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An American National Standard

Standard Practice for Regression Analysis with a Single Predictor Variable[1]

This standard is issued under the fixed designation E3080; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers regression analysis ~~methodology for estimating, evaluating, and using the simple linear regression model~~ of a set of data to define the statistical relationship between two numerical ~~variables.~~variables for use in predicting one variable from the other.

1.2 The regression analysis provides graphical and calculational procedures for selecting the best statistical model that describes the relationship and for evaluation of the fit of the data to the selected model.

1.3 The resulting regression model can be useful for developing process knowledge through description of the variable relationship, in making predictions of future values, in relating the precision of a test method to the value of the characteristic being measured, and in developing control methods for the process generating values of the variables.

1.4 The system of units for this practice is not specified. Dimensional quantities in the practice are presented only as illustrations of calculation methods. The examples are not binding on products or test methods treated.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E178 Practice for Dealing With Outlying Observations

E456 Terminology Relating to Quality and Statistics

E2586 Practice for Calculating and Using Basic Statistics

3. Terminology

3.1 *Definitions*—Unless otherwise noted, terms relating to quality and statistics are as defined in Terminology E456.

~~3.1.1 *coefficient of determination, r^2, n*—square of the correlation coefficient.~~

3.1.1 *degrees of freedom, n*—the number of independent data points minus the number of parameters that have to be estimated before calculating the variance. **E2586**

~~3.1.3 *residual, n*—observed value minus fitted value, when a model is used.~~

3.1.2 *predictor variable, X, n*—a variable used to predict a response variable using a regression model.

3.1.2.1 *Discussion*—

Also called an *independent* or *explanatory* variable.

3.1.3 *regression analysis, n*—a statistical procedure used to characterize the association between two or more numerical variables for prediction of the response variable from the predictor variable.

[1] This practice is under the jurisdiction of ASTM Committee E11 on Quality and Statistics and is the direct responsibility of Subcommittee E11.10 on Sampling / Statistics.
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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the ~~standard's~~standard's Document Summary page on the ASTM website.

3.1.3.1 *Discussion—*

In this practice, only a single predictor variable is considered.

3.1.4 *residual, n*—the observed value minus fitted value, when a regression model is used.

3.1.5 *response variable, Y, n*—a variable predicted from a regression model.

3.1.5.1 *Discussion—*

Also called a *dependent* variable.

3.1.6 *sample coefficient of determination, r^2, n*—square of the sample correlation coefficient.

3.1.7 *sample correlation coefficient, r, n*—a dimensionless measure of association between two variables estimated from the data.

3.1.8 *sample covariance, s_{xy}, n*—an estimate of the association of the response variable and predictor variable calculated from the data.

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *intercept, β_0, n—of a regression model*, ~~β_0,~~ the value of the response variable when the value of the predictor variable is equal to zero.

3.2.2 *regression model parameter, n*—a descriptive constant defining a regression model that is to be estimated.

3.2.3 *residual standard deviation, σ, n—of a regression model*, ~~σ,~~ the square root of the residual variance.

3.2.4 *residual variance, σ^2, n—of a regression model*, ~~σ^2,~~ the variance of the residuals (see *residual*).

3.2.5 *slope, β_1, n—of a regression model*, ~~β_1,~~ the incremental change in the response variable due to a unit change in the predictor variable.

3.3 *Symbols:*

~~b_0~~	=	~~intercept estimate (5.2.2)~~
~~b_1~~	=	~~slope estimate (5.2.2)~~
~~β_0~~	=	~~intercept parameter in model (5.1.2)~~
~~β_1~~	=	~~slope parameter in model (5.1.2)~~
~~E~~	=	~~general point estimate of a parameter (5.4.2)~~
~~e_i~~	=	~~residual for data point *i* (5.2.5)~~
~~ε~~	=	~~residual parameter in model (5.1.3)~~
~~F~~	=	~~*F* statistic (X1.3.2)~~
~~h~~	=	~~index for any value in data range (5.4.5)~~
~~i~~	=	~~index for a data point (5.2.1)~~
~~n~~	=	~~number of data points (5.2.1)~~
~~r~~	=	~~sample correlation coefficient (5.3.2.1)~~
~~r^2~~	=	~~coefficient of determination (5.3.2.2)~~
~~$S(b_0,b_1)$~~	=	~~sum of squared deviations of Y_i to the regression line (X1.1.2)~~
~~s_{b1}~~	=	~~standard error of slope estimate (5.4.3)~~
~~s_{b0}~~	=	~~standard error of intercept estimate (5.4.4)~~
~~s_E~~	=	~~general standard error of a point estimate (5.4.2)~~
~~σ~~	=	~~residual standard deviation (5.1.3)~~
~~s~~	=	~~estimate of σ (5.2.6)~~
~~σ^2~~	=	~~residual variance (5.1.3)~~
~~s^2~~	=	~~estimate of σ^2 (5.2.6)~~
~~s_X^2~~	=	~~variance of *X* data (X1.2.1)~~
~~s_Y^2~~	=	~~variance of *Y* data (X1.2.1)~~
~~S_{XX}~~	=	~~sum of squares of deviations of *X* data from average (5.2.3)~~
~~S_{XY}~~	=	~~sum of cross products of *X* and *Y* from their averages (5.2.3)~~
~~s_{XY}~~	=	~~sample covariance of *X* and *Y* (X1.2.1)~~
~~$s_{\hat{Y}h}$~~	=	~~standard error of $\hat{Y}_h$ (5.4.5)~~
~~$s_{\hat{Y}h(ind)}$~~	=	~~standard error of future individual *Y* value (5.4.6)~~
~~S_{YY}~~	=	~~sum of squares of deviations of *Y* data from average (5.2.3)~~
~~t~~	=	~~Student's *t* distribution (5.4.2)~~
~~X~~	=	~~predictor variable (5.1.1)~~
~~$\bar{X}$~~	=	~~average of *X* data (5.2.3)~~
~~X_h~~	=	~~general value of *X* in its range (5.4.5)~~

