Inverse Sampling of Degenerate Datasets from a Linear Regression Line

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When linear regression generates a relationship between a (dependent) scalar response and one or multiple independent variables, various datasets providing distinct graphical trends can develop resembling relationships based on the same statistical properties. Advanced statistical approaches, such as neural networks and machine learning methods, are of great necessity to process, characterize, and analyze these degenerate datasets. On the other hand, the accurate creation of purposely degenerate datasets is essential to test new models in the research and education of applied statistics. In this light, the present study characterizes the famous Anscombe datasets and provides a general algorithm for creating multiple paired datasets of identical statistical properties.

I. INTRODUCTION

 Originally termed the least-squares fitting, the linear regression method is one of the most widely used analysis tools to primarily investigate trends among variables in various disciplines. Legendre and Gauss initially formulated the regression method from the late 18th to early 19th centuries to understand observed datasets of astronomical phenomena. The modern statistical characteristics of the regression were initially established by Galton’s work that described biological phenomena [1–3], followed by Yule [4]’s and Pearson [5]’s early mathematical formulation. When a linear relationship of a paired dataset provides two fitting coefficients, i.e., the intercept and the slope, the goodness of the regression is quantitatively correlated to the response variable $y$, the linear regression’s inherent problem resides in its statistical degeneracy, such that multiple datasets can have indistinguishable statistical properties.

 A quartet of visually distinct graphs, having identical regression statistics, were investigated by Anscombe [6], who emphasized the equal significances of graphical visualization and quantitative statistics [7,8]. The noticeable heterogeneity of his work’s graph patterns conversely emphasizes the significance of the data degeneracy [9]. Nevertheless, his data generation method was only partially studied [10], and to the best of our knowledge, the full mechanism is still unknown [10,11], even if each dataset has only 11 pairs.

 In principle, simple linear regression between two variables can be easily extended to multiple and non-linear regressions, which include several variables and their power-wise products, respectively. Regardless of the regression type, a regression method uses a single matrix to relate the input(s) and output(s), and the matrix elements consist of, in general, various products of input variables. To investigate relationships between highly correlated data, multiple matrices can be inserted between the input and output layers, and their elements can be calculated using various non-linear functions [12]. Neural networks and machine learning [13–15] are some advanced methods within a category of data exploration [16].

 Once a relationship is made, as either an empirical equation or a matrix form, the range of input variables often limits the applicability of the regression, leaving infinite degrees of degeneracy. There can possibly be many combinations of input variables that provide the same output results. For both preliminary tests of any new, advanced regression algorithm, it is necessary to have a data generator that can create manyfold datasets, satisfying the same statistical constraints. In this light, this work revisits linear regression fundamentals, analyzes Anscombe’s quartet data, and provides a possible algorithm to inversely create degenerate datasets of distinct values with predetermined statistical parameters [17].

II. LINEAR REGRESSION THEORY

 We consider a linear model, such as

$$y = \beta_0 + \beta_1 x + \epsilon$$  \hspace{1cm} (1)

where $x = \{x_1, x_2, \ldots, x_N\}$ and $y = \{y_1, y_2, \ldots, y_N\}$ are vectors of $N$ (observed) elements for the independent and response (dependent) variables, respectively; $\epsilon$ is a vector of randomly distributed errors of zero mean and finite variance, and $\beta_0$ and $\beta_1$ are regression or fitting parameters, so called the $y$-intercept and slope, respectively. Here, we define the regression function, such as

$$Y = \beta_0 + \beta_1 x$$  \hspace{1cm} (2)

that most closely fits the paired data of $(x, y)$ of size $N$. Here, statistically meaningful properties include the mean and variance of $x$, i.e., $\bar{x} = \text{mean}(x)$ and $\sigma_x^2 = \text{var}(x)$, respectively; those of $y$, i.e., $\bar{y} = \text{mean}(y)$ and $\sigma_y^2 = \text{var}(y)$, respectively; and the parameter $\beta_1$ for the $N$ paired points. The goodness of the regression is
estimated using the coefficient of determination, denoted as $R^2$, defined as

$$R^2 = \frac{\sum_k (Y_k - \bar{y})^2}{\sum_k (y_k - \bar{y})^2} = \beta_1^2 \frac{S_{xx}}{S_{yy}} = \beta_1 \frac{\sigma_x^2}{\sigma_y^2}$$

(3)

and

$$\beta_1 = \frac{S_{xy}}{S_{xx}} = \frac{\sigma_{xy}}{\sigma_x^2}$$

(4)

where $\sigma_{xy}$ is a covariance between $x$ and $y$; $S_{xx}$ and $S_{yy}$ are sums of squares of residuals, i.e., $\sum_k (x_k - \bar{x})^2$ and $\sum_k (y_k - \bar{y})^2$, respectively; and $S_{xy}$ is a sum of residual products, i.e., $\sum_k (x_k - \bar{x})(y_k - \bar{y})$. The magnitude and the sign of $\beta_1$ are given as those of $R \sigma_y / \sigma_x$ and $S_{xy}$, respectively. Given a paired dataset, the linear regression process indicates the calculation of $\beta_1$ and $\beta_0$ values that minimize the error $\epsilon$, and is often straightforward, using various spreadsheet programs or numerical/statistical packages, such as Microsoft Excel, Google Sheets, MATLAB/Octave, python, and R-language. In applied statistics disciplines, it is also important to generate manyfold datasets that accurately satisfy the predetermined statistical properties for various testing and training purposes.

