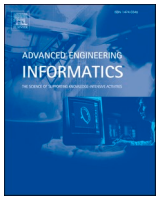
Advanced Engineering Informatics 77 (2027) 105422



Contents lists available at ScienceDirect

Advanced Engineering Informatics

journal homepage: www.elsevier.com/locate/aei



Short Communication

A novel and concise Shu's two–point method for fast least squares and regression analysis and its straightedge–and–compass construction

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ARTICLE INFO

Keywords:
Least squares
Best-fit line
Shu's two-point method
Geometric center
Mass center
Regression analysis
Statistics
Big data
Machine learning
Algorithm optimization
Straightedge-and-compass construction

ABSTRACT

The method of least squares is a core technique widely used in statistics and machine learning to determine the best-fit line through a set of observed data points. Traditional implementations rely on matrix inversion and decomposition; these methods are computationally intensive and inefficient for large-scale data environments. This paper presents a novel, computationally efficient, and easy-to-understand two-point method for fast least squares and regression analysis. This approach determines the best-fit line by joining the geometric center and the mass center of the data, eliminating the need to solve a large system of equations; the paper demonstrates that this method is an algebraically equivalent reconstruction of the method of least squares. Crucially, this approach requires only basic arithmetic operations (addition, subtraction, multiplication, and division), making it highly suitable for teaching basic statistics and machine learning in primary and secondary schools. This stands in stark contrast to the current schoolbook way of least squares and regression analysis based on classical Gaussian approach in statistics, as well as gradient descent in machine learning, all requiring university-level advanced calculus knowledge. Furthermore, this two-point method can be implemented using straightedge-and-compass construction and extended to manage measurement errors involving multiple independent and dependent variables. Its geometric intuitiveness and computational simplicity make it well-suited for big data applications in machine learning, such as knowledge-intensive engineering informatics applications.

1. Introduction

THE method of least squares is one of the oldest and most widely applied statistical techniques, remaining in common use today [1,2]. In 1801, Gauss employed this method to calculate the orbit of the newly discovered planet called Ceres [3,4]. The technique was formally established as a scientific method by Legendre in 1805 [5] and Gauss in 1809 [6], respectively. The method of least squares is one of the most prominent data fitting and classification algorithms; it is used to determine the best-fit line amongst scattered observed data points, assess the existence of correlations between observations, and identify trends within datasets. As a core computational tool, the method of least squares widely serves across numerous modern fields, including statistics [7], machine learning [8], data mining [9], data science [10], and data analysis [11].

The principle behind the method of least squares is straightforward. The least-squares best-fit line is defined as the straight line that lies closest to a set of given observed data points. This line is achieved by minimizing the summation of the squared deviations between the observed data points and the least-squares best-fit line. Suppose the relationship between two variables, x and y, is represented by a least-squares best-fit line of the form $y = ax + b$, where the unknown coefficients, a and b, represent the slope and the y−intercept of the line, respectively. In a two-dimensional space, given m observed data points, $M_1(x_1, y_1)$, $M_2(x_2, y_2)$,⋯, $M_m(x_m, y_m)$, where the ordinate of M_i is y_i, and $y(x_i)$ is the ordinate of a data point on the least-squares best-fit line, which is the same abscissa x_i as M_i, then the quadratic summation S of the differences between the ordinate of each observed data point and the ordinate of the expected straight line for the best least-squares fit can be expressed as:

$$S = \sum_{i=1}^{m} [y_i - y(x_i)]^2 = \sum_{i=1}^{m} (y_i - ax_i - b)^2$$

By minimizing this quadratic summation S, the conditions $\frac{\partial S}{\partial a} = 0$ and $\frac{\partial S}{\partial b} = 0$ are derived as:

$\sum_{i=1}^{m} (y_i - ax_i - b)x_i = 0$ and $\sum_{i=1}^{m} (y_i - ax_i - b) = 0$.