~~X_i~~	~~=~~	~~value of X for data point i (5.2.1)~~
~~Y~~	~~=~~	~~response variable (5.1.1)~~
~~$\bar{Y}$~~	~~=~~	~~average of Y data (5.2.3)~~
~~$\hat{Y}_{h(ind)}$~~	~~=~~	~~predicted future individual Y for a value X_h (5.4.6)~~
~~Y_i~~	~~=~~	~~value of Y for data point i (5.2.1)~~
~~$\hat{Y}_h$~~	~~=~~	~~predicted value of Y for any value X_h (5.4.5)~~
~~$\hat{Y}_i$~~	~~=~~	~~predicted value of Y for data point i (5.2.4)~~

b_0	=	intercept parameter estimate (5.5.1)
b_1	=	slope parameter estimate (5.5)
b_{11}	=	curvature parameter estimate (8.1.1.1)
β_0	=	intercept parameter in model (5.3.1)
β_1	=	slope parameter in model (5.3.1)
β_{11}	=	curvature parameter in model (5.3.3)
E	=	general point estimate of a parameter (5.7)
e_i	=	residual for data point i (5.5.2)
ε	=	error term in model (5.4)
F	=	F statistic (6.5.2)
h	=	index for predicting any value in data range (6.4.3)
i	=	index for a data point (5.2)
L	=	lower confidence limit (5.7.2)
λ	=	Box-Cox parameter (A1.5.4)
n	=	number of data points (5.2)
p	=	number of parameters in regression model (5.7)
r	=	correlation coefficient (6.3.2.1)
r^2	=	coefficient of determination (6.3.2.2)
$S(b_0,b_1)$	=	sum of squared deviations of Y_i to the regression line (A1.1.2)
s_{b1}	=	standard error of slope estimate (6.4.1)
s_{b0}	=	standard error of intercept estimate (6.4.2)
s_E	=	general standard error of a point estimate (5.7)
σ	=	residual standard deviation (5.4.1)
s	=	estimate of σ (6.2.6)
σ^2	=	residual variance (5.4.1)
s^2	=	estimate of σ^2 (6.2.6)
s_X^2	=	variance of X data (A1.2.1)
s_Y^2	=	variance of Y data (A1.2.1)
S_{XX}	=	sum of squares of deviations of X data from average (6.2.3)
S_{XY}	=	sum of cross products of X and Y from their averages (6.2.3)
s_{XY}	=	sample covariance of X and Y (A1.2.1)
$s_{\hat{Y}h}$	=	standard error of $\hat{Y}_h$ (6.4.3)
$s_{\hat{Y}h(ind)}$	=	standard error of future individual Y value (6.4.4)
S_{YY}	=	sum of squares of deviations of Y data from average (6.2.3)
t	=	Student's t distribution (5.7)
U	=	upper confidence limit (5.7.2)
X	=	predictor variable (5.1)
$\bar{X}$	=	average of X data (6.2.3)
X_h	=	general value of X in its range (6.4.3)
X_i	=	value of X for data point i (5.2)
Y	=	response variable (5.1)
$\bar{Y}$	=	average of Y data (6.2.3)
$\dot{Y}$	=	geometric mean of Y data (A1.5.4)
Y'	=	transformed Y (A1.5.2)
$\hat{Y}_{h(ind)}$	=	predicted future individual Y for a value X_h (6.4.4)
Y_i	=	value of Y for data point i (5.2)
$\hat{Y}_h$	=	predicted value of Y for any value X_h (6.4.3)
$\hat{Y}_i$	=	predicted value of Y for data point i (5.5.1)

3.4 *Acronyms:*

3.4.1 *ANOVA, n*—~~Analysis~~analysis of ~~Variance~~variance

3.4.2 *df, n*—~~Degrees~~degrees of ~~Freedom~~freedom

3.4.3 *LOF, n*—~~Lack~~lack of ~~Fit~~fit

3.4.4 *MS, n*—~~Mean Square~~mean square

3.4.5 *MSE, n*—~~Mean Square Error~~mean square error

3.4.6 *MSR, n*—~~Mean Square Regression~~mean square regression

3.4.7 *MST, n*—~~Mean Square Total~~mean square total

3.4.8 *PE, n*—~~Pure Error~~pure error

3.4.9 *SS, n*—~~Sum~~sum of ~~Squares~~squares

3.4.10 *SSE, n*—~~Sum~~sum of ~~Squares Error~~squares error

3.4.11 *SSR, n*—~~Sum~~sum of ~~Squares Regression~~squares regression

3.4.12 *SST, n*—~~Sum~~sum of ~~Squares Total~~squares total

4. Significance and Use

4.1 Regression analysis is a procedure that uses data to study the statistical relationships between two or more variables (**1**, **2**).[3] This practice is restricted in scope to consider only a single numerical response variable and a single numerical predictor variable. The objective is to obtain a regression model for use in predicting the value of the response variable *Y* for given values of the predictor variable *X*.