Revisit to Anscombe’s Quartet

Anscombe’s original quartet, i.e., datasets I–IV, listed in Table III is visualized in Fig. I representing graphically distinct patterns of $y$’s with respect to $x$. A brief analysis of the quartet is as follows. Fig. I(a) shows an apparently linear trend of dataset I, typical in studies of various disciplines. Fig. I(b) (of circular symbols) shows a parabolic, concave-down trend of $y$, having its peak at $(x, y) = (11, 9.26)$. Most points in dataset I and II are closely located near the linear trend line. On the other hand, Fig. I(c) has a noticeable outlier above a linear line that passes through the vicinity of the rest of the 10 points. Fig. I(d) has a bimodal distribution of the 11 data points, i.e., a group of 10 points at one $x$-coordinate and one outlier away from the group. Interestingly, the four datasets of the distinct patterns contain identical statistical properties, summarized in Table III. In each dataset, the sample size is equally $N = 11$; the mean and variance of $x$ are $\bar{x} = 9.0$ and $\sigma_x^2 = 11.00$, respectively; and those of $y$ are $\bar{y} = 7.5$ and $\sigma_y^2 = 4.125$, respectively. (In Anscombe’s original work, sums of $(x_k - \bar{x})^2$ and $(y_k - \bar{y})^2$ are reported, instead of variances, as 111.0 and 41.25, respectively.) The regression statistics provide the same values of $\beta_1 = 0.5$, $\beta_0 = 3.0$, and $R^2 = 0.667$, with acceptable errors. To the best of our knowledge, how Anscombe generated the data quartet has not been well explained in the literature. Because our goal is to create multiple degenerate datasets of the same statistical properties, we here investigate the characteristics of Anscombe’s quartet data in detail.

For a better understanding, we first sorted the datasets in Table III in an ascending order of $x$ and made Table III. Note that the sequences of data pairs do not change the statistical results of the linear regression. For example, even if the first two points of dataset I in Table III, i.e., $(x_1, y_1) = (10.0, 8.04)$ and $(x_2, y_2) = (8.0, 6.95)$, are exchanged to $(x_1, y_1) = (8.0, 6.95)$ and $(x_2, y_2) = (10.0, 8.04)$, the regression statistics of $\beta_0$, $\beta_1$, and $R^2$ values remain invariant. In Table III it is noticed that datasets I–III have an evenly distributed $x$ from 4 to 14 with a fixed interval of 1, and the outliers ($y > 10$) of datasets III and IV are located near the end of the regression line in $x$. Now, we explain how the $x$ and $y$ vectors were possibly generated, keeping the statistical constraints discussed above.

Constraints Applied

The 11 components of $x$ in dataset I–III can be represented as $x_k = x_{k-1} + 1$ for $k = 1, 2, \cdots, N$ with $x_0 = 3$, so that the $k^{th}$ component is described as $x_k = 3 + k$,
Table I. Anscombe’s original quartet datasets.

| Index | I  | II | III | IV  |
|-------|----|----|-----|-----|
| 1     | 10.0 | 8.04 | 9.14 | 7.46 | 8.0 | 6.58 |
| 2     | 8.0 | 6.95 | 8.14 | 6.77 | 8.0 | 5.76 |
| 3     | 13.0 | 7.58 | 8.74 | 12.74 | 8.0 | 7.71 |
| 4     | 9.0 | 8.81 | 8.77 | 7.11 | 8.0 | 8.84 |
| 5     | 11.0 | 8.33 | 9.26 | 7.81 | 8.0 | 8.47 |
| 6     | 14.0 | 9.96 | 8.10 | 8.84 | 8.0 | 7.04 |
| 7     | 6.0 | 7.24 | 6.13 | 6.08 | 8.0 | 5.25 |
| 8     | 4.0 | 4.26 | 3.10 | 5.39 | 19.0 | 12.50 |
| 9     | 12.0 | 10.84 | 9.13 | 8.15 | 8.0 | 5.56 |
| 10    | 7.0 | 4.82 | 7.26 | 6.42 | 8.0 | 7.91 |
| 11    | 5.0 | 5.68 | 4.74 | 5.73 | 8.0 | 6.89 |

