

The Roles of Condition Number in Least Squares Equation.

Abstract. The paper considers nearness to singularity for which the Co-variance matrix in the least squares equation is well known. A synchronization of the condition number with ill-conditioning is made which relates the quality of approximate solution to the described system. Various theoretical lower and upper bounds to the perturbed least squares problems have been described for which, reachability theory has strong representation. In particular, a theorem due to Popova has been revisited and examined in details, and was found to have strong favourable appeals on the resulting linear interval system of equation. A procedure described in Kramer/Rohn is used to crop the corner points solution of the linear interval system of equation based on the appropriate choice of the orthant (where there are 2^n possibilities) by solving systems of linear inequalities. The Rump/Krawczyk method was used to improve the computed corner point solution from Kramer/ Rohn method. The loss function for the result obtained from Popova method for the set of data points is reported.

Keywords : linear least squares, diffeomorphism, reachability theory, condition number, interval arithmetic, regulator in least squares problems

MSC (2000): 65F20, 65 G40

1. Introduction

The paper considers condition numbers associated with solving least squares equations with some noise in the data. The Covariance matrix in least squares interval equations is often Ill-conditioned. Ill-conditioned problems are often encountered in geophysics, signal processing, and medical imaging. For example, Auto-Covariance Least squares are used in the study of Kalma filter. Kalma filter has been widely applied in navigation and control of vehicles, as for example, aircraft and space craft. In its widest application areas, Kalma filter is used in the navigation system of nuclear ballistic missile submarines, and cruise missiles –e.g., the US Navy's Tomahawk missile, US Air Launched Cruise missile are a few typical examples for this purpose to which least squares equations are involved in their formulations . Interval arithmetic has been found useful in the study of fractal mechanics where a fracture in any part of aircraft makes every other part inoperable. Computing reachable set is an essential aspect of nonlinear dynamic and control systems. Reachability is an essential tool in the theory of validation of interval computing, since safety is always a paramount interest in scientific and engineering designs which takes into consideration scenarios of worst case error bounds, [1],[2],[3] and [4]

Reachability problem comes in different flavours as for example, the approximate estimates for the solution to the linear system in least squares equation may be taken as ellipsoids which depends on

the operator parameter. For the exhaustive discussion on theory of reachability, the importance of topological space cannot be underscored.

The least squares problem is formulated in the form:

$$\text{Find } \beta \in R^n \ni Y = f(\beta) = \|Y - T\beta\|_2 = \min_{\beta \in R^n} \|Y - T\beta\|_2 \quad (1.1)$$

where $T \in R^{m \times n}$ matrix, $Y \in R^n$.

In what follows, we signify our notation by the convention: $R^n, IR^n, R^{m \times n}, IR^{m \times n}$ as representing real n -vector, interval n -vector, real $m \times n$ rectangular matrix and interval $m \times n$ matrix respectively. The midpoint of interval matrix T as well as interval vector b is respectively defined in the form

$$T_c = 0.5(T + \bar{T}),$$

$$b_c = 0.5(b + \bar{b}).$$

The interval radius of interval matrix T as well as interval vector b is given by

$$\Delta T = 0.5(\bar{T} - T), \Delta b = 0.5(\bar{b} - b)$$

We note that R^n itself is convex, and all interval boxes in R^n are convex. A subset $D \subseteq R^n$ is convex if there are points $\beta, z \in D \ni t\beta + (1-t)z \in D \forall t \in [0,1]$.

Interval arithmetic operations possess strict validation of every computed result in any calculation and any such computed result is always perfectly correct when faithfully implemented. This captures all possible conversion errors, rounding errors, approximation errors which are always vigorously estimated, [4].

The separation theorem for convex set, [5], states that a point outside a closed convex set is separated from D by a hyper plane.

It is expected that readers acquaint themselves with the concept of well known implicit function theorem which gives necessary conditions under which a continuously differentiable function has an inverse. This leads us to the concept of a diffeomorphism [6], that transforms a nonlinear system in equation 1.1 to a linear system

$$T^T T \beta = T^T b \Rightarrow \hat{\beta} = (T^T T)^{-1} T^T b = T^T Y \quad (1.2)$$

Here, it is assumed that if $X \in ID \subset IR^m$ be closed in IR^m . A function $f: ID \rightarrow IR^n$ is a diffeomorphism of ID onto its image $Y = f(ID)$ if it is one-to-one, smooth, and of full rank n .