4.2 ~~Regression analysis is a statistical procedure~~A regression model consists of: (*1* ~~that~~) a ~~*studies the*~~*regression function* ~~statistical relationships between two or more variables Ref.~~ that relates the mean values ~~(1, 2). In general, one of these variables is designated as a response variable and the rest of the variables are designated as~~of the response variable distribution to fixed values of the predictor variable, and (*2* ~~predictor~~) a ~~*variables. Then*~~*statistical distribution* ~~the objective of the model is to predict the response from the predictor variables.~~that describes the variability in the response variable values at a fixed value of the predictor variable.

~~4.1.1 This standard considers a numerical response variable and only a single numerical predictor variable.~~

~~4.1.2 The regression model consists of: (*1*) a mathematical function that relates the mean values of the response variable distribution to fixed values of the predictor variable, and (*2*) a description of statistical distribution that describes the variability in the response variable at fixed levels of the predictor variable.~~

4.2.1 The regression ~~procedure~~analysis utilizes either *experimental* or *observational* data to estimate the *parameters* defining a regression model and their precision. Diagnostic procedures are utilized to assess the resulting model fit and can suggest other models for improved prediction performance.

~~4.1.4 The regression model can be useful for developing process knowledge through description of the variable relationship, in making predictions of future values, and in developing control methods for the process generating values of the variables.~~

4.3 ~~Section~~The ~~5 in this standard deals with the simple linear regression model using a straight line mathematical relationship between the two variables where variability of the response variable over the range of values of the predictor variable is described by a normal distribution with constant variance.~~ information in this practice is arranged as follows.~~Appendix X1 provides supplemental information.~~

4.3.1 Section 5 gives a general outline of the steps in the regression analysis procedure. The subsequent sections cover procedures for estimation of specific regression models.

4.3.2 Section 6 assumes a straight line relationship between the two variables. This is also known as the simple linear regression model or a first order model. This model should be used as a starting point for understanding the *XY* relationship and ultimately defining the best fitting model to the data.

4.3.3 Section 7 considers a proportional relationship between the variables, where the ratio of one variable to the other is constant. The intercept is constrained to be zero. This model is useful for single point calibration, where a reference material is run periodically as a standard during routine testing to correct for drift in instrument performance over a given range of test results.

4.3.4 Section 8 discusses a regression function that considers curvature in the *XY* relationship, the second order polynomial model.

4.3.5 Annex A1 provides supplemental information of a more mathematical nature in regression.

4.3.6 Appendix X1 lists calculations for the curvature model estimates and exhibits a worksheet for these calculations.

5. Regression Analysis Procedure for a Single Predictor Variable

5.1 *Choose the response variable Y and the predictor variable X*. The predictor variable *X* is assumed to have known values with little or no measurement error. For given values of *X*, the response variable *Y* has a distribution of values representing the random effect of measurement errors, and these distributions are defined within a given range of the *X* values.

[3] The boldface numbers in parentheses refer to a list of references at the end of this standard.

5.2 *Obtain a data set* consisting of *n* pairs of values designated as (X_i,Y_i), with the sample index *i* ranging from 1 through *n*. The data can arise in two different ways. Observational data consists of *X* and *Y* values measured on a set of *n* random test units. Experimental data consists of *Y* values measured on *n* test units with *X* values set at controlled values in an experimental study.

5.2.1 When designing an experiment for defining the *XY* association some considerations are:

(1) Range of *X* values.

(2) Number of distinct *X* values.

(3) Spacing of *X* values.

(4) Number of *Y* observations for each *X* value.

The answers depend on the objectives of the investigation, whether determining the nature of the regression function, estimating the slope or intercept of the simple linear model, or estimating the measurement error of *Y*, as well as other objectives.

5.2.1.1 The *X* values should cover the entire range of interest. Extrapolation beyond the range of observed *X* values may fail due to expanding estimation error outside the range and the uncertainty of whether the model gives an adequate description of the *XY* relationship outside the range. When inference is required for the *Y* intercept (the value of *Y* when *X* is zero) the range of *X* should extend down to zero or near zero.

5.2.1.2 Two *X* levels are necessary when the objective is to determine if there is an effect of *X* on *Y*, and to give an estimate of the effect (slope). Three *X* levels are necessary to evaluate any curvature in the relationship. Four or more *X* levels give better definition of the model shape, particularly if there is a possible asymptote or a threshold in the relationship. The *X* levels should be equally spaced. If *X* is transformed, such as to logarithms, the equal spacing should be with respect to the transformed *X*.

5.2.1.3 Usually the number of *Y* observations should be equal at each *X* level. When the objective is to estimate *Y* variance or evaluate variance constancy, then at least four observations are recommended at each *X* level.

5.3 *Choose a regression function that fits the data.* A *scatter plot* of the data is recommended for a visual look at the *XY* relationship, and most computer packages have this as an option. This is a plot of points on the *XY* plane having a value of *Y* (on the vertical axis) and a value of *X* (on the horizontal axis) for each data pair, where it is useful for evaluating the quality of the data and suggesting an appropriate regression function to define the *XY* relationship. Fig. 1 gives examples of four scatter plots that illustrate different situations.

5.3.1 Fig. 1A shows a cluster of points that appear to be elongated in a particular direction along a straight line that does not pass through the *origin* (X=0, Y=0). This pattern suggests the straight line regression function $Y=\beta_0+\beta_1X$. The two *parameters* for this function are the *intercept* β_0 and the *slope* β_1. The slope is the amount of incremental change in *Y* units for a unit change in *X*. The intercept is the value of *Y* when $X = 0$. Both parameters are necessary to define this regression function.

5.3.2 Fig. 1B suggests a straight line that appears to go through the origin, thus *Y* is proportional to *X*, and the regression function is $Y=\beta_1X$. An intercept term is not required because the *Y* intercept is constrained to equal zero, that is, the line goes through the origin.