Table II. Statistical properties of Anscombe’s quartet data in Table I.

| Index | Property          | Value |
|-------|-------------------|-------|
| 1     | The sample size   | N = 11 |
| 2     | The mean of x     | \( \bar{x} = 9.0 \) |
| 3     | The variance of x | \( \sigma_x^2 = 11.00 \) |
| 4     | The mean of y     | \( \bar{y} = 7.5 \) |
| 5     | The variance of y | \( \sigma_y^2 = 4.125 \) |
| 6     | The slope         | \( \beta_1 = 0.5 \) |
| 7     | The y-intercept   | \( \beta_0 = 3.0 \) |
| 8     | The coefficient of determination \( R^2 \) | 0.667 |

and the mean of \( \bar{x} \) is calculated as

\[
\bar{x} = 3 + \frac{1}{2} (N + 1) \tag{5}
\]

that provides \( \bar{x} = 9 \) for \( N = 11 \). Now, one can use a more flexible relationship between \( x_k \) and \( x_{k+1} \) by having an arbitrary interval \( a \), such as

\[
x_k = x_{k-1} + a \quad \text{for} \quad k = 1, 2, \ldots, N \tag{6}
\]

Table III. Anscombe’s quartet data sorted by \( x \) (for datasets I–III), followed by \( y \) (for dataset IV).

| Index | I  | II | III | IV  |
|-------|----|----|-----|-----|
| 1     | 1.0 | 4.95 | 3.10 | 5.39 | 8.0 | 5.25 |
| 2     | 5.0 | 5.68 | 1.74 | 5.73 | 8.0 | 5.56 |
| 3     | 6.0 | 7.24 | 6.13 | 6.08 | 8.0 | 5.76 |
| 4     | 7.0 | 4.82 | 7.26 | 6.42 | 8.0 | 6.58 |
| 5     | 8.0 | 6.95 | 8.14 | 6.77 | 8.0 | 6.89 |
| 6     | 9.0 | 8.81 | 8.77 | 7.11 | 8.0 | 7.04 |
| 7     | 10.0 | 9.96 | 9.14 | 8.46 | 8.0 | 7.71 |
| 8     | 11.0 | 8.33 | 9.26 | 7.81 | 8.0 | 7.91 |
| 9     | 12.0 | 10.84 | 9.13 | 8.15 | 8.0 | 8.47 |
| 10    | 13.0 | 7.58 | 8.74 | 12.74 | 8.0 | 8.84 |
| 11    | 14.0 | 9.96 | 8.10 | 8.84 | 19.0 | 12.50 |

Table IV. Data of three points satisfying Anscombe’s statistical restriction. Note that \( \delta x_k = -\delta x_1 \) and \( \delta y_k^{(1)} = -\delta y_1^{(1)} \) for \( k = 1 \) to 3.

| \( k \) | \( x_k \) | \( y_k^{(1)} \) | \( y_k^{(2)} \) |
|--------|----------|----------|----------|
| 1      | 5.6834   | 6.5187   | 5.1647   |
| 2      | 9.0000   | 6.1460   | 8.8540   |
| 3      | 12.3166  | 9.8353   | 8.4813   |

and then the two parameters of \( a \) and \( x_0 \) can be determined by preset constraints of \( \bar{x} \) and \( \sigma_x^2 \), such as

\[
a = \sigma_x \sqrt{\frac{6}{N m}} \tag{7}
\]

\[
x_0 = \bar{x} - am \tag{8}
\]

where \( m = \frac{1}{2} (N + 1) \) is an mid-point index. Here, we restrict ourselves to odd \( N \) cases for simplicity. Substitution of \( N = 11, \sigma_x = \sqrt{11} \) (obtained from \( S_{xx} = 110 \)), and \( \bar{x} = 9 \) into Eqs. (7) and (8) results in \( a = 1 \) and \( x_0 = 3 \), as shown in Table III. On the other hand, dataset IV has a special set of \( x_k \), containing only two values, denoted as \( x_a (= x_1 = \cdots = x_{N-1}) \) and \( x_b (= x_N) \). Because the sequential indices of \( x_a \) do not influence any statistical analysis, the mean of \( x \) is written as

\[
\bar{x} = \frac{(N - 1) x_a + x_b}{N} \tag{9}
\]

and further

\[
(N - 1) \delta x_a + \delta x_b = 0 \tag{10}
\]

where \( \delta x_j = x_j - \bar{x} \) for \( j = a, b \). Anscombe used the fixed value of \( S_{xx} \), which is represented below, using \( \delta x_a \) and \( \delta x_b \), as

\[
S_{xx} = (N - 1) \delta x_a^2 + \delta x_b^2 = (N - 1) N \delta x_b^2 \tag{11}
\]

using Eq. (10). Finally, we obtain (for \( N = 11 \))

\[
(x_a, x_b) = (9 \pm 1, 9 \mp 10) = (-1, 10) \text{ or } (8, 19) \tag{12}
\]

where the latter case of \( (x_a, x_b) = (8, 19) \) was chosen in Anscombe’s original work [6].