By full rank, would imply the maximal possible rank, e.g., the case of a rectangular matrix of size $m \times n$, the full rank is given by $\min\{m, n\}$. Solving least squares problems in interval form is not without some combinatorial difficulties. As a typical example, the Co-Variance matrix is sometimes always nearly singular or, even singular.

A case of how to resolve problem of singularity in the least squares problem, the regulator parameter has been discussed [7]. The solution could be written in the form

$$\hat{\beta} = (T^T T + \tau^k I)^{-1} T^T Y, p \geq 2 \quad (1.3)$$

The term τ is taken to be $\frac{1}{\|T^+\|}$, where T^+ is the pseudo inverse operator. Interestingly, [7] proved that the best value for k in equation 1.3 is 2.

In what follows the matrix product $T^T T$ will be denoted by another matrix B, and $T^T Y = b$ as a vector. The inverse of the matrix B is the Co-Variance matrix. It will play a major role in our analysis hence forth.

In the mean time, the paper is categorized as follows: Section 2 gives the condition numbers associated with linear least squares problems. Section 3 discusses the perturbation error bounds for the lower and upper chain reachable set of the approximate solution to the least squares problems wherein, the residual error plays vital roles in their formulation. In section 4 the theorem of [8], re-examined and was adopted for a useful purpose in the realization of numerical results.

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2. CONDITION NUMBERS OF LINEAR LEAST SQUARES PROBLEM

Condition number has very useful property in both Scientific and Engineering designs. It is also used in economics.

The quality of results computed from the least squares equation is based on the condition numbers of the system of equation 1.2. Condition number shows how the solution to the described system fits the data under study. Condition number measures how a change in input is propagated to change in output. High condition number implies high non linearity in the obtained solution to the system.

For a real matrix B which is not singular and whose norm $\|\cdot\|$ is known, the condition number [9, 10], was defined to be

$$K(B) = \lim_{\varepsilon \rightarrow 0^+} \sup_{\|\Delta B\| \leq \varepsilon \|B\|} \frac{\|(B + \Delta B)^{-1} - B^{-1}\|}{\varepsilon \|B^{-1}\|}, \quad (2.1)$$

Whereas, the traditional condition number is known to be

$$K(B) = \|B^{-1}\| \cdot \|B\| \quad (2.2)$$

If condition number $K(B)$ of a matrix B is known in advance, it is possible to calculate the loss function, the digits of accuracy of solution in the variable β compared to precision of B by taking the logarithm of $K(B)$.

The derivation of condition number in equation (2.2) may be obtained as follows: Suppose that $\beta^{(sle,abs)}$ denotes the least squares solution to equation 1.1. Then, following [11], it is that

$$\begin{aligned} \beta^{(sle,abs)}(B) &= \lim_{\beta \rightarrow \beta_0} \sup \frac{\|\beta - \beta_0\|}{\beta^{(sle)}(x)} \\ &= \lim_{\beta \rightarrow \beta_0} \frac{\|\beta - \beta_0\| \|\beta_0\|}{\|B\beta - b\|} = \lim_{\delta \beta \rightarrow 0} \sup \frac{\|\delta \beta\| \|\beta_0\|}{\|B \delta \beta\|} = \|B^{-1}\| \cdot \|\beta_0\|. \end{aligned}$$

As a result, the relative condition number is then the quantity

$$\beta^{(sle,rel)}(B) = \frac{\|B\|}{\|\beta_0\|} \beta^{(sle,abs)}(B) = \|B^{-1}\| \|B\|.$$

The problem of computing β , given b has a condition number

$$\begin{aligned} K_\beta &= \frac{\|B^{-1}\| \|\beta\|}{\|b\|} \quad \text{Whereas, the problem of computing } b \text{ given } \beta \text{ has a condition number,} \\ K_b &= \frac{\|B\| \cdot \|\beta\|}{\|b\|}. \end{aligned}$$