5.3.3 Fig. 1C indicates curvature in the relationship, and there are several regression functions that can be used. For slight

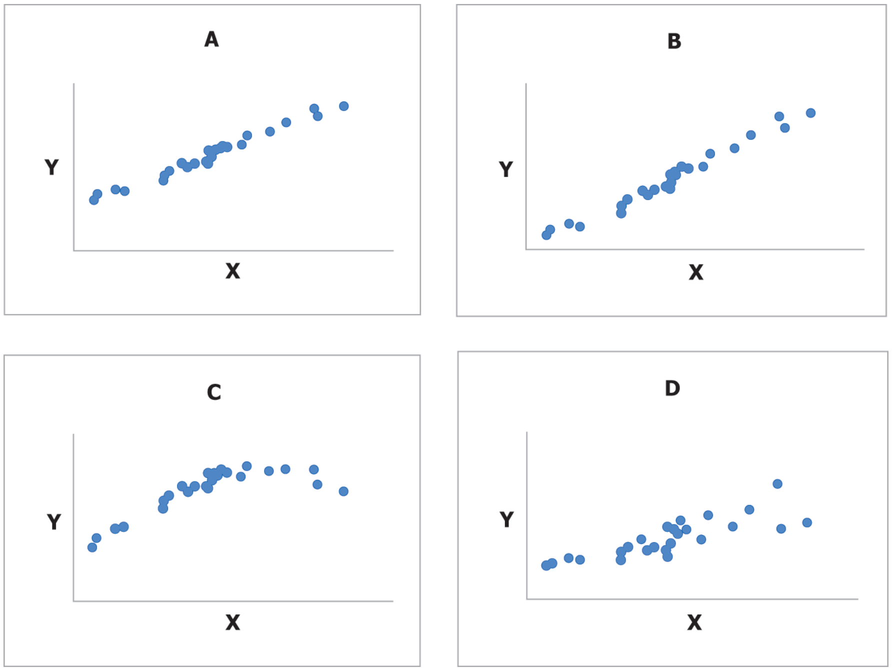


FIG. 1 Scatter Plots

curvature, a simple model is to add a second order (X^2) term to the straight line function as $Y=\beta_0+\beta_1X+\beta_{11}X^2$.

5.3.4 Fig. 1D shows data with increasing variability with larger mean values. This suggests the need for a weighted regression procedure discussed in A1.4.2.

5.3.5 Data points appearing outside the swarm of data (*outliers*) can have an adverse effect on estimation of regression function parameters. For the straight-line function, outliers at the extremes of the *X* range can greatly affect the estimate of the slope and intercept parameters, and outliers in the middle of the range tend to affect the intercept estimate more than the slope. Outliers can be formally identified by statistical procedures (see Practice E178).

5.3.6 A special situation occurs when there are two data swarms separated by a gap. This may indicate that there were two sources of data with different values of a second lurking predictor variable. Such a data set consists essentially of two data points in cases of a large gap.

5.4 *Define the regression model* by adding an error term to the regression function that describes the variation in *Y* through a statistical distribution. For example, the *simple linear regression model* using the regression function in 5.3.1 is then stated as $Y=\beta_0+\beta_1X+\varepsilon$, where ε is a random error having a distribution with mean zero and standard deviation σ (variance σ^2).

5.4.1 The distribution for ε can often be assumed to have a normal (Gaussian) distribution with a constant standard deviation over the range of *X*. Thus, the distribution of *Y* at a given *X* is a normal distribution with a mean of $\beta_0+\beta_1X$ and a standard deviation of σ. An example of such a linear regression model is shown in Fig. 2 over a range of *X* from 0 to 40 *X* units. Normal distributions of response *Y* with σ = 1.3 *Y* units are depicted at *X* = 10, 20, and 30 *X* units.

5.4.2 Distributions other than the normal distribution may also be considered, depending on knowledge of the application. For example, low microbial counts may use a Poisson error distribution.

5.5 *Parameter estimation* uses the data set to provide the parameter estimates. For the simple regression functions described above, the procedures used are given in the following sections. In this practice, the parameters are lower-case Greek letters and the estimates are the corresponding lower-case Roman letters. For example, the estimate of the slope parameter β_1 is b_1.

5.5.1 The *fitted values of Y*, denoted $\hat{Y}_i$ (read *Y*-hat), for each data point (X_i,Y_i) are calculated from the estimated regression function. For the straight-line model, the fitted values of Y_i are $\hat{Y}_i=b_0+b_1X_1$. The right-hand function defines the regression line, which may be shown on the scatter plot of the data to evaluate model fit.

5.5.2 The estimates of the error term values ε are the *residuals* ε_i, calculated as $e_i=Y_i-\hat{Y}_i$, and these are used to estimate the standard deviation parameter σ. Note that the residual values are the vertical distances of the points from the regression line.

5.6 *Evaluation of the regression model* is performed to diagnose departure from model assumptions, such as model fit to the data, constancy of variance over the range of *X*, and conformance to the assumed error distribution. Residual plots are useful for these diagnostics.

5.6.1 A plot of the residuals against their *X* values (or equivalently, against their $\hat{Y}_i$ values) will detect certain departures from the assumptions. Residuals may also be plotted against time of testing (if available) or against another known variable. Fig. 3 shows some of these patterns and discusses remedies for these departures. (The horizontal line on the plots indicates a value of zero for the average of the residuals.)