When a paired dataset \( \{(x_k, y_k)\}_{k=1}^N \) is fitted on a straight line, the goodness of the linear regression is often estimated using the coefficient of determination \( R^2 \) of Eq. (3). Alternatively, the slope coefficient \( \beta_1 \) can be set as the last constraint, in addition to \( \bar{y} \) and \( \sigma_y^2 \), requiring the minimum sample size of \( N = 3 \) to fully implement the six statistical constrains. In the next section, we discuss how to generate the three \( x - y \) data points that hold the six statistical constrains.

A minimum data set of three components

Let’s consider three consecutive values of \( x \), with the predetermined constraints of \( \bar{x} = 9 \) and \( \sigma_x^2 = 11 \), to have

\[
x_k = x_0 + a \cdot k \quad \text{for} \quad k = -1, 0, 1 \tag{13}
\]
where \( x_0 = \bar{x} = 9 \), \( a = \sqrt{11} = 3.3166 \), so that \( \delta x_1 = -3.3166 = -\delta x_3 \) and \( \delta x_2 = 0 \). The following equations are obtained for \( y \) of three components, such as
\[
\delta y_1 + \delta y_2 + \delta y_3 = 0
\]
\[
\delta y_1^2 + \delta y_2^2 + \delta y_3^2 = 2\sigma_y^2
\]
\[
\delta x_1 \cdot (\delta y_1 - \delta y_3) = 2\beta_1 \sigma_y^2
\]
using \( \delta x_2 = 0 \) and \( \delta x_3 = -\delta x_1 \). Analytic solutions of \( \delta y_k \) for \( k = 1 \) to \( 3 \) are obtained as
\[
\delta y_2 = \pm \frac{2}{\sqrt{3}} \sqrt{\sigma_y^2 - B_1^2}
\]
\[
\delta y_1 = -\frac{1}{\sqrt{3}} \delta y_2 - B_1
\]
\[
\delta y_3 = -\frac{1}{\sqrt{3}} \delta y_2 + B_1
\]
where \( B_1 = \beta_1 \sigma_y^2 / \delta x_3 = \sqrt{\frac{3}{2}} \).

Table IV shows two sets of solutions, denoted as \( y_k^{(1)} \) and \( y_k^{(2)} \), while both satisfy all of the constraints indicated above. This degeneracy is due to the squared feature of the variance of Eq. (15). Fig. 2 shows the two sets of \( y \) versus \( x \) with \( N = 3 \), following the same Anscombe’s constraints, except for the sample size. Even with this smallest number of the sample size for a linear regression, two possible cases of degenerate \( y \)’s co-exist, having the identical statistical properties. A trivial case is that if \( \sigma_y^2 = B_1^2 \), then \( \delta y_2 = 0 \) and \( \delta y_1 = -\delta y_3 = -\beta_1 \delta x_3 \), so that \( y_k^{(1)} \) and \( y_k^{(2)} \) become identical, and so will be located on the regression line.