Let B be perturbed by ΔB and β be the solution to system of equation 1.1, the perturbation in b would be approximately bounded by

$$\frac{\|\delta b\| / \|b\|}{\|\Delta B\| / \|B\|} \approx K_b \leq K(B) \Rightarrow \|\delta b\| \leq \frac{K(B) \|b\| \cdot \|\Delta B\|}{\|B\|} \quad (2.3)$$

Similarly, assuming B is perturbed by ΔB and b is given, then the perturbation in β is also approximately equal to :

$$\frac{\|\delta \beta\| / \|\beta\|}{\|\Delta B\| / \|B\|} = K_\beta \leq K(B) \Rightarrow \|\delta \beta\| \approx \frac{K(B) \|\beta\| \|\Delta B\|}{\|B\|} \quad (2.4)$$

The product norm for the data space which holds for $\|\beta\|_2$ as the solution space, [12] is given by the equation

$$\|(B, b)\|_F = \sqrt{\|B\|_F^2 + \|b\|_2^2} \quad (2.5)$$

120 Via the definition of relative condition number, as the quantity

$$121 \quad \beta^{(sle,abs)}(B) = \frac{\|B\|}{\|\beta_0\|} \beta^{(sle,abs)}(B) = \|B^{-1}\| \|B\|, \quad \text{the relative condition number obtained in [13,14] for}$$

122 **using some iterative methods is given by** the quantity

$$123 \quad K^{(rel)}(B, b) = \|B^+\|_2 \left(\|B^+\|_2^2 \|r\|_2^2 + \|\beta\|_2^2 + 1 \right)^{\frac{1}{2}} \frac{\|(A, b)\|_2}{\|\beta\|_2}, \quad (2.6)$$

124 **for any** $r = b - B\beta$.

125 The reciprocal of condition number is equal to the distance to the nearest singular matrix for all
126 structured perturbations.

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128 Most importantly, [9] used the Bauer-Skeel condition number for a weighted matrix to show that

$$129 \quad Cond_{BS}(B, E) = \left\| \left| B^{-1} \right| E \right\| \quad (2.8)$$

130 **E, being** defined as $|B|$ and relates condition number with spectral radius by the equation:

$$131 \quad Cond(B, E) = \rho\left(\left| B^{-1} \right| E\right) = \inf_{D_1, D_2}^{cond_{\infty}} (D_1 B D_2) \quad (2.9)$$

132 D_1, D_2 are diagonal scaling. It follows [9] that

$$133 \quad \frac{1}{\rho\left(\left| B^{-1} \right| E\right)} \leq \delta(B, E) < \frac{(3 + 2\sqrt{2})}{\rho\left(\left| B^{-1} \right| E\right)} \quad (2.10)$$

134 The expression $\delta(B, E)$ in equation 2.10 is the familiar singular value of (B,E) . In any case, [9]

135 warned that the factor $(3 + 2\sqrt{2})$ cannot be replaced by 1 since computationally,

$$136 \quad \delta(|B|, E) = \frac{n}{\rho\left(\left| B^{-1} \right| |B|\right)}.$$

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138 3. Backward perturbation error bound for Least squares equation

139 The smallest Frobenius perturbation ΔB which makes a given non-zero β into a solution space of

140 the perturbed problem $\min_{\beta} \|b - (B + \Delta B)\beta\|_2$ in a sense due to [15] was estimated to be

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$$X_F^{(LS)}(\beta) = \left(\frac{\|r\|_2^2}{\|\beta\|_2^2} + \min\{0, \lambda\} \right)^{\frac{1}{2}} \quad (3.1)$$

Where ,

$$\lambda = \lambda_{\min} \left(BB^T - \frac{rr^T}{\|\beta\|_2^2} \right) \quad (3.2)$$

The number λ is the smallest eigenvalue of the $m \times n$ matrix. The lower bound for equation 3.1 was found to be

$$\frac{1}{\sqrt{2}} X_F^{(LS)}(\beta) \leq X_2^{(LS)} \leq X_F^{(LS)}(\beta) \quad (3.3)$$

More complicated upper error bound for the least squares solution set was later found in [15] to be

$$\left(X_2^{(LS)}(\beta) \right)^2 = W \frac{(r^T B \beta)^2}{\|\beta\|_2^2 (\|B\beta\|_2^2 + \|r\|_2^2)} \quad (3.4)$$

Wherefrom,

$$W = \frac{2}{1 + \sqrt{1 - \eta}}, \quad (3.5)$$

$$\eta = \frac{4(r^T B \beta)^2}{(\|B\beta\|_2^2 + \|r\|_2^2)^2} \quad (3.6)$$

Two conditions may be adduced for least squares problem to be ill-conditioned namely, either b could be nearly orthogonal to the column space of B, or, B itself is ill-conditioned, [16].