(1) Plot A – the desired horizontal pattern – indicates no model deficiencies

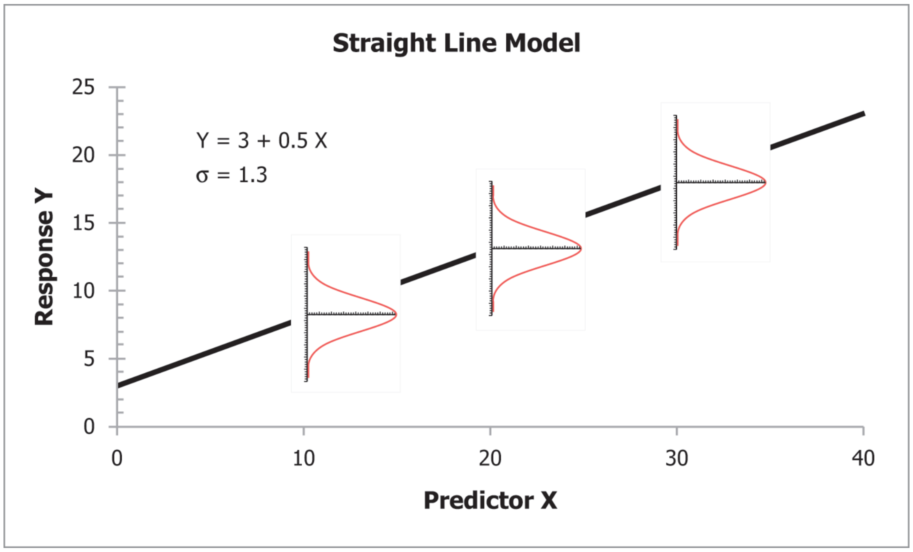


FIG. ~~1~~2 Graphical Depiction of a Straight Line Regression Model

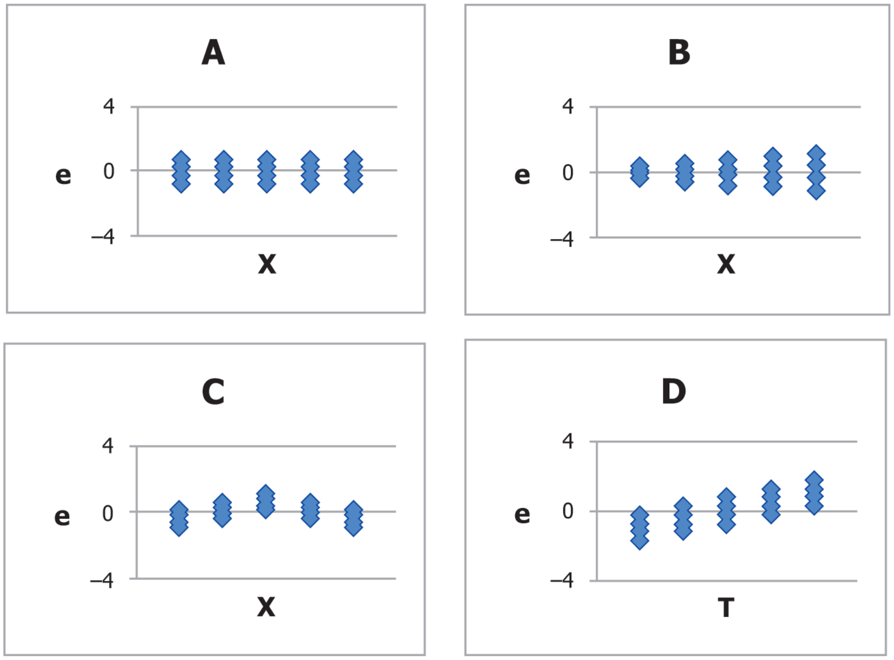


FIG. ~~2~~3 ~~Dot Plot of the Predictor Value~~ Residual Plots – Some Patterns~~X~~

(2) Plot B – increasing variance with *X*, consider weighted regression (see A1.4.2) or data transformations (see A1.5)

(3) Plot C – curvature in the relationship, consider adding a quadratic term or using a nonlinear model (see Section 8)

(4) Plot D – possible effect of time order of testing or the effect of another variable denoted as *T*

5.6.2 Plotting the residuals against a vertical scale of the cumulative percentage of the normal distribution checks the assumption of normality in the model. The fitted cumulative normal distribution from the data is shown as a straight line on the plot if the residuals fit a normal distribution. Computer packages provide these plots and can also perform a more rigorous statistical test for normality. If the plot indicates a curve, a data transformation may be required to achieve a normal distribution.

5.6.3 Outlier testing in regression analysis takes two forms. Outlier testing can be performed upon any sets of multiple *Y*'s collected at each unique value of *X* studied. Additionally, outlier analysis can be performed on the entire set of residuals. In the latter case, finding an outlier could indicate an issue in either the *X* or *Y* value of the point in question or it may indicate other issues with the regression analysis.

5.7 *Use of the model for interval estimates of regression parameters and predicted Y values.*

5.7.1 The estimates of model parameters and fitted *Y* values are *point estimates*. For example, the estimate of the slope parameter β_1 is the estimate b_1 that has been calculated from the data. To give a sense of the precision for these estimates, *interval estimates*, or confidence intervals, can be provided. A general form for the *confidence interval* for a general point estimate *E* is:

$$E \pm t s_E \tag{1}$$

where s_E is the *standard error* of the estimate and *t* is a tabulated multiplier that is dependent upon *the degrees of freedom* of the standard error and the desired *confidence level*, stated as a percentage. Thus, we may state that the true value of the parameter being estimated lies within the confidence interval at a given confidence level. The degrees of freedom for the standard error are generally $n - p$, where *p* is the number of parameters in the regression model.