**Generation of degenerate datasets with constraints**

**Satisfying three constraints using three arbitrary points**

After the \( x \) vector of a size of \( N \) is determined with constraints of \( \bar{x} \) and \( \sigma_x^2 \), other three constraints should be satisfied by \( y \) vector, which include finite \( \bar{y} \) and \( \sigma_y^2 \), alternately represented as
\[
\sum_{k=1}^{N} \delta y_k = 0
\]
and
\[
\sum_{k=1}^{N} \delta^2 y_k = S_{yy} = (N - 1) \sigma_y^2
\]
respectively; and finally, \( \beta_1 \) defined as a ratio of a covariance between \( x \) and \( y \) to a variance of \( x \), i.e., \( \sigma_{xy}/\sigma_x^2 \), such as
\[
\sum_{k=1}^{N} \delta x_k \cdot \delta y_k = (N - 1) \sigma_{xy} = (N - 1) \sigma_x^2 \beta_1
\]
Because the \( x \) vector is generated independently, all the constraints for an arbitrary \( N \) are satisfied by the creation of the \( y \) vector, having a degree of freedom of \( N - 3 \). In our approach, we generate an initial \( y \) vector (as a function of the \( x \) vector), having a specific pattern near the preset regression line of Eq. (2). Then we select the minimum, maximum, and mid-point of the \( x \) vector and adjust the three values of the corresponding \( y \)-components to satisfy the constraints of Eqs. (20)–(22). Assume that we already have a sorted \( x \) vector, i.e., \( x_{k-1} < x_k \) for \( k = 1 - N \), and have decided \( y_k \), except \( k = 1 \), \( m \), and \( N \), where \( m \) is theoretically any index between 1 and \( N \), i.e., \( 2 \leq m \leq N - 1 \). For simplicity, an index of the mid-point can be used, such as
\[
m = \frac{N + \text{mod}(N, 2)}{2} = \begin{cases} \frac{N}{2} (N + 1) & \text{if } N \text{ is even} \\ \frac{N}{2} (N + 1) & \text{if } N \text{ is odd} \end{cases}
\]
where \( \text{mod}(N, 2) \) is a remainder when \( N \) is divided by 2, or simply
\[
m = \text{floor} \left[ \frac{1}{2} (N + 1) \right]
\]
which is to round off \( \frac{1}{2} (N + 1) \), especially for odd \( N \). The above three equations can be rewritten as
\[
\delta y_1 + \delta y_N = -\sum_k' \delta y_k
\]
\[
\delta y_1^2 + \delta y_N^2 = -\sum_k' \delta y_k^2 + S_{yy}
\]
\[
\delta x_1 \delta y_1 + \delta x_N \delta y_N = -\sum_k' \delta x_k \delta y_k + S_{xx} \beta_1
\]
where \( \sum_k' = \sum_{k=2}^{N-1} \) is defined as a summation over \( k \), except the first and last indices. Combining Eqs. (25) and (27), we represent \( \delta y_1 \) and \( \delta y_N \) as linear functions of \( \delta y_m \), such as
\[
\delta y_1 = a_1 + b_1 \delta y_m
\]
\[
\delta y_N = a_N + b_N \delta y_m
\]
where

\[ a_1 = \frac{\beta_1 (N - 1) \sigma_y^2 + \sum_{k, k \neq m} (\delta x_n - \delta x_k) \cdot \delta y_k}{\delta x_1 - \delta x_N} \]  

\[ a_N = a_1 \]  

\[ b_1 = \frac{\delta x_N - \delta x_m}{\delta x_1 - \delta x_N} \]  

\[ b_N = \frac{\delta x_1 - \delta x_m}{\delta x_N - \delta x_1} \]  

and substitute Eqs. (28) and (29) into (26) to derive for \( \delta y_m \), such as

\[ \delta y_m = -B \pm \sqrt{s_{yy}^' + B^2 - C^2} \]  

where

\[ s_{yy}^' = \left[ (N - 1) \sigma_y^2 - \sum_k \delta^2 y_k \right] / \left( 1 + b_N^2 + b_N^2 \right) \]  

\[ B = \left( a_1 b_1 + a_N b_N \right) / \left( 1 + b_1^2 + b_N^2 \right) \]  

\[ C^2 = \left( a_1^2 + a_N^2 \right) / \left( 1 + b_1^2 + b_N^2 \right) \]  

In this case, two sets of \( \{ \delta y_1, \delta y_m, \delta y_N \} \), and hence \( \{ y_1, y_m, y_N \} \), are generated, depending on the sign of the square-root term in Eq. (34). Furthermore, there are no mandatory conditions that the first and last points should be included to meet the constraints. Instead, three arbitrary points within a dataset \( \{ x_k, y_k \}_{k=1}^N \), e.g., \( k = p_1, p_2, \) and \( p_3 \), can be selected as long as they are different, i.e., \( p_1 \neq p_2 \neq p_3 \). Nevertheless, if the x-positions of the three points are closely located, then large differences between their y-values are expected.

**Selection of a shape function**

In previous sections, we discussed how to determine the components of the y vector, especially three points, assuming that the rest \( N - 3 \) points are already properly located near the given regression line of Eq. (2). The predetermination of \( N - 3 \) points is to have the equal numbers of constraints (3) and unknown points (3). Because \( N - 3 \) is also the degree of freedom of the pre-positioned y values, the number of patterns that the \( N - 3 \) elements of y can make is theoretically infinite. In addition, having \( \sigma_y^2 \) as one of the constraints doubles the degeneracy of the created dataset. Here, we consider a function that determines the initial distribution of N points, among which \( y_1, y_m, \) and \( y_N \) are updated to meet the three statistical constraints (\( \tilde{y}, \sigma_y^2, \) and \( \beta_1 \)). We name this function as a shape function and discuss how shape functions are used in Anscombe’s datasets in the following.