In what follows, given that $BB^+ \Delta B = \Delta B$, and $B^+ B (\Delta B)^T = (\Delta B)^T$, if range $((\Delta B)^T) \subseteq \text{range}(B^T)$ and $\text{range}(\Delta B) \subseteq \text{range}(B)$, then $(B + \Delta B)^T$ can be approximated [17] by the truncated Taylor Series as

$$(B + \Delta B)^T = B^+ - B^+ (\Delta B) B^+ + O(\varepsilon^2) \quad (3.7)$$

Therefore, since

$$\beta + \delta\beta = (B + \Delta B)^+ (b + \delta b) = \beta + B^+ \delta b - B^+ (\Delta B) B^+ b + O(\varepsilon^2), \quad (3.8)$$

$$\delta b = - \frac{\|b\|}{\|B\| \|\beta\|} \Delta B \beta, \quad (3.9)$$

162 $\delta\beta$ be approximated by the equation

$$163 \quad \delta\beta = -B^+ \Delta B \beta \left(1 + \frac{\|b\|}{\|B\|\|\beta\|} \right) \quad (3.10)$$

164 **Thus the condition number for the solution set is**

$$165 \quad K^S(B, b) = \|B^+\| \|B\| + \|B^+\| \frac{\|b\|}{\|\beta\|} \approx \|B^+\| \|B\| + \|B^+\| \frac{\|B\beta\|}{\|\beta\|} \quad (3.11)$$

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169 **4. Computability of Reachable Sets**

170 As said earlier at the beginning of the paper, computability set is a very important issue in nonlinear
171 dynamic and control theory, [18,19]. Reach-ability problem comes in different flavours, for instance,
172 given a diffeomorphism which transforms a nonlinear system to a linear system, the approximate
173 estimates for the solution set may be considered in the form of ellipsoids which depends on the
174 operator. Various values of parameter will lead to a family of ellipsoids whose intersection is the
175 exact reach set.

176 As it were, one can apply ellipsoid on linear system to obtain the reach set where the inverse
177 operator becomes very necessary to approximate the nonlinear system for the convex bodies.

178 The only worry one has is " which is the best operator" as a tool to achieve this objective? Thus we
179 need the best selection of interval Hull $\sum(B, b)$ as solution set to the given problem.

180 In what follows, we introduce the parametrised linear interval system

$$181 \quad B(p) \cdot \beta = b(p) \quad (4.1)$$

182 where $B(p) \in R^{m \times n}$ and $b(p) \in R^n$ all depend on parameter vector $p \in R^k$, and p varies within a
183 range $[p] \in IR^k$, the set of solution to all $B(p) \cdot \beta = b(p)$, $p \in [p]$. It is in a sense due to [8] and is
184 given by the equation

$$185 \quad \sum.^p = \sum(B(p), b(p), [p]) = \{\beta \in R^n \mid B(p) \cdot \beta = b(p)\}, (for \text{ some } p \in [p]), \quad (4.2)$$

186 That each individual component $\{B(p)\}_{ij}$ and $\{b(p)\}_j$ of B(p), respectively, b(p) depends linearly on
187 p means that there are vectors

$$188 \quad \omega(i, j) \in R^k \text{ for } 0 \leq i \leq n, 1 \leq j \leq \text{ with}$$

$$\{B(p)\}_{ij} = \omega(i, j)^T \cdot p \text{ and } \{b(p)\}_j = \omega(0, j)^T \cdot p$$

In what follows, we review the following theorem for an invariant set such that, $F(\beta) \subset \beta$. This relates Brouwer Fixed point theorem to contraction mapping. We are interested in an interval vector β that is chain reachable from β_0 to β for which the ε -chain holds good.