5.7.2 To calculate these interval estimates, the form of the statistical distribution for *Y* is required, and the normal distribution is often assumed. The widths of the interval estimates, given here as two-sided confidence intervals, are dependent on (*1*) the standard errors of the estimates, and (*2*) the level of confidence. The standard errors depend on the number of data pairs *n* and the values of the X_i.

The confidence level is defined as 100(1 – α) %, where α is the probability that the confidence interval does not contain the parameter value. For example, α = 0.05 (or a risk of 5 % non-coverage) corresponds to a confidence level of 95 %, which shall be used for the examples in this practice. The value of *t* is the upper (1 – α/2)th quantile of the Student's *t* distribution with $n - p$ degrees of freedom, for a confidence level of 100(1 – α) %. Values of *t* are found in statistical texts and in commercial statistical software packages.

5.7.3 The confidence interval can also be stated as the interval (L, U) between lower (L) and upper (U) confidence limits for the parameter being estimated. Practice E2586 provides discussion of confidence intervals, standard error, and degrees of freedom.

6. Simple Linear Regression Analysis

6.1 *Simple Linear Regression Model:*

6.1.1 ~~Select the response variable~~This model defines the functional relationship ~~Y~~between ~~and the predictor variable *X*. *The predictor* *X* is assumed to have known values with little or no measurement error. The response~~ and *Y* ~~has a distribution of values for a given~~ as a straight line in the ~~*X*~~*XY* ~~value, and this distribution is defined for all~~ plane.~~X values in a given range.~~

6.1.2 The *regression function* for the straight line relationship is:

$$Y=\beta_0+\beta_1X \tag{2}$$

where the two *parameters* for the function are the *intercept* β_0 and the *slope* β_1.

The ~~regression function for the straight line relationship is $Y=\beta_0+\beta_1X$. The two parameters for the function are the intercept β~~intercept ~~$_0$ and the slope β_1. The intercept~~ is the value of *Y* when *X* = 0, but this parameter may not be of practical interest when the range of *X* is far removed from zero. The slope is the amount of incremental change in *Y* units for a unit change in *X*.

6.1.3 The statistical distribution for *Y* is usually assumed to be a normal (Gaussian) distribution having a mean of $\beta_0+\beta_1X$ with a standard deviation σ. The *simple linear regression model* is then stated ~~as~~ as:~~$Y=\beta_0+\beta_1X+\varepsilon$, where ε is a random error that is normally distributed with mean zero and standard deviation σ (variance σ^2).~~

$$Y=\beta_0+\beta_1X+\varepsilon \tag{3}$$

where ε is a random error that is normally distributed with mean zero and standard deviation σ (variance σ^2).

~~5.1.4 An example of a linear regression model is depicted in Fig. 1 over a range of *X* from 0 to 40 *X* units. Normal distributions of response *Y* with σ = 1.3 *Y* units are depicted at *X* = 10, 20, and 30 *X* units.~~

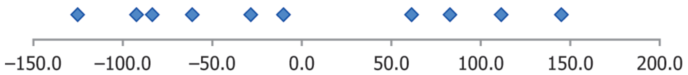


FIG. ~~5~~6 Dot Plot of Residuals

6.2 *Estimating Regression Model Parameters:*

6.2.1 The model parameters β_0, and β_1, are estimated from a sample of data consisting of *n* pairs of values designated as (X_i,Y_{ii}), with the sample number *i* ranging from 1 through *n*. The data can arise in two different ways. Observational data consists of *X* and *Y* values measured on a set of *n* random samples. Experimental data consists of *Y* values measured on *n* experimental units with *X* values set at fixed values. In both cases the *Y* values may have measurement error, but the *X* values are assumed known with negligible measurement error.

6.2.2 The regression line parameters β_0, and β_1 are estimated by the method of least squares, which finds their corresponding estimates b_0 and b_1 that minimize the sum of the squares of the vertical distances between the Y_{ii} values and their respective line values at X_i. (For a further discussion of the least squares method, see ~~X1.1.2~~A1.1.2.)

6.2.3 Calculate the following statistics from the *X* and *Y* values in the data set.

6.2.3.1 Calculate the averages of *X* and *Y*:

$$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n} \quad (1)$$

$$\bar{Y} = \frac{\sum_{i=1}^{n} Y_i}{n} \quad (2)$$

$$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n} \quad (4)$$

$$\bar{Y} = \frac{\sum_{i=1}^{n} Y_i}{n} \quad (5)$$

6.2.3.2 Calculate the sums of squared deviations S_{XXXX} and S_{YYYY} of *X* and *Y* from their respective averages and the sum of cross products S_{XYXY} of the *X* and *Y* deviations from their averages:

$$S_{XX} = \sum_{i=1}^{n} \left(X_i - \bar{X}\right)^2 \quad (3)$$

$$S_{YY} = \sum_{i=1}^{n} \left(Y_i - \bar{Y}\right)^2 \quad (4)$$

$$S_{XY} = \sum_{i=1}^{n} \left(X_i - \bar{X}\right)\left(Y_i - \bar{Y}\right) \quad (5)$$

$$S_{XX} = \sum_{i=1}^{n} \left(X_i - \bar{X}\right)^2 \quad (6)$$

$$S_{YY} = \sum_{i=1}^{n} \left(Y_i - \bar{Y}\right)^2 \quad (7)$$

$$S_{XY} = \sum_{i=1}^{n} \left(X_i - \bar{X}\right)\left(Y_i - \bar{Y}\right) \quad (8)$$

S_{XXXX} is a known fixed constant. S_{YYYY} and S_{XYXY} are random variables.