**Random distribution** In Fig. [1(a)] for dataset I, five points (of index 2, 5, 7, 8, and 11 in Table [II]) are located very close to the regression line of Y: among the rest, half of them are above the regression line, and the other half are below it. The subset consisting of the closest five pairs \( (x_j, y_j) \) of \( j = 2, 5, 7, 8, \) and 11 has a regression line of \( 3.235 + 0.4746x \) with \( R^2 = 0.9950 \). In this case, the shape function of dataset I is a linear line, similar to the predetermined regression line plus random biases, such as

\[ f_I (x_k) = \tilde{Y} (x_k) + \eta_k (0, s) \]  

where \( \tilde{Y} \sim Y \) and \( \eta \) is a random vector, having normally distributed random components with zero mean and a finite variance, denoted as \( s^2 \). For dataset I, \( \eta \) should consist of 11 components, selected from a population of normally distributed random numbers, with a mean of \( \mu \sim 0 \) and standard deviation of \( s \sim \sqrt{1.376} \).

**Quadratic function** In Fig. [1(b)], the parabolic pattern of dataset II is best fitted using a quadratic shape function

\[ f_{II} (x) = q (x) = q_0 + \alpha (x - x^*)^2 \]  

and plotted using star symbols. In this case, the three constants of \( q_0, \alpha, \) and \( x^* \) should be simultaneously determined to satisfy the three constraints. Eqs. (20), (21), and (22) are satisfied as follows:

\[ \alpha = \frac{\beta_1 (N - 1) \sigma_y^2}{\sum_{k=1}^N (x_k - x^*)^3} \]  

\[ q_0 = \tilde{y} - \frac{\alpha}{N} \sum_{k=1}^N (x_k - x^*)^2 \]  

\[ \sigma_y^2 = \frac{\alpha^2}{N - 1} \sum_{k=1}^N (x_k - x^*)^4 - \frac{N (\tilde{y} - q_0)^2}{N - 1} \equiv \sigma_y'^2 \]  

indicating that \( \alpha = \alpha (x^*), \) \( q_0 = q_0 (\alpha, x^*), \) and \( \sigma_y'^2 \) as a function of \( \alpha, q_0, \) and \( x^* \) with the predetermined constraint \( \sigma_y^2 \). Therefore, \( x^* \) can be obtained by plotting

\[ \Delta \sigma^2 = \sigma_y'^2 - \sigma_y^2 \]  

with respect to \( x^* \) and graphically finding \( x^* \) of \( \Delta \sigma^2 = 0 \), as shown in Fig. [3]. Here, \( \alpha = -0.1267 \) and \( q_0 = 9.2616 \) are calculated using Eqs. (41) and (42), respectively, using visually found \( x^* = 10.972 \). Similarly, for \( x^* = 7.027 \), we obtained \( \alpha = 0.1267 \) and \( q_0 = 5.7405 \). These two parameter sets of \( \alpha, q_0, \) and \( x^* \) are used to plot \( f_{II} \) and \( f_{III}, \) shown in Fig. [1(b)].

In Fig. [1(c)], a subset of 10 points, excluding the outlier of \( (x_{10}, y_{10}) = (13, 12.74) \), are aligned on a straight line, of which the regression line is calculated as

\[ f = \beta_0' + \beta_1' x \rightarrow f_{III} \]
where $\beta_0' = 4.01, \beta_1' = 0.3454$, and $R^2 = 0.999$, which can be considered as a shape function of dataset III. Compared to the given regression line of Eq. (2), $f_{III}$ has a higher intercept and a gentler slope, as compared to those of Eq. (2), as well as $Y$ of dataset I. A condition can be suggested, such as $(\beta_0' - \beta_0)(\beta_1' - \beta_1) < 0$, so that if the slope $\beta_1'$ is stiffer than $\beta_1$, i.e., $(\beta_1' - \beta_1) > 0$; then the intercept $\beta_0'$ is located below $\beta_0$, and vice versa. After locating $N$ points on or near the linear shape function of Eq. (45), one arbitrary point, such as $(x_p, y_p)$ for $p = 10$ in dataset III, can be made as an outlier by changing the $y_p$ value. In theory, relocating an outlier position cannot fully satisfy the three constraints. Instead, this outlier can be included as one of the three points used for the degenerate dataset’s creation by replacing the mid-point, i.e., $\{\delta y_1, \delta y_m, \delta y_N\} \rightarrow \{\delta y_1, \delta y_p, \delta y_N\}$. Furthermore, the first and last points can also be replaced by any two distinct points, if needed.

In Fig. 3(d) of dataset IV, a group of ten points is located at a same x-positions, i.e., $x_1 = \cdots = x_{10} = 8$. These ten points have a mean of 7.0 and a variance of 1.527, which increased to the preset values of $\bar{x} = 7.5$ and $\sigma^2_x = 4.125$, respectively, by including the outlier of $(x_{11}, y_{11}) = (19, 12.5)$ that already satisfies $y_{11} = 3 + 0.5x_{11}$. At $x = 8$, $\{y_{11}\}_{k=1}^{10}$ can be modeled as normally distributed random numbers of zero mean and finite variance $s$, such as $\eta(0, s)$, similar to Eq. (28), such as

$$f_{IV}(x_k) = \begin{cases} Y(x_k) + \eta_k(0, s) & \text{if } k \neq 11 \\ 3 + 0.5x_{11} & \text{if } k = 11 \end{cases} \quad (46)$$

Because the last point $(x_{11}, y_{11})$ is fixed, any three points at $x = 8$ should be (randomly) selected and updated to meet the given constraints.

