TREND REMOVAL IN SOIL PROPERTY

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Abstract: It is often that trend in the form of linear or curvature appears in soil properties. Trend removal is necessary in many engineering applications where the residuals obtained would be used for further analyses. If trend in the data is not removed, a larger inherent soil variability compare to the actual one would be obtained. In this paper, a guideline relates the necessity of trend removal to the magnitude of \( R^2 \) (coefficient of determination) is established. A parametric study is also done in order to investigate the effect of trend removal on the accuracy of standard deviation.

Keywords: Soil properties; trend removal; standard deviation

1.0 Introduction

Soil is a geological material formed by various processes and subject to different stresses, pore fluids, physical changes and chemical changes. Thus, there is considerable variability in soil properties. The variability not only exists from site to site, but even within apparently homogeneous deposits at a single site (Baecher and Christian, 2003). The natural variation exhibits in soils from one location to another as a result of the myriad and complex processes that form them is known as spatial variability (Jaksa et al., 1997). The spatial variability of a soil property could happen in the vertical direction (‘down-the-hole’) and horizontal direction (‘parallel-to-the-ground’). A certain trend might also appear in the soil property if the data are extracted from a homogeneous soil layer. For example, a soil profile that displays an increasing trend with depth is shown in Figure 1. The trend could be a straight-line (Figure 1a) or a line with curvature (Figure 1b).
The spatial variability of a soil property can be separated into two parts: (a) trend function and (b) fluctuating component. Hence, a statistical model that is used to describe the spatial variability of the soil property at location $x$ can be written as

$$z(x) = t(x) + u(x),$$

(1)
where \( z(x) \) is the soil property, \( t(x) \) is a trend function formed by a polynomial function and \( u(x) \) is the fluctuating component formed by the residual. The fluctuating component is assumed to be a stationary random variable with zero mean and constant variance (Baecher and Christian, 2003; Phoon et al., 2003).

In many engineering applications, the trend in the data is removed and the residuals are used for further analyses. The statistical analysis performed on detrended data (i.e. residuals) provides a result that is valid and has higher accuracy. For instance, the statistical parameters such as standard deviation, coefficient of variation and scale of fluctuation are used to describe the inherent soil variability. If the trend in the data is not removed, then a larger inherent soil variability compare to the actual one would be obtained (Phoon and Kulhawy, 1999; Phoon et al., 2003). Hence, trend removal is necessary in order to obtain the statistical parameters that are well represented the soil variability. In addition, geostatistical and random field analyses are also facilitated by the data being stationary (Jaksa et al., 1997). By removing the trend in the data, the residual obtained should represent a stationary data set. The residual would then be used for further geostatistical and random field analyses.

In geotechnical engineering, the trend function formed by low-order polynomial function using regression analysis based on the method of ordinary least squares (OLS) was widely used. The trend estimation with polynomial up to the order of 2 is predominant and recommended (Lumb, 1974; Asaoka and A-Grivas, 1982; Ravi, 1992; Jaksa et al., 1997; Cafaro and Cherubini, 2002; Uzielli et al., 2005). A polynomial function with order 1 represents a straight-line relationship between the soil property and depth while a polynomial function with order 2 represents a relationship with curvature. Trend function that is formed by polynomial function with order 1 and order 2 can be expressed as Equations (2) and (3), respectively.

\[
t(x) = \beta_0 + \beta_1 x \quad (2)
\]

\[
t(x) = \beta_0 + \beta_1 x + \beta_2 x^2 \quad (3)
\]

The examples of the straight-line trend function \((t(x) = \beta_0 + \beta_1 x)\) and trend function with curvature \((t(x) = \beta_0 + \beta_1 x + \beta_2 x^2)\) are given in Figure 1a and 1b, respectively.
The coefficient of determination ($R^2$) is a statistical measure that is commonly used to show how well is the trend function fitted to the data (Jaksa et al., 1997;). The $R^2$ is ranging from 0 to 1. $R^2 = 0$ implies a complete lack of fit of the model to the data while $R^2 = 1$ implies a perfect fit, with the model passing through every data point (Mendenhall and Sincich, 2003).

As discussed previously, trend removal is necessary in many engineering applications. Trend removal is deemed important for a data set where its trend function is associated with a large $R^2$. On the other hand, the necessity of trend removal becomes relatively low if a data set having a trend function with small $R^2$. In most studies, how large or how small of the values of $R^2$ is remained subjective.

In general, the larger the value of $R^2$, the better the trend function fits the data. However, we can hardly find a deterministic guideline on the magnitude of $R^2$ that implies a well-fitted model. Should it be $R^2 > 0.5$, or $R^2 > 0.7$, or $R^2 > 0.9$, or some other ranges? Therefore, it is found that the interpretation on the $R^2$ is quite subjective. The element of subjectivity leads to the ambiguity in determining whether the trend function really well-fits the data. In order to solve this ambiguity, a guideline related to the magnitude of $R^2$ is established and it is presented in this paper. This guideline on the magnitude of $R^2$ would directly imply the necessity of trend removal of a data set.

