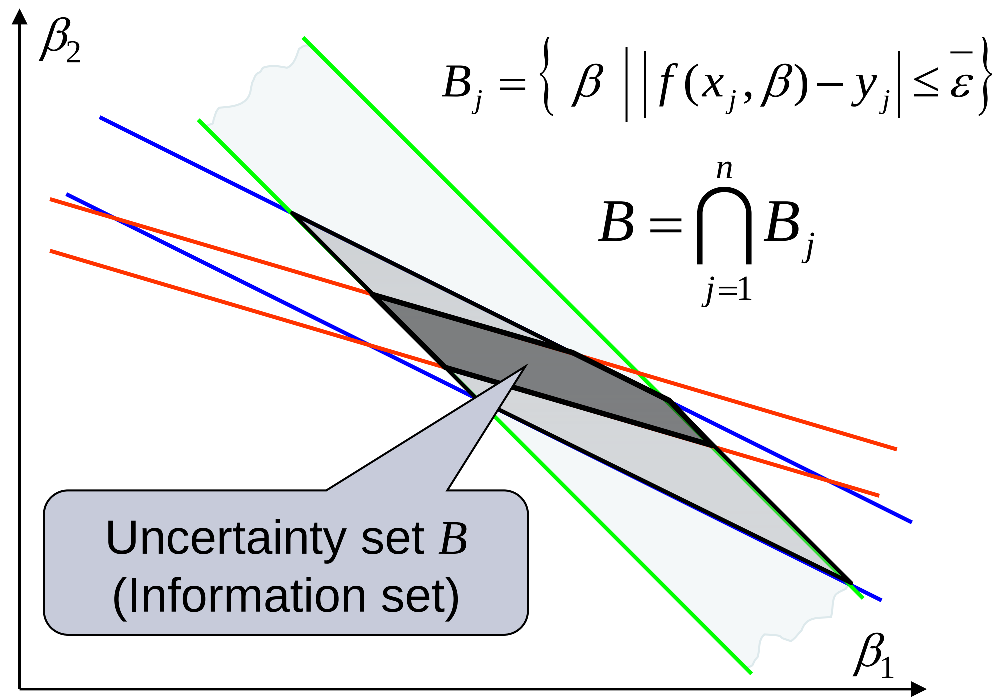
Linear Regression under Interval Error

- Building model $y = \beta_1 + \beta_2 x + \varepsilon, \quad \varepsilon \in [-\bar{\varepsilon}, \bar{\varepsilon}]$

In (x, y) domain



In (β_1, β_2) domain



Linear Regression under Interval Error

- Problems stated with respect to uncertainty set B
  - Prediction of the response value for fixed values of input variables
    - Interval estimates of y

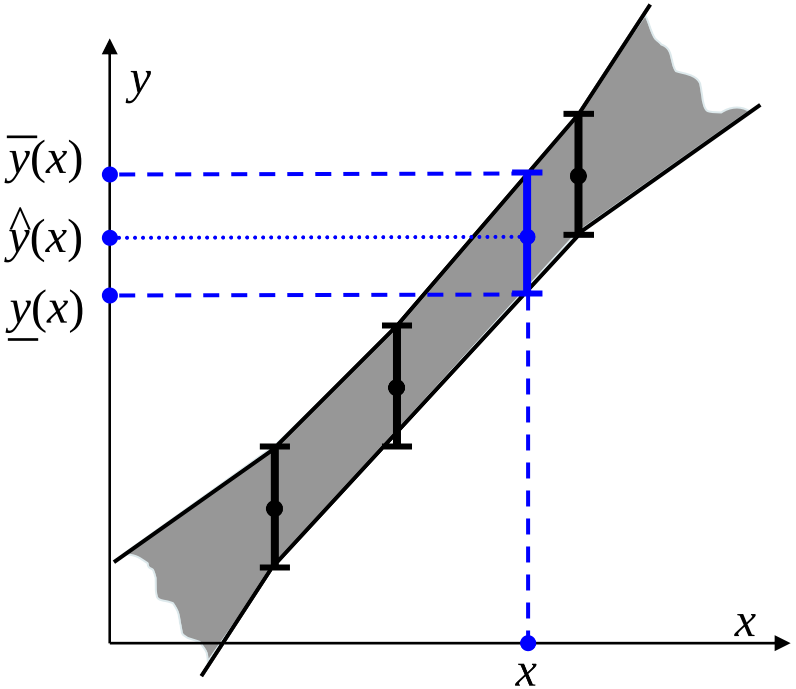
$$\mathbf{y}(x) = \left[\underline{y}(x), \overline{y}(x)\right]:$$

$$\underline{y}(x) = \min_{\beta \in B} \beta^T x,$$

$$\overline{y}(x) = \max_{\beta \in B} \beta^T x,$$

    - Point estimates of y

$$\hat{y}(x) = \tfrac{1}{2}\left(\underline{y}(x) + \overline{y}(x)\right)$$



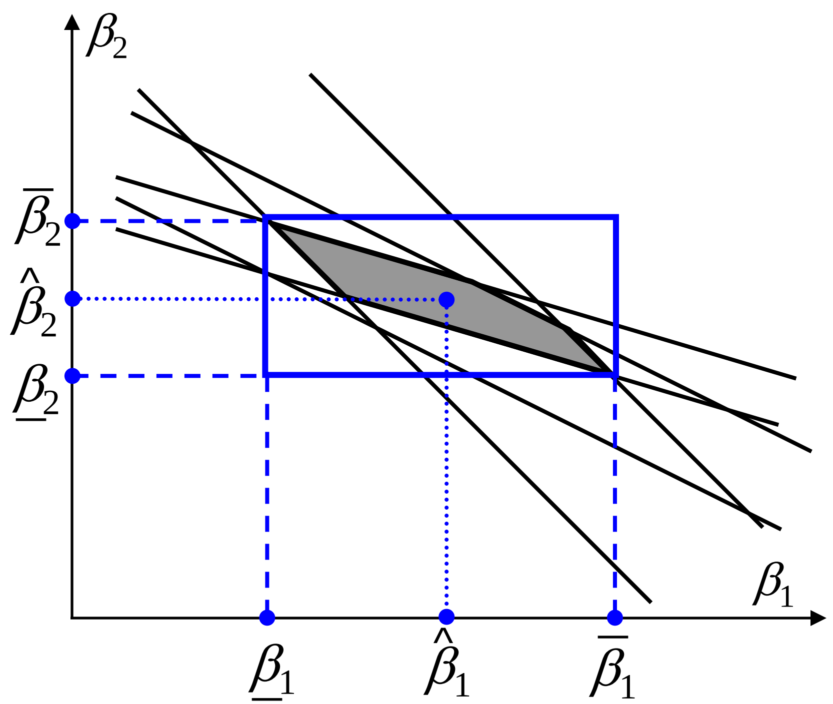
Linear Regression under Interval Error

- Problems stated with respect to uncertainty set B
  - Model parameters estimation
    - Interval estimates of β