Solving these above two linear equations simultaneously yields the

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https://doi.org/10.1016/j.aei.2026.105422
Received 8 June 2026; Received in revised form 16 September 2026; Accepted 21 October 2026
Available online 25 October 2026
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classic analytical expressions: $a = \frac{m\sum_{i=1}^{m} x_i y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} y_i}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2}$ and $b = \frac{\sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i - \sum_{i=1}^{m} x_i \sum_{i=1}^{m} x_i y_i}{m\sum_{i=1}^{m} x_i^2 - \left(\sum_{i=1}^{m} x_i\right)^2}$; however, calculating the values of a and b using these formulas requires $2m$ multiplication operations during the summation phase (computing $\sum_{i=1}^{m} x_i y_i$ and $\sum_{i=1}^{m} x_i^2$ for each data point) and six multiplication operations in the post-summation phase (computing products of the accumulated summations). Traditional least-squares algorithms typically involve matrix inversion and decomposition; however, when dealing with high-density matrices or repetitive solutions, the computational overhead of these matrix inversion and decomposition is immense, resulting in high overall computational complexity. As the problem scale increases (due to factors such as a vast number of data points, data sparsity, streaming data transmission, and distributed data acquisition), the solution time of these algorithms depends not only on the number of floating-point operations but also on communication, memory data movement, and numerical stability under finite-precision arithmetic.

To overcome these limitations, this paper develops a novel two-point method technique to determine the least-squares best-fit line, $y = ax + b$, by identifying two geometrically significant points: the geometric center and the mass center of the data, instead of using the formulas described above. Consequently, in terms of execution time and memory footprint, this novel approach reduces the number of multiplication operations required for each data point during the summation process, thereby lowering the overall computational complexity of implementing least squares (a term from linear algebra) and regression analysis (a term from statistics), particularly when processing large numbers of observed data points. Crucially, the method relies solely on basic arithmetic operations (addition, subtraction, multiplication, and division), distinguishing it fundamentally from the classical Gaussian approach [6] in statistics and gradient descent [12] in machine learning, both of which require knowledge of calculus. Thus, this two-point method serves as an ideal introductory teaching tool for statistics and machine learning courses at the primary and secondary education levels, as it requires no mathematical knowledge beyond basic arithmetic.

Furthermore, this work is significant due to its applicability to knowledge-intensive engineering tasks. Regression analysis underpins various data-driven applications, such as predictive maintenance, structural health monitoring, sensor data fusion, and digital twin modeling. The geometric simplicity of the two-point method facilitates efficient deployment on embedded systems and edge computing platforms, while its intuitive geometric interpretation aids in the development of interpretable machine learning models for engineering applications. Consequently, this paper not only deepens theoretical understanding but also provides a practical tool for applications across diverse fields, including science, engineering, medicine, and social science.

2. Methods

2.1. Best-fit line passing through both the geometric center and the mass center

To avoid the cumbersome steps involved in the traditional implementation of the least squares, this paper develops a simple and easy-to-implement two-point method that utilizes both the geometric center and the mass center of all observed data points. The theorem below rigorously proves that the line joining these two points is the best-fit line in the least-squares sense.

Theorem: Given m observed data points in a two-dimensional space, $M_1(x_1, y_1)$, $M_2(x_2, y_2)$,⋯, $M_m(x_m, y_m)$, the least-squares best-fit line necessarily passes through the following two points:

Point 1 (geometric center): $\begin{cases} \overline{x} = \frac{\sum_{i=1}^{m} x_i}{m} \\ \overline{y} = \frac{\sum_{i=1}^{m} y_i}{m} \end{cases}$,

Point 2 (mass center): $\begin{cases} \overline{\overline{x}} = \frac{\sum_{i=1}^{m} x_i^2}{\sum_{i=1}^{m} x_i} \\ \overline{\overline{y}} = \frac{\sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} x_i} \end{cases}$.