The chain reachable set F from β_0 is defined as $\text{Chain-Reach}(F, \beta_0) = \bigcap_u \text{Reach}(F, \beta_0, u)$ where u runs over all open covers of β .

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Theorem 4.1,[20,8]. Let $B(p) \cdot \beta = b(p)$ with $B(p) \in R^{n \times n}, b(p) \in R^n, p \in R^k$ be a parametrised linear system, where $B(p), b(p)$ are given. Let $R \in R^{n \times n}, [Y] \in IR^n, \beta \in R^n$, define $[Z] \in IR^n, [C] \in IR^{n \times n}$ by

$$[Z]_i = \left(\sum \left\{ R_{ij} \cdot \left(\omega(0, j) - \bar{\beta}_v \cdot \omega(j, v) \right) \right\}^T \right) [p],$$

$$[C] = I - R \cdot B([p]).$$

Define $[V] \in IR^n$ by means of the following iteration enclosure

$$1 \leq i \leq n : V_i = ([Z]) + [C] \cdot [U],$$

$$[U] = (V_1, V_2, \dots, V_{i-1}, Y_i, \dots, Y_n)^T,$$

If, $[V] \overset{\subset}{\neq} [Y]$, then R and every matrix $B(p), p \in [p]$ are regular, and for every $p \in [p]$ the unique solution

$$\hat{\beta} = B^{-1}(p) \cdot b(p), \quad (4.3)$$

the point system satisfies $\beta = \beta_c + [V]$ with $[\Delta] = \{[C] \cdot [V] \in IR^n\}$ and the solution set $\sum.^p$ as defined by equation 4.2, the following inner and outer estimation hold true

$$[\beta_c - \inf([Z]) + \sup([\Delta]), \beta_c + \sup([Z]) + \inf([\Delta])] \subseteq [\inf(\sum.^p), \sup(\sum.^p)] \quad (4.4)$$

We also used the discussion in [21] as a prelude to crop the corner point solution of $\sum(B, b) \cap O_k$, where O is the sign vector $s = (s_i) \in S^n, (s_i \in \{-1, +1\}, i=1(1)n)$, corresponds to the signs of the components of an interior point of O. It is supposed that O is an orthant, [22].

By theory of linear inequalities proven in [22], the solution to the linear interval system of equation 4.1 becomes

$$\sum(B, b) \cap O = \bigcap_{i=1}^n \left(H_i \cap \bar{H}_i \right) \cap O. \quad (4.5)$$

The $H_i, \bar{H}_i$ are half spaces computable systems of linear inequalities and they are dependent on the choice of orthant O (2^n possibilities). As in [21], exact solution set of the linear interval system of equation 4.1 is in the form

$$\sum(B, b) = \bigcup_{k=1}^{2^n} \left[\bigcap_{i=1}^n \left(H_i^k \cap \bar{H}_i^k \right) \cap O_k \right] \quad (4.6)$$

The expression in the right hand side bracket $[.]$ is either $\emptyset$ or a convex polytope. As a result, we are led to the following theorem.

Theorem 4.2, [23]. Let $B = [B_c - \Delta B, B_c + \Delta B]$ be an $n \times n$ interval matrix, $b = [b_c - \delta, b_c + \delta]$ an interval n-vector, and let Z be a subset of S_n having the following properties:

(i) $\text{sgn}(\beta_0) \in Z$ for some $\beta_0 \in \sum(B, b)$,

(ii) for each $z \in Z$ the inequalities

$$(QB_c - I)O_z \geq |Q|\Delta B, \quad (4.7)$$

$$(QB_c - I)O_{-z} \geq |Q|\Delta B, \quad (4.8)$$

have matrix solutions Q_z and Q_{-z} , respectively.

(iii) if $z \in Z, Q_{-z}b_c - |Q_{-z}|\delta \leq Q_z b_c + |Q_z|\delta$, and $(Q_{-z}b_c - |Q_{-z}|\delta)_j (Q_z b_c + |Q_z|\delta)_j \leq 0$

for some j , then $z - 2z_j e_j \in Z$.