$$\square B = \left(\left[\underline{\beta}_1, \overline{\beta}_1 \right], \ldots, \left[\underline{\beta}_p, \overline{\beta}_p \right] \right):$$

$$\underline{\beta}_i = \min_{\beta \in B} \beta_i, \quad \overline{\beta}_i = \max_{\beta \in B} \beta_i,$$

$$i = 1, \ldots, p.$$



    - Point estimates of β

$$\hat{\beta} = \left(\hat{\beta}_1, \ldots, \hat{\beta}_p \right):$$

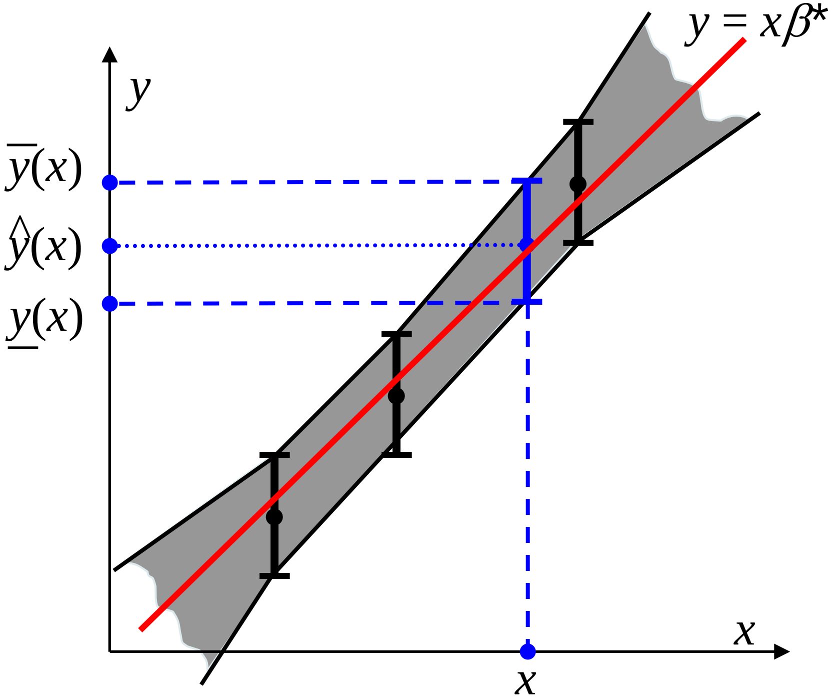
$$\hat{\beta}_i = \tfrac{1}{2} \left(\underline{\beta}_i + \overline{\beta}_i \right), \; i = 1, \ldots, p.$$

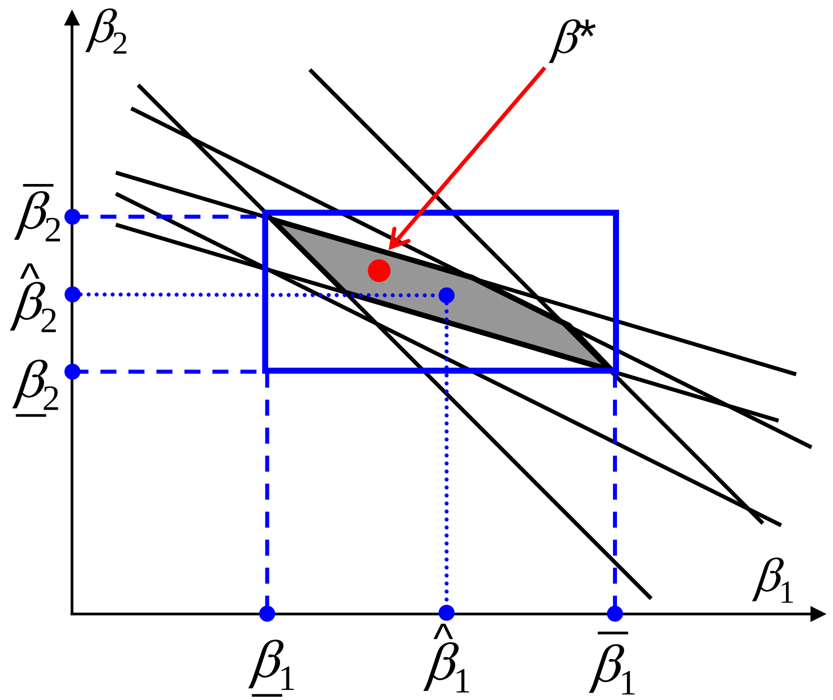
Fitting Experimental Data under Unknown-But-Bounded Error

- Years and Authors
  - 1962 L.V. Kantorovich
  - 1970 S.I. Spivak et al.
  - 1982 G. Belforte, M. Milanese et al.
  - 1983 N.M. Oskorbin et al.
  - 1986 J.P. Norton
  - 1987 S.I. Kumkov et al.
  - 1987 E. Walter, H. Piet-Lahanier
  - 1989 A.P. Voshchinin et al.
  - 1993 P.L. Combettes
  - 2000 O.E. Rodionova, A.L. Pomerantsev
  - 2003 A.A. Podruzhko, A.S. Podruzhko

Linear Regression under Interval Error

- Problems stated with respect to uncertainty set B
  - Prediction of the response for fixed values of input variables
  - Model parameters estimation





Validity of Prior Assumptions

- Interval regression assumptions
  - Structure of modeling function is fixed
  - Upper error bound is equal to $\bar{\varepsilon} \in [-\bar{\varepsilon}, \bar{\varepsilon}]$

- Milanese M., Novara C.:
  - **Definition***. Prior assumptions are considered validated if $B \neq \varnothing$.
  - The fact that the prior assumptions are validated (are consistent with the *present* data) does not exclude that they may be invalidated by *future* data**.

*Milanese M., Novara C. *Set membership identification of nonlinear systems* // Automatica 40 (2004), 957-975.

**Popper K.R. *Conjectures and Refutations: The Growth of Scientific Knowledge*. London: Rontedge and Kegan Paul, 1969.

Uncertainty Center Method
(Oskorbin, 1983)

- If data are inconsistent ($B = \varnothing$) for certain model structure and upper error bound $\bar{\varepsilon}$
  - Find minimal feasible error ε_{min} (expand error bound until $B \neq \varnothing$)
  - Analyze ε_{min} and boundary samples of $B(\varepsilon_{\text{min}})$ to detect outliers or to modify model structure.

Oskorbin, N.M., Maksimov, A.V., and Zhilin, S.I., *Construction and Analysis of the Empirical Dependences Using the Uncertainty Center Method*, Izv. Alt. Gos. Univ., 1998, No. 1, pp. 35–38. (in Russian).

Simple Method for Outlier Detection
(Zhilin, 2004)

- Core idea
  - An outlier may be treated as a measurement with the underestimated error (i.e. the actual measurement error is greater than the declared error ε_j for it)
  - What are the lower bounds ε_j' for actual errors which provide non-empty uncertainty set?