Proof (step-by-step):

Step 1: Formulate the normal equations based on the minimization principle of the least squares. To minimize the objective function, $S = \sum_{i=1}^{m} [y_i - y(x_i)]^2 = \sum_{i=1}^{m} (y_i - ax_i - b)^2$, take partial derivatives with respect to a and b, respectively, and set them to zero, yielding two necessary conditions:

$$\frac{\partial S}{\partial a} = 0 : \sum_{i=1}^{m} (y_i - ax_i - b)x_i = 0, \tag{1}$$

$$\frac{\partial S}{\partial b} = 0 : \sum_{i=1}^{m} (y_i - ax_i - b) = 0 \tag{2}$$

Step 2: Verify that Point 1 (geometric center) lies on the best-fit line. Expand Eq. (2): $\sum_{i=1}^{m} y_i - a\sum_{i=1}^{m} x_i - mb = 0$. Divide both sides of the equation by m: $\frac{\sum_{i=1}^{m} y_i}{m} - a\frac{\sum_{i=1}^{m} x_i}{m} - b = 0$. Substitute $\overline{x} = \frac{\sum_{i=1}^{m} x_i}{m}$ and $\overline{y} = \frac{\sum_{i=1}^{m} y_i}{m}$: $\overline{y} = \frac{\sum_{i=1}^{m} y_i}{m} = a\frac{\sum_{i=1}^{m} x_i}{m} + b = a\overline{x} + b$. This confirms that the geometric center $(\overline{x}, \overline{y})$ lies on the best-fit line $y = ax + b$.

Step 3: Verify that Point 2 (mass center) lies on the best-fit line. Expand Eq. (1): $\sum_{i=1}^{m} x_i y_i - a\sum_{i=1}^{m} x_i^2 - b\sum_{i=1}^{m} x_i = 0$. Divide both sides by $\sum_{i=1}^{m} x_i$ (assuming $\sum_{i=1}^{m} x_i \neq 0$): $\frac{\sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} x_i} - a\frac{\sum_{i=1}^{m} x_i^2}{\sum_{i=1}^{m} x_i} - b = 0$. Substitute $\overline{\overline{x}} = \frac{\sum_{i=1}^{m} x_i^2}{\sum_{i=1}^{m} x_i}$ and $\overline{\overline{y}} = \frac{\sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} x_i}$: $\overline{\overline{y}} = \frac{\sum_{i=1}^{m} x_i y_i}{\sum_{i=1}^{m} x_i} = a\frac{\sum_{i=1}^{m} x_i^2}{\sum_{i=1}^{m} x_i} + b = a\overline{\overline{x}} + b$. This confirms that the mass center $(\overline{\overline{x}}, \overline{\overline{y}})$ lies on the best-fit line $y = ax + b$.

Step 4: Uniqueness of the line. Since both Point 1 and Point 2 lie on the unique best-fit line $y = ax + b$ (determined uniquely by the least-squares normal equations) and generally $\overline{x} \neq \overline{\overline{x}}$ (meaning they are distinct points), the line joining Point 1 and Point 2 coincides exactly with the least-squares best-fit line. ■.

Note: This two-point method is an algebraically equivalent formulation of the least-squares estimator. It provides a geometric characterization of the least-squares solution that is both computationally convenient and intuitively understandable.