Then B is regular and

$$\sum(B, b) \subseteq \bigcup_{z \in Z_0} [\beta_z, \bar{\beta}_z] \quad (4.9)$$

holds, where

$$Z_0 = \{z \in Z \mid \sum(B, b) \cap R_z^n \neq \emptyset\} \quad (4.10)$$

Let us note that an improvement on the computed results from methods 4.6 and 4.10 can be made by further using Rump/Krawczyk method [20]

$$Rb + (I - RB)z^k \subset \text{int}(z^k), (z^k \supset \sum(B, b)) \quad (4.11)$$

238 5. NUMERICAL EXAMPLE

239 Planetary elliptical orbit of ten observations of its position in the (X,Y) plane is considered based
240 on the sample data taken from [24].

241 TABLE 1

X	Y
1.02	0.39
0.95	0.32
0.87	0.27
0.77	0.22
0.67	0.18
0.56	0.15
0.44	0.13
0.30	0.12
0.16	0.13
0.01	0.15

242

243 Take Gaussian noise $|p| = 0.0005$ for the data set. We use a polynomial of order three for the
244 data fit.

245 Using cubic polynomial fit, the result for the Least squares problem 1 without noise in the data is

246 $\hat{\beta} = (0.1550, -0.2578, 0.4694, -0.0295)^T$.

247 Results computed from the Table 1 using the Theorem due to [8] is hereby displayed in Table 2

248 TABLE 2 SHOWING RESULTS COMPUTED FROM TABLE 1.

RESULT FROM POPOVA METHOD [8] FOR $\hat{\beta}$	
[0.1549994,	0.15500067]
[-0.25780655,	-0.2577921]
[0.46940375,	0.46940565]
[-0.02950075,	-0.0294949]

249

250

251 TABLE 3 SHOWING RESULTS COMPUTED FROM METHOD 4.6 AND IMPROVED RESULTS WITH
252 RUMP/KRAWCZYK METHOD

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CORNER POINT SOLUTION WITH CROPPING	IMPROVED RESULTS WITH RUMP/ KRAWCZYK [
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FROM METHOD 4.6 FOR $\hat{\beta}$	METHOD [20] $\hat{\beta}$
[0.1553, 0.1553]	[0.1552891, 0.1553112]
[-0.2611, -0.2620]	[-0.2617332, -0.2614201]
[0.4772, 0.4803]	[0.4787567, 0.4790004]
[-0.0367, -0.0342]	[-0.0355532, -0.0353243]

254

255 We computed $\frac{\|\beta_c - \hat{\beta}\|}{\|\hat{\beta}\|}$ and obtained the loss function to be [6.8446, 6.8446] for the method [8].

256 The condition number for the solution without noise using equation 3.11 is 1.1684×10^4 .

257 The polynomial fit of order three used for [8] is given by

$$f(\beta) = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$$

258 $= [0.1549994, 0.15500067] + [-0.25780655, -0.2577921]X + [0.46940275, 0.46940565]X^2 +$
 $[-0.02950075, -0.0294949]X^3$

259 For arbitrary $X=0.12$ we have that $f(\hat{\beta}) = [0.1308, 0.1308]$ for method [8]. The same analogy
 260 goes for Kramer method [21] as given in equation 4.6. All results were computed using MATLAB
 261 Version 2007.

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263 6. CONCLUSION

264 The paper considered the roles of condition number in the studies of least squares interval
 265 equations using polynomial fit of order three. Possible areas of applications of least squares were
 266 highlighted. The backward perturbation errors in least squares problems were discussed. A
 267 diffeomorphism is made to relate the reachability for the computable set of resulting linear
 268 interval system from which, an ellipsoid may be applied. Here, in the paper the theorem due to
 269 [20] as exemplified by Popova in [8] was adopted to provide validated bounds to the linear
 270 interval system. The loss function was computed based on the results from Table 2. Theoretical
 271 approximation technique for cropping corner points solution in the sense of [21,22,23] was
 272 adopted in the paper to verify the obtained results. The Rump/Krawczyk method was used to
 273 refine the computed approximate solution from Kramer/Rohn method as showed in Table 3.
 274 Finally result computed for the data set when there is absence of noise in the described least
 275 squares problem was also discussed. Further insight is given on how to estimate $f(\hat{\beta})$ based on
 276 the given value of input data.

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