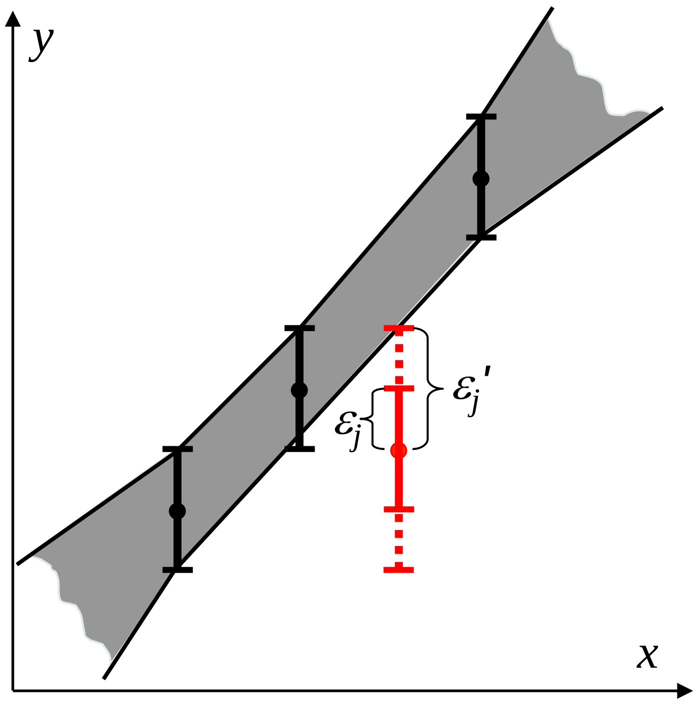
Zhilin S.I. On Fitting Empirical Data Under Interval Error // Reliable Computing (2005) 11 (5) 433-442.

Zhilin S.I. Simple Method for Outlier Detection in Fitting Experimental Data Under Interval Error // Chemometrics and Intelligent Laboratory Systems (2007) 88 (1) 60-68.

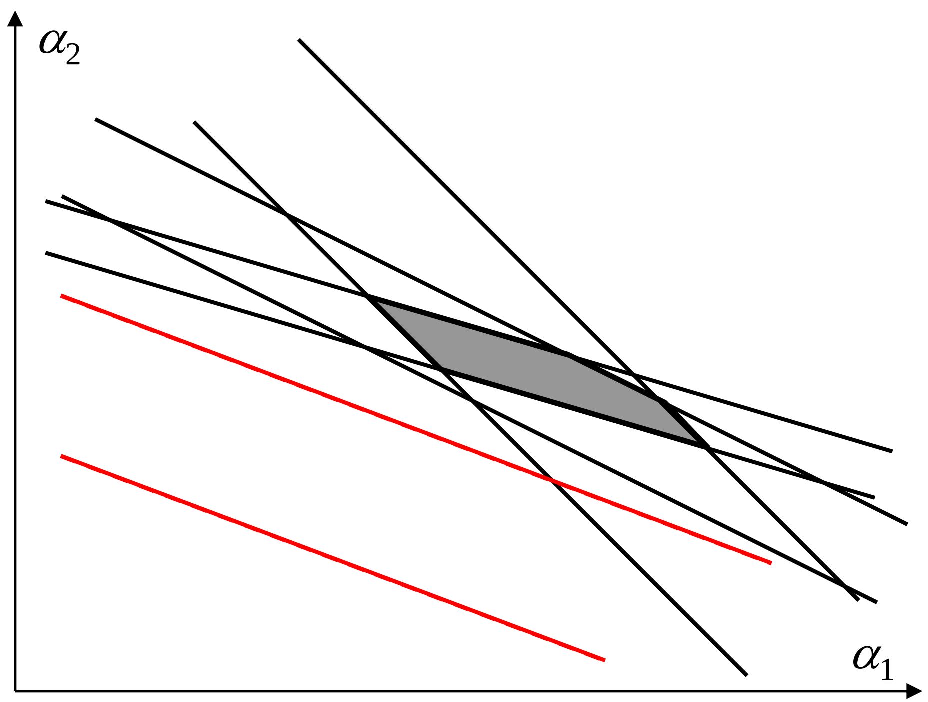
Simple Method for Outlier Detection
(Zhilin, 2004)

- How much must we stretch the declared error interval in order to «correct» an outlier?

In variables domain



In parameters domain



Simple Method for Outlier Detection
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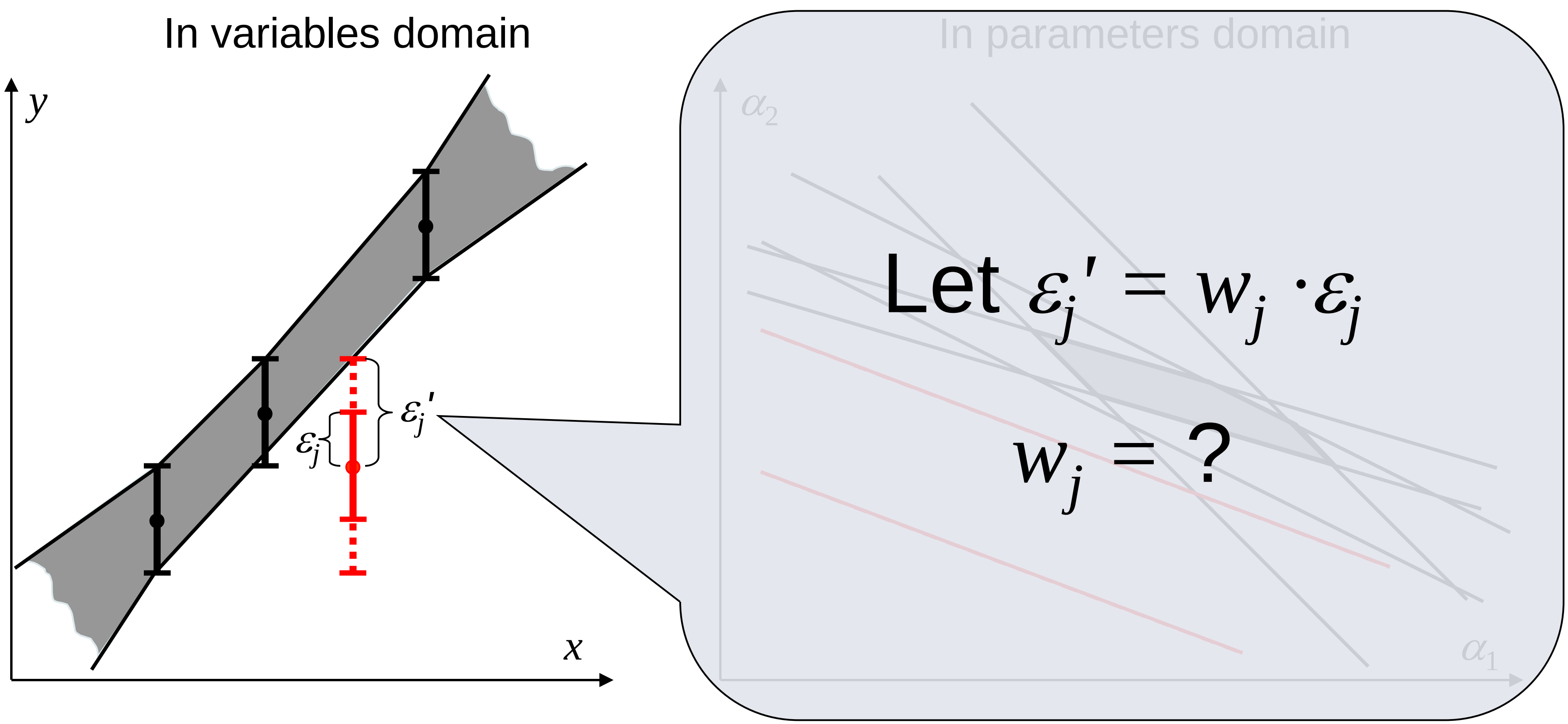