In this theorem, the two-point form of the least-squares best-fit line

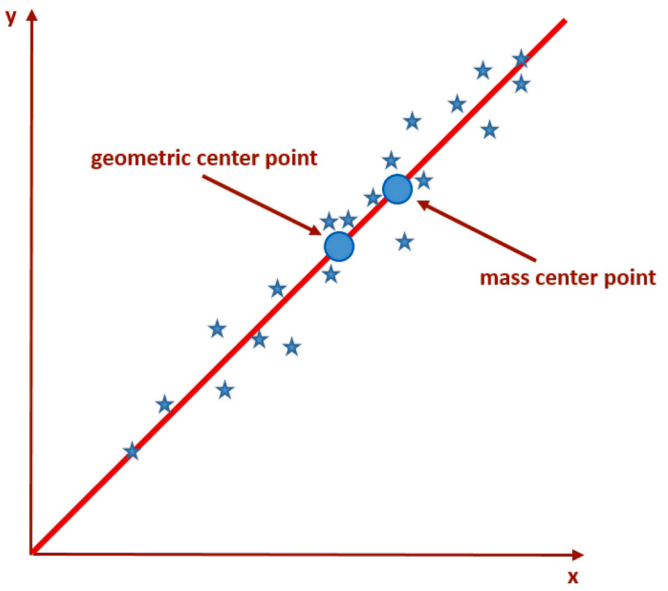

Fig. 1. The straight line passing through both the geometric center point and the mass center point is the least-squares best-fit line.

can be expressed as $\frac{y-\bar{y}}{x-\bar{x}} = \frac{\bar{\bar{y}}-\bar{y}}{\bar{\bar{x}}-\bar{x}}$, or equivalently as $\frac{y-\bar{\bar{y}}}{x-\bar{\bar{x}}} = \frac{\bar{\bar{y}}-\bar{y}}{\bar{\bar{x}}-\bar{x}}$ (as shown in Fig. 1). Using this simple and easy-to-implement two-point method to achieve the least squares makes finding the best-fit for experimental and observational data more convenient and simplifies the calculation process. This novel two-point technique, focusing on both the geometric center point and the mass center point, requires only $2m$ multiplication operations per data point to calculate the mass center during the summation process to determine the least-squares best-fit line: specifically, calculating x_i^2 (one multiplication operation per data point) and $x_i y_i$ (one multiplication operation per data point). In contrast, when calculating the slope a and intercept b using the classical closed-form formulas involves additional multiplication operations after the summation stage (specifically, multiplying the accumulated summations), thereby bringing the total number of multiplication operations involved in the full calculation to $2m + 6$. The two-point method, however, eliminates post-summation multiplication operations: the line is geometrically defined by joining two calculated points; determining the slope requires only a single division operation, with no additional multiplication operation needed. Consequently, the two-point method reduces the total number of multiplication operations in the overall calculation process.

This simple and intuitive two-point method facilitates the best-fit analysis of experimental and observational data, thereby streamlining the calculation workflow. Furthermore, as it requires solely basic arithmetic operations, the method is highly suitable for teaching primary and secondary school students, standing in stark contrast to the classical Gaussian approach [6] and gradient descent [12], both of which require knowledge of calculus.

2.2. Straightedge-and-compass construction

The approach of straightedge-and-compass construction is a geometric construction technique for drawing points, lines, and circles using only an unmarked straightedge and a compass. This novel and concise two-point method determines the best-fit line by joining the geometric center point and the mass center point of all observed data points; thus, the approach of straightedge-and-compass construction identifies these geometric center point and the mass center point by geometrically representing the data points as line segment lengths, performing addition operation by joining the end-to-end of line segments, and performing multiplication/division operations by constructing similar triangles based on the intercept theorem. The specific procedural steps are as follows:

Constructing a unit length: Define a line segment of arbitrary length on a straight line as "1″.

Representing data points: For each data point in the observed data, use a compass to mark off a line segment of the corresponding length.

Addition operation: Use the straightedge and compass to join the end-to-end of all line segments, resulting in a single line segment representing the total summation.

Multiplication/division operations: Apply the intercept theorem to construct similar triangles involving parallel lines; specifically, establish a proportional relationship to determine the new length (*i.e.*, the product or quotient).

This geometric construction method requires no complex algebraic knowledge, only an understanding of line segments and proportions, further highlighting the educational value of the two-point method in primary and secondary school instruction.

2.3. Regression analysis

This concept can be extended to various problems involving the least squares and regression analysis, including (A) uncertain variables [13] and (B) multidimensional spaces [14]. Traditional approaches to these problems require formulating the necessary conditions for minimization, which can be expressed as a system of equations involving partial derivatives. This process entails matrix inversion and decomposition, resulting in an overall computational complexity proportional to the cube of the total number of observed data points, that is, $O(m^3)$. In contrast, the newly developed, easy-to-implement two-point method resolves these issues simply by identifying only a few key points and performing basic arithmetic operations, thereby reducing the overall computational complexity to the square of the total number of observed data points, that is, $O(m^2)$. Consequently, the overall computational complexity is significantly reduced. The following formulas are presented as corollaries applicable to uncertain variables and multidimensional spaces.