**General algorithm**

If a paired dataset shows a monotonous variation of $y$ with respect to $x$, or vice versa, then the above-mentioned algorithms can be generalized and used to create degenerate datasets of the same constraints, as follows

1. determine six statistical parameters: $N$, $\bar{y}$, $\sigma^2_x$, $\sigma_y$, $\sigma^2_y$, and $\beta_1$ and calculate $\beta_0 = \bar{y} - \beta_1 \bar{x}$;
2. make an $x$ vector of $N$ components, having predetermined $\bar{y}$ and $\sigma^2_y$;
3. use a shape function to initialize $y$-components near the given regression line, $Y(x)$, of Eq. (2);
4. update the $y$-values of any three points, as needed, using Eqs. (28), (29), and (34) to satisfy the three constraints of $\bar{y}$, $\sigma_y$, and $\beta_1$;
5. confirm that the generated dataset is characterized by the six parameters listed above.

In general, when $n_C (\geq 3)$ constraints are implemented, $N_n - n_C$ points are determined using a shape function, and the rest of the $n_C$ points can be determined by analytically solving the constraint equations. The availability of analytic solutions will be limited as the number of constraints increases. In this case, the problem can be described as a linear regression with constraint functions of

$$g_{\alpha} \left( y^1_1, \ldots, y^1_\beta, \ldots, y^1_{n_C} \right) = 0 \quad \text{for} \quad \alpha, \beta = 1 - n_C \quad (47)$$

where $y^1_\beta$ is one of $n_C$ components of $y$, chosen to satisfy $n_C$ constraints. A general root-finding algorithm can be used to numerically find $y^1_\beta$.

**III. RESULTS AND DISCUSSIONS**

**Inverse Sampling of Degenerate Datasets**

The creation of one of degenerate paired datasets requires six constraints, such as $N$, $\bar{x}$, $\sigma^2_x$, $\bar{y}$, $\sigma^2_y$, and $\beta_1$. For a given sample size $N$, the mean and standard deviation of $x$ and $y$ determine their central locations and spread degrees. If more than three constraints are considered, the degrees of degeneracy are theoretically infinite, and therefore, one can create as many as degenerate datasets as needed, disregarding their graphical similarities or dissimilarities. If a trend line is made by a linear regression of multiple datasets of the same size, then it is highly probable that the degenerate datasets created from the calculated trend line do not include the original datasets used for the linear regression, but instead can include unexpected forms of meaningful datasets.

In statistical physics, the importance sampling technique is frequently used for efficient Monte Carlo simulations [18, 19], which indicates sampling from only specific
distributions that over-weigh the important region. In a microcanonical ensemble of a thermodynamic system, sampling of particles’ positions and velocities are under a constant total energy \[20\]. Once particle positions are determined, a specific value of kinetic energy \( K \) is calculated as the total energy subtracted by the position-dependent potential energy, such as \( K = \frac{1}{2} \sum m_i v_i^2 \), and particle velocities are randomly assigned and carefully adjusted to maintain the kinetic energy. There are many distinct configurations of velocities in the phase space that give the same kinetic energy value. This specific sampling is called inverse sampling, which is analogous to the present work that inversely calculates and samples datasets of specific statistical constraints.

Paired datasets generated using shape functions

In this section, we create a few paired datasets having the same statistical properties of Anscombe’s quartet. A test shape function we employed is a fourth-order polynomial with respect to \( x \), such as

\[ f(x) = Y(x) + f_0(x-h_1)(x-h_2)(x-h_3)(x-h_4) \]  

(48)

where \( h_1 = 4.150, h_2 = 7.480, h_3 = 10.710, \) and \( h_4 = 13.850 \) are chosen slightly away from the (integer) \( x_k \) value; and \( f_0 \) is a weight factor of the shape function, which is either 0 or \( \pm \sqrt{2} \times 10^{-2} \). The non-zero magnitude of \( f_0 \) is selected by trial and error. If \( f_0 = 0.0 \), then the predetermined regression line \( Y(x) \) becomes the shape function.