Simple Method for Outlier Detection
(Zhilin, 2004)

- Weights w_j may be found from the following optimization problem

$$\min_{\alpha,w} \sum_{j=1}^{n} w_j \qquad (1)$$

Uncertainty set constraints with movable bounds

$$y_j - w_j\varepsilon_j \le f(x_j,\beta) \le y_j + w_j\varepsilon_j, \qquad j=1,\ldots,n \qquad (2)$$

$$w_j \ge 1, \quad j=1,\ldots,k \qquad (3)$$

$$w_j = 1, \quad j=k+1,\ldots,n \qquad (4)$$

$$\begin{aligned} & w_1 = w_2 = \ldots = w_{j_1}, \\ & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots, \\ & w_{j_m+1} = w_{j_m+2} = \ldots = w_n \end{aligned} \qquad (5)$$

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Uncertainty set constraints with movable bounds

We can only enlarge error intervals…

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$$w_j \ge 1, \quad j = 1, \ldots, k \qquad (3)$$

…or “freeze” some of error intervals

$$w_j = 1, \quad j = k+1, \ldots, n \qquad (4)$$

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$$w_j \ge 1, \quad j = 1, \ldots, k \qquad (3)$$

$$w_j = 1, \quad j = k+1, \ldots, n \qquad (4)$$

Some of the measurements are obtained with equal errors

$$\begin{aligned} & w_1 = w_2 = \ldots = w_{j_1}, \\ & \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots, \\ & w_{j_m+1} = w_{j_m+2} = \ldots = w_n \end{aligned} \qquad (5)$$

Simple Method for Outlier Detection
(Zhilin, 2004)

- Relations to robust estimation

$$\min_{\alpha,w} \sum_{j=1}^{n} w_j \qquad (1)$$

$$y_j - w_j\varepsilon_j \le f(x_j, \beta) \le y_j + w_j\varepsilon_j, \qquad j = 1,\ldots,n \qquad (2)$$

$$w_j \ge 0, \quad j = 1,\ldots,n \qquad (3')$$

Uncertainty set constraints with movable bounds

~~We can only enlarge error intervals…~~

We allow free scale of error intervals (to expand and to contract)

Simple Method for Outlier Detection
(Zhilin, 2004)

- Relations to robust estimation

$$\min_{\alpha,w} \sum_{j=1}^{n} w_j \qquad (1)$$

$$y_j - w_j\varepsilon_j \le f(x_j,\beta) \le y_j + w_j\varepsilon_j, \qquad j=1,\ldots,n \qquad (2)$$

$$w_j \ge 0, \quad j=1,\ldots,n \qquad (3')$$

Uncertainty set constraints with movable bounds

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Solution (β', w') of (1)-(3') gives
β^* is M-estimator for parameters β (known as L_1)

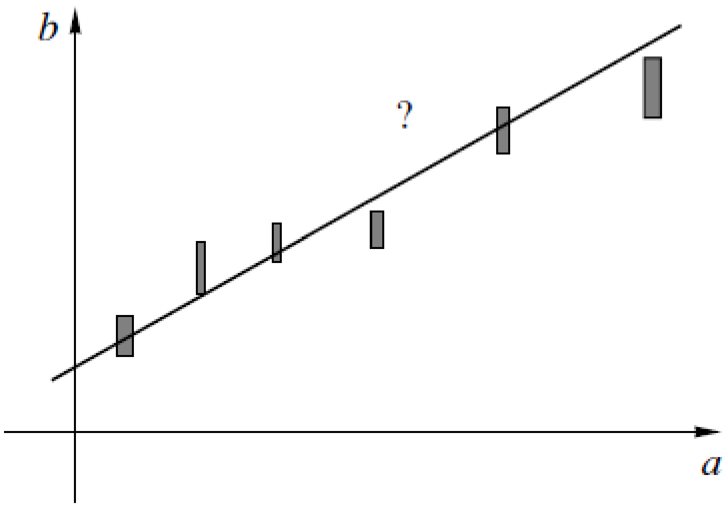
Weight function: $W(x) = 1/|x|$.

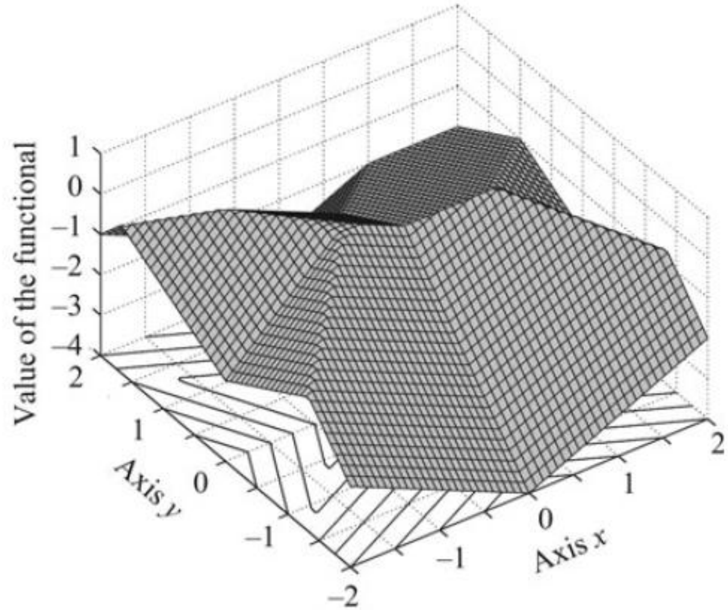
Residuals: $w_j^* \cdot \varepsilon_j$.