2.0 The Relationship between the $R^2$ and the F-test

Firstly, the relationship between the $R^2$ and the F-test is studied. Both of $R^2$ and F-test are usually used to check the usefulness of a regression model. In many applications, a linear regression model, $y = \beta_0 + \beta_1 x_1 + ... + \beta_k x_k + \epsilon$, is used to predict the dependent variable ‘$y$’ from $k$ independent variables, $x_1, x_2, ..., x_k$. Note that $\epsilon$ is the error term in the model. Once the model is shown to be statistically useful, the model can be used for prediction.
2.1 The F-test

The F-test is a test of utility of the model, that is a test to determine whether the model is adequate for predicting ‘y’ (Ryan, 1997; Mendenhall and Sincich, 2003). The regression model is said to be statistically useful at the significance level $\alpha = 5\%$ if the test statistic of the F-test, a $F$ statistic, is greater than a critical value, $F_{0.05,k,n-k-1}$. In short, the hypothesis test can be summarized as follows:

Hypothesis: $H_0 : \beta_1 = \beta_2 = \ldots \beta_k = 0$

$H_1 : \text{At least one } \beta_i \neq 0$

Test statistic: $F = \frac{(SST - SSE) / k}{SSE / (n - k - 1)}$, where $n$, $k$, $SST$ and $SSE$ refer to the sample size, number of independent variables in the model, total sum of squares and sum of squares of errors

Conclusion: If $F > F_{0.05,k,n-k-1}$, the regression model is said to be statistically useful at $\alpha = 5\%$. Or else, the regression model is not statistically useful.

2.2 The Derivation of the Relationship between $R^2$ and F Statistic

The coefficient of determination, $R^2$, is a measure of how well a model fits a set of data. $R^2$ is defined as

$$R^2 = \frac{SST - SSE}{SST}.$$  (4)

Based on the definition of $F$ statistic and $R^2$, it is found that there is a relationship between the $R^2$ and $F$ statistic, that is:

$$F = \frac{(SST - SSE) / k}{SSE / (n - k - 1)}$$

$$= \left( \frac{SST - SSE}{SST} \right) / k$$

$$= \frac{SSE / SST}{1} / (n - k - 1)$$

$$= \frac{R^2 / k}{(1 - R^2) / (n - k - 1)}.$$  (5)
In F-test, the regression model is said to be statistically useful at \( \alpha = 5\% \) if \( F > F_{0.05,k,n-k-1} \). Or else, the regression model is not statistically useful. Hence, F-test is able to give us a deterministic conclusion based on a rejection condition that involves the critical value \( F_{0.05,k,n-k-1} \).

Therefore, by using the relationship in Equation (5), we may obtain an equivalent critical value of \( R^2 \), say \( R_0^2 \), that give us same conclusion in F-test. That is, the regression model is said to be statistically useful at \( \alpha = 5\% \) if \( R^2 > R_0^2 \). Or else, the regression model is not statistically useful if \( R^2 < R_0^2 \).

The expression of \( R_0^2 \) in \( R^2 > R_0^2 \), that corresponds to \( F > F_{0.05,k,n-k-1} \), is derived as follows:

\[
F > F_{0.05,k,n-k-1}
\]

\[
\frac{R^2}k > \frac{(n-k-1)R^2}{1-R^2}\frac{(1-R^2)/(n-k-1)} > F_{0.05,k,n-k-1}
\]

\[
(n-k-1)R^2 > k F_{0.05,k,n-k-1}(1-R^2)
\]

\[
(n-k-1)R^2 > k F_{0.05,k,n-k-1} - (k F_{0.05,k,n-k-1})R^2
\]

\[
(n-k-1)R^2 + (k F_{0.05,k,n-k-1})R^2 > k F_{0.05,k,n-k-1}
\]

\[
(n-k-1+k F_{0.05,k,n-k-1})R^2 > k F_{0.05,k,n-k-1}
\]

\[
R^2 > \frac{k F_{0.05,k,n-k-1}}{n-k-1+k F_{0.05,k,n-k-1}}
\]

where \( R_0^2 = \frac{k F_{0.05,k,n-k-1}}{n-k-1+k F_{0.05,k,n-k-1}} \).

(a) Case 1: A Linear Regression Model with an Independent Variable

A linear regression model with an independent variable \( k = 1 \) can be written as \( y = \beta_0 + \beta_1 x + \epsilon \).