(A) Uncertain variables

Corollary 1. Given m observed data points in a two-dimensional space, $M_1(x_1, y_1)$, $M_2(x_2, y_2)$,⋯, $M_m(x_m, y_m)$, the least-squares best-fit line passes through the following two points:

(a) *Point 1:* $\begin{cases} \bar{x} = \frac{\sum_{i=1}^m x_i}{m} \\ \bar{y} = \frac{\sum_{i=1}^m y_i}{m} \end{cases}$ *Point 2:* $\begin{cases} \bar{\bar{x}} = \frac{\sum_{i=1}^m x_i^2}{\sum_{i=1}^m x_i} \\ \bar{\bar{y}} = \frac{\sum_{i=1}^m x_i y_i}{\sum_{i=1}^m x_i} \end{cases}$ *for fixed* x_i *and uncertain* y_i*;*

(b) Point 1: $\begin{cases} \bar{x} = \frac{\sum_{i=1}^m x_i}{m} \\ \bar{y} = \frac{\sum_{i=1}^m y_i}{m} \end{cases}$ Point 2: $\begin{cases} \bar{\bar{x}} = \frac{\sum_{i=1}^m x_i y_i}{\sum_{i=1}^m y_i} \\ \bar{\bar{y}} = \frac{\sum_{i=1}^m y_i^2}{\sum_{i=1}^m y_i} \end{cases}$ for uncertain x_i and fixed y_i;

(c) Point 1: $\begin{cases} \bar{x} = \frac{\sum_{i=1}^m x_i}{m} \\ \bar{y} = \frac{\sum_{i=1}^m y_i}{m} \end{cases}$ Point 2: $\begin{cases} \bar{\bar{x}} = \frac{\sum_{i=1}^m x_i \sqrt{x_i^2 + y_i^2}}{\sum_{i=1}^m \sqrt{x_i^2 + y_i^2}} \\ \bar{\bar{y}} = \frac{\sum_{i=1}^m y_i \sqrt{x_i^2 + y_i^2}}{\sum_{i=1}^m \sqrt{x_i^2 + y_i^2}} \end{cases}$ for uncertain x_i and y_i.

3. (B) *Multidimensional spaces*

Corollary 2. Given m observed data points in an $N-$dimensional space, defined by a set of N orthogonal coordinates $\left\{\vec{e}_1, \vec{e}_2, \cdots, \vec{e}_N\right\}$, $M_1\left(\vec{x}_1, \vec{y}_1\right)$, $M_2\left(\vec{x}_2, \vec{y}_2\right)$,⋯, $M_m\left(\vec{x}_m, \vec{y}_m\right)$, the least-squares best-fit line passes through the following two points:

(a) *Point 1:* $\overline{M}\cdot\vec{e}_j = \frac{\sum_{i=1}^m M_i\cdot\vec{e}_j}{m}$ *Point 2:* $\overline{\overline{M}}\cdot\vec{e}_j = \frac{\sum_{i=1}^m \left(M_i\cdot\vec{e}_j\right)\left(\vec{x}_i\cdot\vec{e}_j\right)}{\sum_{i=1}^m \left(\vec{x}_i\cdot\vec{e}_j\right)}$ *for fixed* $\vec{x}_i$ *and uncertain* $\vec{y}_i$*;*

(b) Point 1: $\overline{M}\cdot\vec{e}_j = \frac{\sum_{i=1}^m M_i\cdot\vec{e}_j}{m}$ Point 2: $\overline{\overline{M}}\cdot\vec{e}_j = \frac{\sum_{i=1}^m \left(M_i\cdot\vec{e}_j\right)\left(\vec{y}_i\cdot\vec{e}_j\right)}{\sum_{i=1}^m \left(\vec{y}_i\cdot\vec{e}_j\right)}$ for uncertain $\vec{x}_i$ and fixed $\vec{y}_i$;