6.2.3.3 The least squares solution gives the parameter estimates:

~~$b_1 = S_{XY}/S_{XX}$ (6)~~

~~$b_0 = \bar{Y} - b_1\bar{X}$ (7)~~

~~[S_{YY} is not used here but will be used in subsequent sections.]~~

$$b_1 = S_{XY}/S_{XX} \quad (9)$$

$$b_0 = \bar{Y} - b_1\bar{X} \quad (10)$$

6.2.4 The *fitted values*$\hat{Y}_i$ for each data point Y_{ii} are calculated from the estimated regression function as:

~~$\hat{Y}_i = b_0 + b_1X_i$ (8)~~

$$\hat{Y}_i = b_0 + b_1X_i \quad (11)$$

6.2.5 The *residual*e_{ii} is the difference between the response data point Y_{ii} and its fitted value $\hat{Y}_i$:

$$e_i = Y_i - \hat{Y}_i \quad (12)$$

Residuals are graphically the vertical distances on the scatter plot between the response data points $Y_{\cancel{i}\bar{i}}$ and the estimated regression line.

6.2.6 The estimates s^2 of the variance σ^2 and s of the standard deviation σ of the Y distribution are calculated as the sum of the squared residuals divided by their degrees of freedom:

$$s^2 = \frac{\sum_{i=1}^{n} e_i^2}{(n - 2)} = \sum_{i-1}^{n} \left(Y_i - \hat{Y}_i\right)^2 / (n - 2) \tag{10}$$

~~$s = \sqrt{s^2}$ (11)~~

$$s^2 = \frac{\sum_{i=1}^{n} e_i^2}{(n - 2)} = \frac{\sum_{i-1}^{n} \left(Y_i - \hat{Y}_i\right)^2}{(n - 2)} \tag{13}$$

$$s = \sqrt{s^2} \tag{14}$$

These estimates have $n - 2$ degrees of freedom because of prior estimation of two parameters, the slope and intercept of the line, which removed two degrees of freedom from the data set of n data points prior to calculation of the residuals.

6.2.7 ~~*Regression Analysis Procedure with*~~ *Example*—A data set from Duncan, Ref. (**3**) lists measurements of shear strength (inch-pounds) and weld diameter (mils) measured on 10 random test specimens, so this is an observational data set with $n = 10$ pairs. Regression analysis will be used to investigate the relationship between weld diameter and shear strength, with the objective of predicting shear strength Y from weld diameter X. The ~~steps in the regression analysis procedure for the simple linear model, that are illustrated~~weld diameters are considered to be measured with small error. The data are listed in Table 1~~the example below, are as follows:~~.

~~*(1)* Choose the predictor variable X and response variable Y.~~

~~*(2)* Obtain data pairs of X and Y from available data or by conducting an experiment.~~

~~*(3)* Evaluate the distribution of the predictor variable and the XY relationship using plots.~~

~~*(4)* If the model is supported by the data plots, estimate the model parameters from the data.~~

~~*(5)* Evaluate the fitted model against the model assumptions.~~

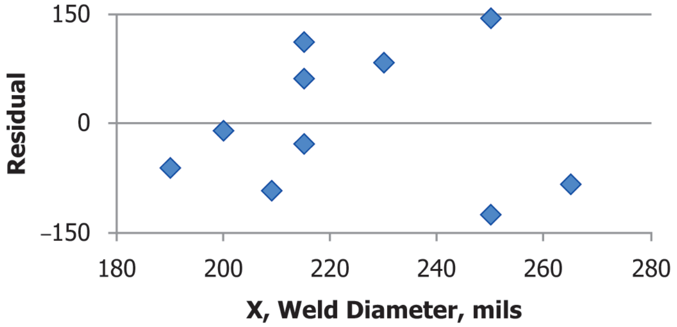
~~*(6)* Use the regression model for future prediction of Y from X.~~

~~5.2.7.1 A data set from Duncan, Ref. (**3**) lists measurements of shear strength (inch-pounds) and weld diameter (mils) measured on 10 random test specimens, so this is an observational data set with $n = 10$ pairs. Regression analysis will be used to investigate the relationship between weld diameter and shear strength, with the objective of predicting shear strength Y from weld diameter X. The weld diameters are considered to be measured with small error. The data are listed in Table 1.~~

~~5.2.7.2 A dot plot of the X data is shown as Fig. 2, and the plot indicated that the data was spread out fairly evenly across the range of 190–270 mils and some of the parts had the same diameters.~~