Method of Maximal Consistency
(Shary, 2012)

- Measure of consistency := USS recognizing functional

$$\mathrm{Uni}\,(x, \boldsymbol{A}, \boldsymbol{b}) = \min_{1\leqslant i\leqslant m} \left\{ \mathrm{rad}\, \boldsymbol{b}_i - \left\langle \mathrm{mid}\, \boldsymbol{b}_i - \sum_{j=1}^{n} \boldsymbol{a}_{ij}\, x_j \right\rangle \right\}$$

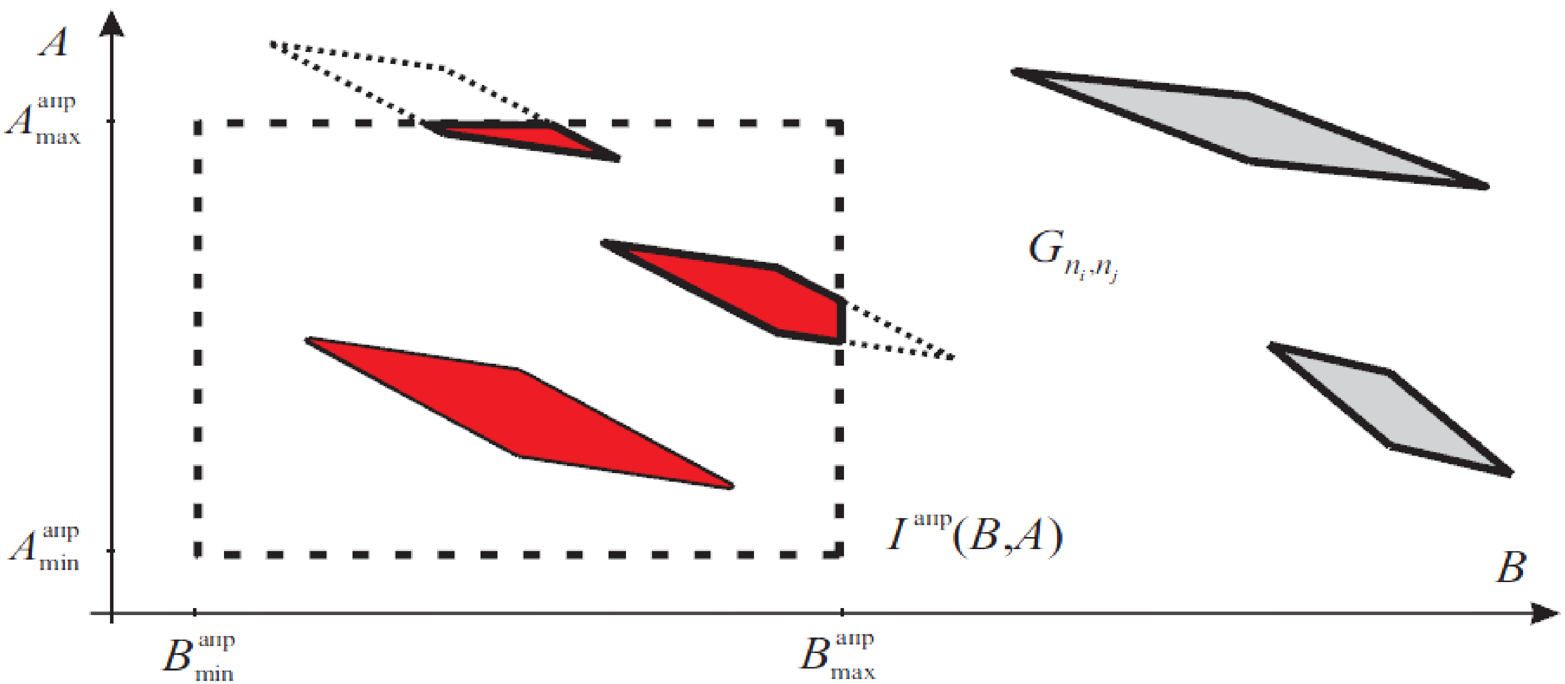




Shary S.P. *Solvability of Interval Linear Equations and Data Analysis under Uncertainty* // Automation and Remote Control (2012) 73 (2), 310–322.

Partial Information Sets
(Kumkov, 1987)

- Analysis of consistent subsamples



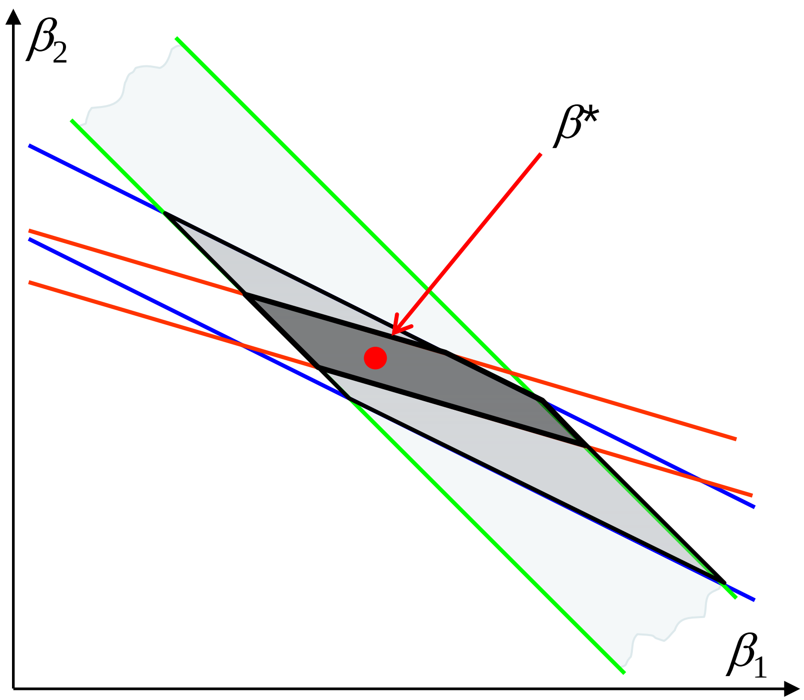
Kumkov S.I. *Processing of Experimental Data on Ionic Conductivity of Molten Electrolyte by the Interval Analysis Methods* // Rasplavy (2010), No. 3, pp. 86–96.

Potapov A.M., Kumkov S.I., and Y. Sato. *Processing of Experimental Data on Viscosity under One-Sided Character of Measuring Errors* // Rasplavy (2010), No. 3, pp. 55–70.