Further Considerations

While \( x \) is predetermined independently, the three effective constraints provide the same number of closure equations, reducing the degrees of freedom of \( y \) from \( N \) to \( N-3 \). It is worth noting that the degeneracy is originated not only by the number of elements, but also from the squared form of \( n \). Not determined not only by the number of elements, but also from the equations, reducing the degrees of freedom of \( n \). Effective constraints provide the same number of closure terms. While there are in principle an infinite number of available shape functions and multiple ways to locate data points near the shape functions, identifying data patterns seems to be challenging work, even if the trend seems to follow a noticeable shape. Nevertheless, this work provides in-depth analysis of Anscombe’s original work in terms of data creation and a straightforward algorithm to reproduce his work, as well as to perform the inverse sampling of regressive datasets.

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datasets to visually compare. However, if the created datasets are tested for various indices, they can easily be classified into several groups of similarities \[29\].

Table \[V\] shows the third and fourth moments of the \( z \)-scores of \( x \) and \( y \), denoted as \( z_x = (z - \bar{z}) / \sigma_x \) and \( z_y = (y - \bar{y}) / \sigma_y \), respectively. The \( n \)th moment of \( z \) is defined as a mean value of \( z^n \), i.e., \( \langle z^n \rangle \), and the third and fourth moments are called standard skewness and kurtosis, respectively. Because the \( x \)’s of datasets I–III are equally evenly distributed, their mean, variance, skewness, and kurtosis are identical, which is not observed in dataset IV. The \( y \)-skewness of dataset I and II have negative values, indicating that more \( y \)-values are located below \( \bar{y} \). The larger magnitude of \( \langle z^3 \rangle_{y} = -0.97882 \) than \( \langle z^3 \rangle_{y} = -0.04837 \) indicates the quadratic shape function of dataset II locates more data points lower than the regression line than that of dataset I. The two largest \( y \)-skewnesses of dataset III and IV are ascribed to their outliers. The \( x \)-kurtosis values of the four datasets show a similar trend to those of skewnesses, and the \( y \)-Kurtosis values increase from dataset I to dataset IV, also following the similar trend of absolute \( y \)-skewnesses. Including higher order moments will require the same number of additional constraints to make multiple datasets statistically identical within the range of constraints applied.

1. These shape functions of positive, negative, and zero \( f_0 \) values are made and shown in Fig. (4a), (b), and (c), respectively. Figs. (4a) and (b) show smooth shape functions with opposite signs, and Fig. (4c) shows the predetermined linear regression line \( Y(x) \) as the shape function so that initial points are located on the regression line. Fig. (4d) combines all the datasets and shape functions, generated in (a)–(c), and shows the overall trend.

2. In each of Figs. (4a)–(c), \( N \) points initially on the shape function (filled circles) are randomly relocated to new neighboring positions (hollow diamonds) above or below the original positions.

3. Three vertical positions of \( y_j \) for \( j = 1, m \), and \( N \) are adjusted to two distinct groups (hollow circles and rectangles), of which both satisfy the given constraints using the algorithm discussed above.
Figure 4. Created data using the shape function of Eq. (48) with (a) \( f_0 = +\sqrt{2} \times 10^{-2} \), (b) \( f_0 = -\sqrt{2} \times 10^{-2} \), and (c) \( f_0 = 0 \): filled circles are points on the shape function; blank diamonds are randomly deviated from the shape functions; three filled diamonds are replaced by either hollow squares or circles, adjusted to meet the statistical constraints listed in Table II; and (d) a collection of all hollow symbols in (a)–(c), where specific patterns become unnoticeable.

Table V. The third and fourth moments of Anscombe’s quartet.

| Dataset | \( \langle z_3^y \rangle \) | \( \langle z_4^y \rangle \) | \( \langle z_3^x \rangle \) | \( \langle z_4^x \rangle \) |
|---------|----------------|----------------|----------------|----------------|
| I       | 0.000          | 1.471          | -0.048         | 1.801          |
| II      | 0.000          | 1.471          | -0.979         | 2.486          |
| III     | 0.000          | 1.471          | 1.377          | 4.228          |
| IV      | 2.467          | 7.521          | 1.119          | 3.622          |

IV. CONCLUSION

Testing the similarities or identicalness of two datasets from distinct origins is an ubiquitously important issue in statistics, applicable to various studies. When a paired dataset is linearly regressed, the trend line indicates correlation degrees of how the response variable \( y \) depends on the independent variable \( x \), assuming that one is a cause and the other is an effect, or vice versa. In reality, it is rare to have two or more visually different datasets that provide an identical regression equation. On the other hand, a given regression equation can interpret or explain a number of datasets from various sources. Here, we recognized that a robust method to sample many degenerate datasets satisfying the given constraints is of great necessity, not only in advanced data sciences and applications, but also in applied statistics education at college and graduate levels. In this work, we presented an algorithm to sample many degenerate datasets having the identical six constraints used for a linear regression. Our method is extendable for an arbitrary number of constraints, including higher-order statistical moments, to create statistically closer datasets.

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