TABLE 1 Data and Calculations for Straight Line Regression Model Example

Sample, i	X_i	Y_i	$X_i-\bar{X}$	$Y_i-\bar{Y}$	$\hat{Y}_i$	e_i	Statistics	Results	EQ
~~1~~	~~190~~	~~680~~	~~–33.9~~	~~–295.0~~	~~741.2~~	~~–61.2~~	~~S_{XX}~~	~~5268.90~~	~~Eq 3~~
1	190	680	–33.9	–295.0	741.2	–61.2	S_{XX}	5268.90	Eq 6
~~2~~	~~200~~	~~800~~	~~–23.9~~	~~–175.0~~	~~810.1~~	~~–10.1~~	~~S_{YY}~~	~~330550.00~~	~~Eq 4~~
2	200	800	–23.9	–175.0	810.1	–10.1	S_{YY}	330550.00	Eq 7
~~3~~	~~209~~	~~780~~	~~–14.9~~	~~–195.0~~	~~872.2~~	~~–92.2~~	~~S_{XY}~~	~~36345.00~~	~~Eq 5~~
3	209	780	–14.9	–195.0	872.2	–92.2	S_{XY}	36345.00	Eq 8
~~4~~	~~215~~	~~885~~	~~–8.9~~	~~–90.0~~	~~913.6~~	~~–28.6~~	~~Slope, b_1~~	~~6.8980~~	~~Eq 6~~
4	215	885	–8.9	–90.0	913.6	–28.6	Slope, b_1	6.8980	Eq 9
~~5~~	~~215~~	~~975~~	~~–8.9~~	~~0.0~~	~~913.6~~	~~61.4~~	~~Intercept, b_0~~	~~–569.47~~	~~Eq 7~~
5	215	975	–8.9	0.0	913.6	61.4	Intercept, b_0	–569.47	Eq 10
~~6~~	~~215~~	~~1025~~	~~–8.9~~	~~50.0~~	~~913.6~~	~~111.4~~	~~Variance, s^2~~	~~9980.16~~	~~Eq 10~~
6	215	1025	–8.9	50.0	913.6	111.4	Variance, s^2	9980.16	Eq 13
~~7~~	~~230~~	~~1100~~	~~6.1~~	~~125.0~~	~~1017.1~~	~~82.9~~	~~St. Dev., s~~	~~99.90~~	
7	230	1100	6.1	125.0	1017.1	82.9	St. Dev., s	99.90	Eq 14
~~8~~	~~250~~	~~1030~~	~~26.1~~	~~55.0~~	~~1155.0~~	~~–125.0~~			
8	250	1030	26.1	55.0	1155.0	–125.0			
9	250	1300	26.1	325.0	1155.0	145.0			
~~10~~	~~265~~	~~1175~~	~~14.1~~	~~200.0~~	~~1258.5~~	~~–83.5~~			
10	265	1175	14.1	200.0	1258.5	–83.5			
	$\bar{X}$	$\bar{Y}$							
Average	223.9	975.0	0.0	0.0	975.0	0.0			
~~Equation~~	~~Eq 1~~	~~Eq 2~~			~~Eq 8~~	~~Eq 9~~			
Equation	Eq 4	Eq 5			Eq 8	Eq 9			



~~FIG. 6 Residual Plots – Some Patterns~~
FIG. 7 Plot of Residuals versus *X* — Duncan Example

6.2.7.1 ~~A scatter plot of the data is recommended as a first or concurrent step for a visual look at the relationship, and most computer packages have this as an option. This is a plot of *Y* (on the vertical axis) versus *X* (on the horizontal axis) for each data pair. If a straight line relationship exists, the cluster of points will appear to be elongated in a particular direction along a straight line, and the plot will visually reveal any curvature or any other deviations from a straight line relationship, as well as any outlying data points. The estimated regression line can also be included on the plot to give a visual impression of the fit of the model to the data.~~

The scatter plot for this example is shown in Fig. ~~3~~4. The shear strength appears to be increasing in a linear fashion with weld diameter. There is some scatter but no apparent outlying data points.

6.2.7.2 The calculations, with equation numbers for each calculation, are shown in Table 1. The averages of *X* and *Y* are respectively 233.9 mils and 975.0 inch-pounds. The deviations of *X* and *Y* from their averages are listed for each observation, and these are used to calculate values of the statistics S_{XX}, S_{YY}, and S_{XY}. The least squares estimates of the slope and intercept are calculated, resulting in the estimated model equation giving fitted values $\hat{Y}_i$=-569.47+6.898 X_i, and these values are listed for each observation. The residuals e_i=Y_i=$\hat{Y}_i$ are also listed for each observation. Estimates of the variance and standard deviation of the *Y* distribution are calculated from squares of the residuals. The estimated standard deviation is 99.90 inch-pounds.

6.2.7.3 The least squares straight line is depicted with the scatter plot in Fig. ~~3~~4, and indicates that a straight line model appears to give a reasonable fit to this data set. Some additional comments from Table 1 are:

(1) The least squares estimated model equation is *Y* = –569.47 + 6.898 *X*. Clearly the negative intercept is not a plausible value for shear strength. This is apparently due to the fact that the data are so far removed from the origin (0, ~~0). It is~~ 0) that the estimate is poorly defined. It is also possible that there is some nonlinear behavior in the relationship approaching the origin.

(2) The averages of the deviations of *X* and *Y* from their averages are zero, and the average of the residuals are zero. These results follow from the property that sums of deviations from averages are zero.

(3) The average of the fitted values, $\hat{Y}_i$ ~~of~~, ~~Y~~is the same as the average of the *Y* data.

6.3 *Evaluation of the Model:*

6.3.1 This section discusses model evaluation through measures of association and plots of the residuals to check for departures from the model assumptions and the presence of data outliers.

6.3.2 *Measures of Association Between X and Y:*

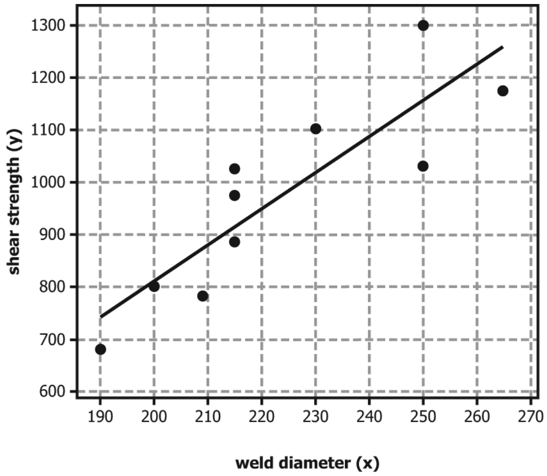


FIG. ~~3~~4 Scatter Plot of Data with Fitted Linear Model