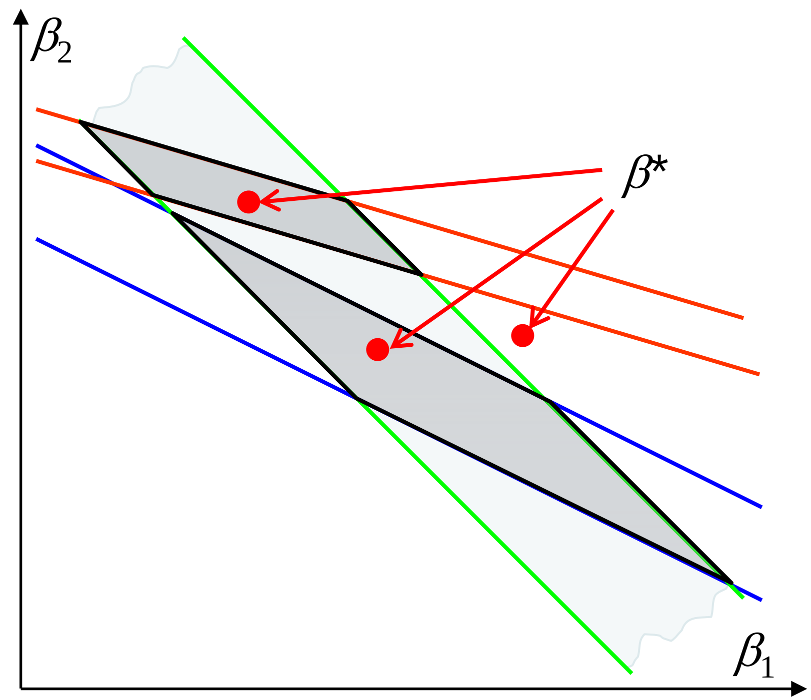
Data Consistency is Necessary But Not Sufficient

- Estimating model $y = \beta_1^* + \beta_2^* x$

$\beta^* \in B$



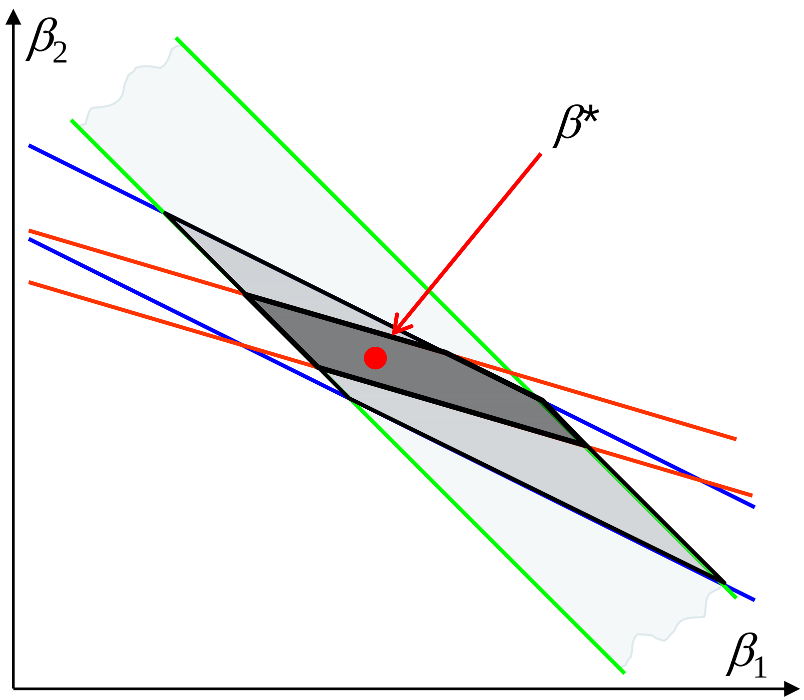
$B = \varnothing$



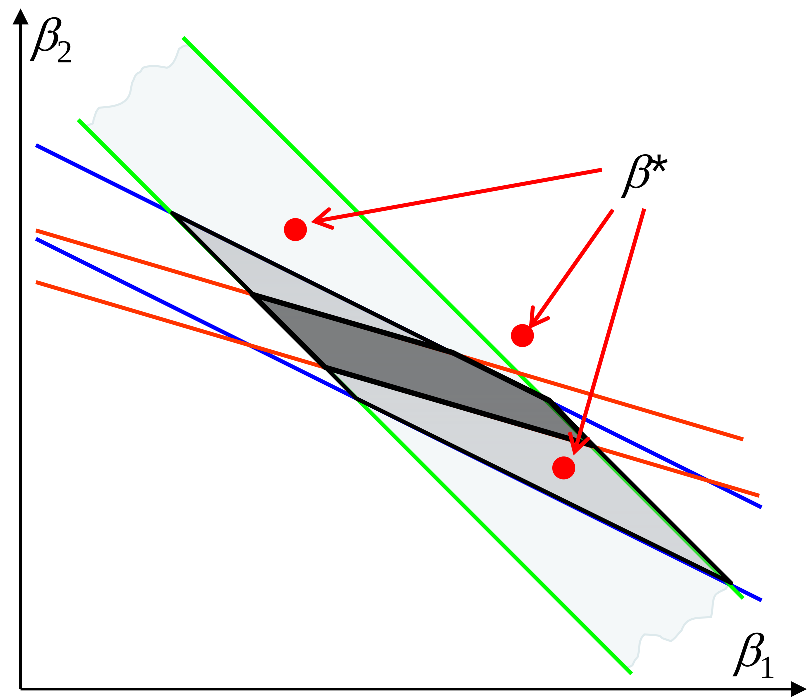
Data Consistency is Necessary But Not Sufficient