(c) Point 1: $\overline{M}\cdot\vec{e}_j = \frac{\sum_{i=1}^m M_i\cdot\vec{e}_j}{m}$ Point 2: $\overline{\overline{M}}\cdot\vec{e}_j = \frac{\sum_{i=1}^m \left(M_i\cdot\vec{e}_j\right)\sqrt{\|\vec{x}\|^2+\|\vec{y}\|^2}}{\sum_{i=1}^m \sqrt{\|\vec{x}\|^2+\|\vec{y}\|^2}}$ for uncertain $\vec{x}_i$ and $\vec{y}_i$,

where $\cdot$ and $\|\ \|$ denote the vector dot product and Euclidean norm, respectively.

4. Conclusion

This paper aims to improve one of the most important data fitting and classification techniques, least squares and regression analysis, by introducing a novel two-point method with intuitive geometric significance. Traditional algorithms for implementing least squares and regression analysis construct the necessary conditions for minimization, which can be written as a system of equations containing partial derivatives and solved by using matrix inversion and decomposition techniques. In cases where the matrix is highly concentrated and needs to be solved repeatedly, the computational overhead of matrix inversion and decomposition is immense, resulting in an overall computational complexity that is the cube of the total number, m, of observed data points, that is, $O(m^3)$. In contrast, the newly developed two-point method is far more streamlined; it focuses on a few key points and relies solely on basic arithmetic operations, thereby reducing the overall computational complexity to the square of the total number, m, of observed data points, that is, $O(m^2)$. Consequently, this novel approach significantly lowers the overall computational complexity and simplifies the cumbersome calculations inherent in the traditional way. In the current era of big data, where rapid and efficient processing is essential, this method enables the determination of the least-squares best-fit line simply by calculating the geometric center and the mass center of all observed data points.

This paper provides complete formal proof demonstrating that the geometric center and the mass center are, in fact, direct algebraic consequences of the two normal equations used in the least squares. Thus, the two-point method represents an algebraically equivalent reformulation of the least squares, offering a representation that is both geometrically intuitive and computationally transparent. The elegance of this novel method lies in its simplicity: it relies exclusively on the four basic arithmetic operations (addition, subtraction, multiplication, and division) without the need to solve a large system of equations, making it highly suitable as instructional material for statistics and machine learning at the primary and secondary school levels. This stands in stark contrast to the classical Gaussian approach [6] in statistics and gradient descent [12] in machine learning, both of which typically require knowledge of advanced calculus, topics usually taught only at the university level.

Notably, this novel concept can not only be realized through straightedge-and-compass construction but has also been extended to address a wide variety of regression analysis involving uncertain variables and multidimensional spaces [15–19]. This fundamental two-point method performs exceptionally well in simple linear regression scenarios.

From the perspective of knowledge-intensive engineering informatics, the two-point method offers significant practical value. In engineering domains such as structural health monitoring, predictive maintenance, manufacturing quality control, and sensor-based diagnostics, there is often a need to perform real-time analysis on massive streaming datasets under constraints of limited computational resources. The geometric simplicity of the two-point method allows for its direct integration into lightweight embedded systems, digital twin frameworks, and edge computing platforms, environments where matrix operations typically entail prohibitive computational overheads. Furthermore, the geometric intuitiveness of this construction method imparts strong interpretability to the regression model; this characteristic is particularly crucial for knowledge engineering and intelligent engineering design systems that rely heavily on model trustworthiness and physical interpretability. Future research could explore the method's application in "physics-informed machine learning" for engineering systems; in such scenarios, the algebraic simplicity of the two-point construction method can accelerate parameter estimation within data-driven digital twin models, thereby facilitating real-time engineering monitoring and decision-making.

CRediT authorship contribution statement

Jian-Jun Shu: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The author declares that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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