- Estimating model $y = \beta_1{}^* + \beta_2{}^* x$

$$\beta^* \in B$$



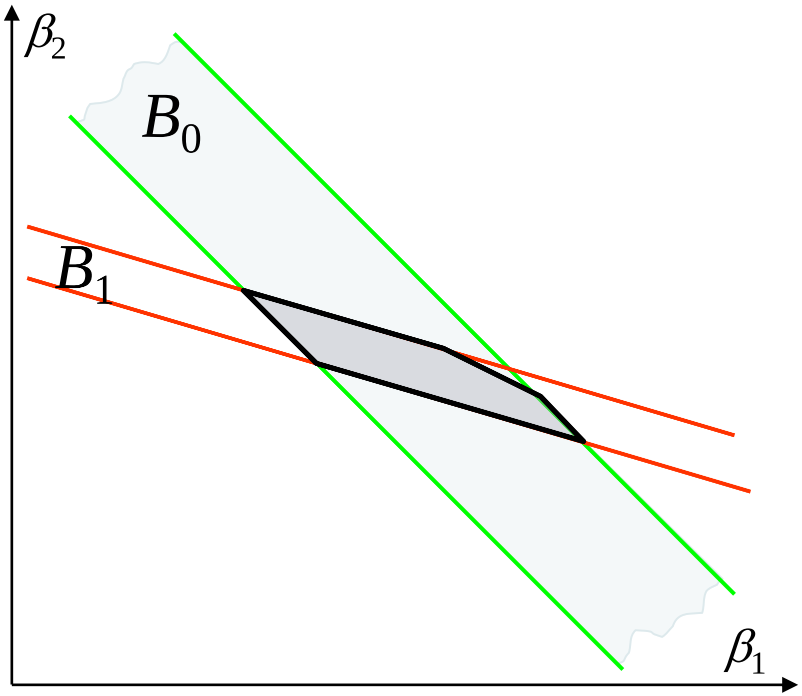
$$\beta^* \notin B \neq \emptyset$$

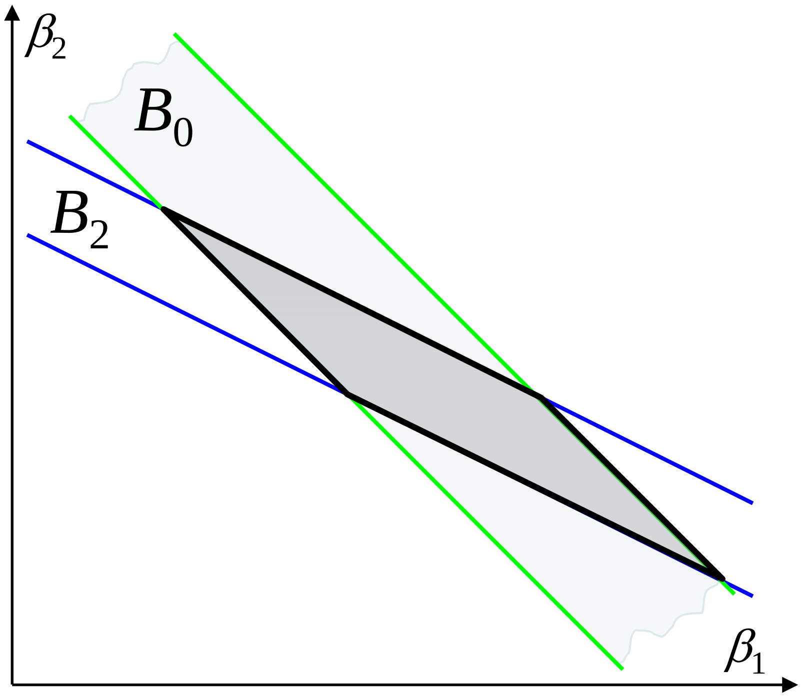


Revealing inconsistencies: possible additional indicators

- Estimate an informational value of each portion of data and knowledge with respect to the selected basic set

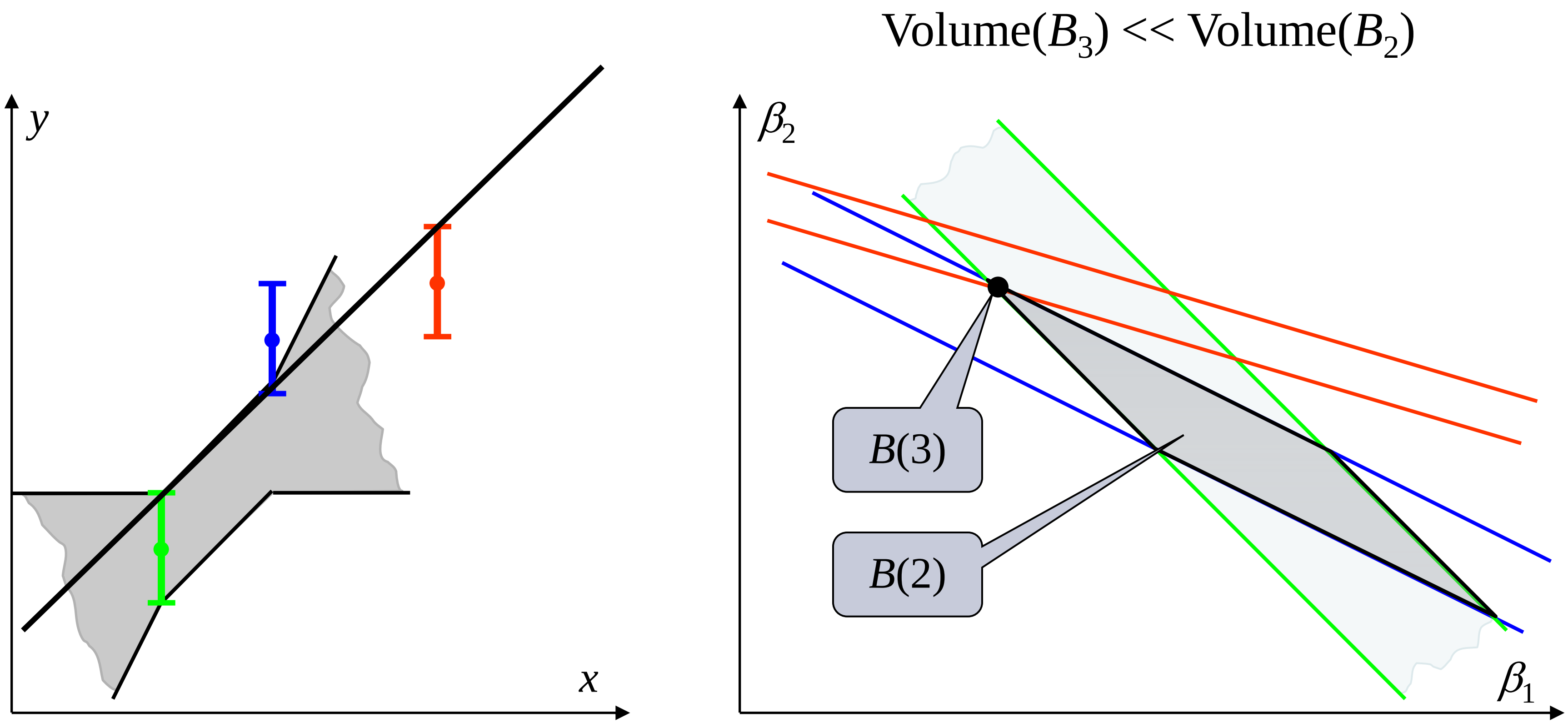
$$\text{Informativity}(B_i) = 1 - \frac{\text{Volume}(B_0 \cap B_i)}{\text{Volume}(B_0)}$$





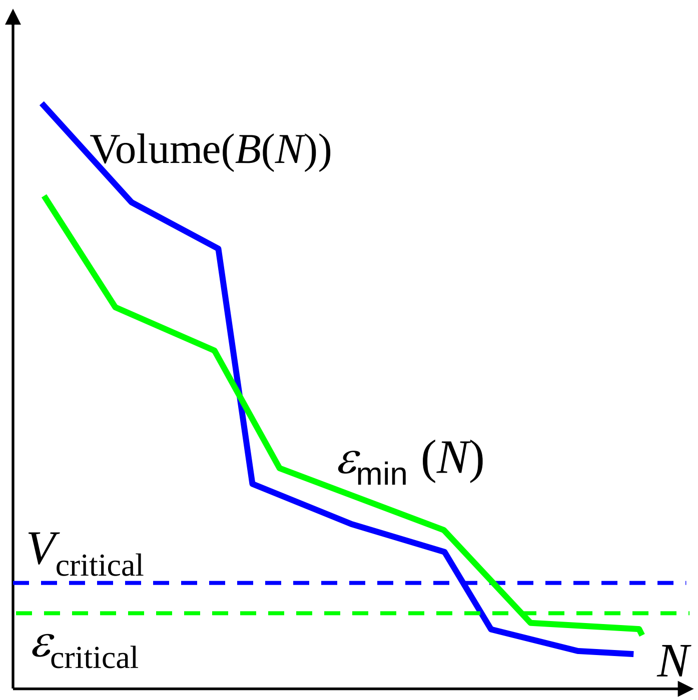
Revealing inconsistencies: possible additional indicators

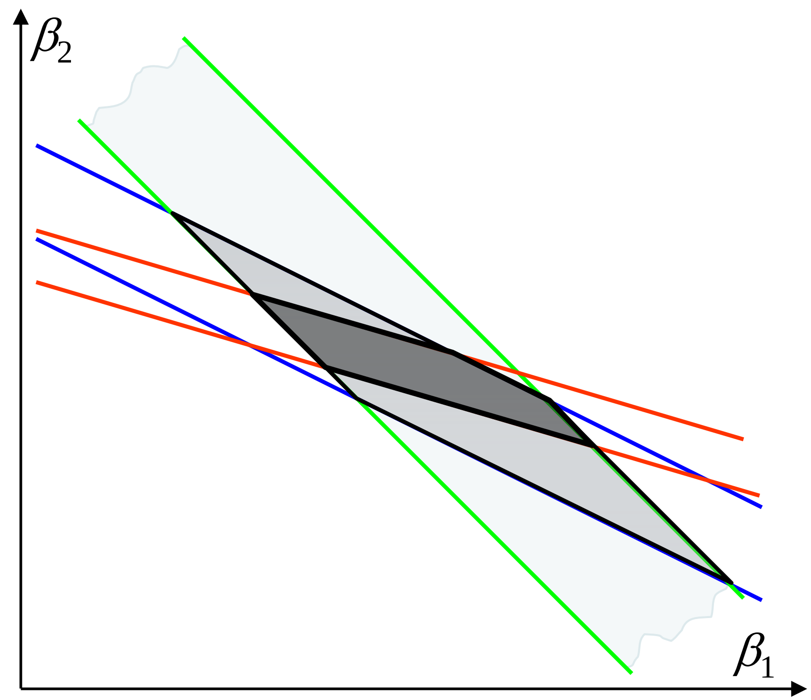
- Relate the volume of $B(N)$ to the value of N



Revealing inconsistencies: possible additional indicators

- Investigate the dynamics depending on N:
  - volume of $B(N)$
  - $\varepsilon_{\min}(N)$





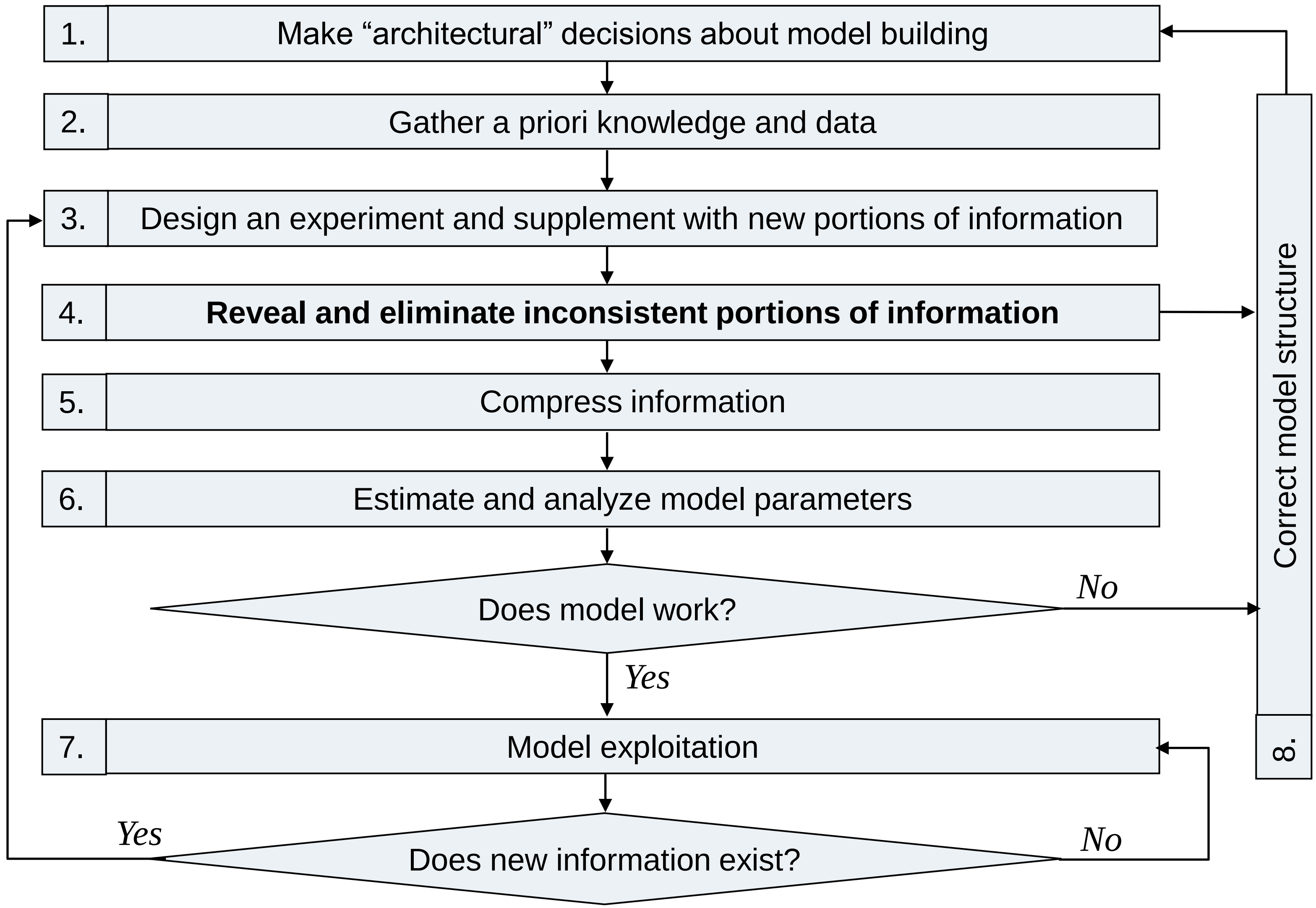
Revealing inconsistencies: possible additional indicators

- To discover inconsistencies one can
  - Estimate an informational value of each portion of data and knowledge with respect to the selected basic set
  - Relate the volume of $B(N)$ to the value of N
  - Investigate the dynamics of the volume of $B(N)$ and $\varepsilon_{min}(N)$ depending on N

Basic Principles

- It is impossible to obtain reliable estimates of process (object) parameters using an inconsistent set of data and knowledge about the process (object)
- Data consistency is necessary but not sufficient condition for reliable estimates
- None of the inner mathematical needs can be a ground for any kind of modifications of analyzed data and knowledge

General Scheme



Conclusions

- We propose
  - Basic principles and general scheme of building and analysis of empirical dependencies using interval analysis
  - Possible additional indicators of inconsistencies in data and knowledge

- Implementation of the proposed approach demands for the development of suitable mathematical tools and accumulation of experience in specific applications