We may use F statistic in F-test to check whether the regression model is statistically useful. As an alternative, we may also obtain same conclusion by evaluating the value of \( R^2 \). From Equation (6) (using \( k = 1 \), the regression
model is said to be statistically useful at $\alpha = 5\%$ if $R^2 > R^2_0$, where
\[
R^2_0 = \frac{F_{0.05,1,n-2}}{n - 2 + F_{0.05,1,n-2}}.
\]

It is observed that the critical value, $R^2_0$, depends on the sample size $n$. The values of $R^2_0$ for different sample size $n$ are tabulated in the Table 1.

Table 1: The critical value ($R^2_0$) for linear model $y = \beta_0 + \beta_1 x + \varepsilon$

<table>
<thead>
<tr>
<th>Sample size, $n$</th>
<th>Critical value, $R^2_0$</th>
<th>The model is statistically useful at $\alpha = 5%$ if $R^2 &gt; R^2_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.20</td>
<td>$R^2 &gt; 0.20$</td>
</tr>
<tr>
<td>30</td>
<td>0.13</td>
<td>$R^2 &gt; 0.13$</td>
</tr>
<tr>
<td>40</td>
<td>0.10</td>
<td>$R^2 &gt; 0.10$</td>
</tr>
<tr>
<td>50</td>
<td>0.08</td>
<td>$R^2 &gt; 0.08$</td>
</tr>
</tbody>
</table>

For instance, a linear regression model ($y = \beta_0 + \beta_1 x + \varepsilon$) with sample size $n = 50$ is statistically useful at $\alpha = 5\%$ when $F > F_{0.05,1,48} = 4.04$ by using $F$-test. Equivalently, if its $R^2 > 0.08$ (refer Table 1), then we may obtain same conclusion in $F$-test, i.e. the model is statistically useful at $\alpha = 5\%$. Hence, Table 1 can be used as a guideline for $R^2$ to check the usefulness of the linear regression model with an independent variable.

A graph of $p$-value of $F$-test versus $R^2$ for a sample size of $n = 50$ is given in Figure 2. We can see that the $p$-value < 0.05 when $R^2 > 0.08$, implying the linear regression model is statistically useful at $\alpha = 5\%$.
Figure 2: Graph of $p$-value of $F$-test versus $R^2$ for a linear regression model ($y = \beta_0 + \beta_1 x + \varepsilon$) with sample size of $n = 50$

(b) Case 2: A Quadratic Model

The linear regression model, $y = \beta_0 + \beta_1 x + \varepsilon$, represents a straight-line relationship between ‘$y$’ and ‘$x$’. On the other hand, a quadratic model, $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$, represents a relationship with curvature. In this quadratic model, $k = 2$.

The corresponding values of $R_0^2 = \frac{2 F_{0.05, 2, n-3}}{n-3 + 2 F_{0.05, 2, n-3}}$ for different sample size $n$ are tabulated in the Table 2.
Table 2. The critical value ($R^2_0$) for quadratic model $y = \beta_0 + \beta_1x + \beta_2x^2 + \varepsilon$

<table>
<thead>
<tr>
<th>Sample size, $n$</th>
<th>Critical value, $R^2_0$</th>
<th>The model is statistically useful at $\alpha = 5%$ if $R^2 &gt; R^2_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.30</td>
<td>$R^2 &gt; 0.30$</td>
</tr>
<tr>
<td>30</td>
<td>0.20</td>
<td>$R^2 &gt; 0.20$</td>
</tr>
<tr>
<td>40</td>
<td>0.15</td>
<td>$R^2 &gt; 0.15$</td>
</tr>
<tr>
<td>50</td>
<td>0.12</td>
<td>$R^2 &gt; 0.12$</td>
</tr>
</tbody>
</table>

(c) The Summary of the Critical Value, $R^2_0$

Refer to Table 1, a linear regression model $y = \beta_0 + \beta_1x + \varepsilon$ where the sample size is $n = 30$, $n = 40$ and $n = 50$ is said to be statistically useful at $\alpha = 5\%$ if $R^2 > 0.13$, $R^2 > 0.10$ and $R^2 > 0.08$, respectively. A statistical rule-of-thumb always suggest that a sample size of at least $n = 30$ should be used so that the sample is large enough to represent the population. Therefore, we may conclude that, for a data set with sample size of $n \geq 30$, a linear regression model $y = \beta_0 + \beta_1x + \varepsilon$ with $R^2 > 0.13$ is said to be statistically useful at $\alpha = 5\%$.

Similarly, we may see from Table 2 that, for a data set with sample size of $n \geq 30$, a quadratic model $y = \beta_0 + \beta_1x + \beta_2x^2 + \varepsilon$ with $R^2 > 0.20$ is said to be statistically useful at $\alpha = 5\%$.

In previous discussion, it is stated that the trend estimation with polynomial function up to the order of 2 is predominant and recommended in geotechnical engineering. Hence, the trend functions $t(x) = \beta_0 + \beta_1x$ (Equation 2) and $t(x) = \beta_0 + \beta_1x + \beta_2x^2$ (Equation 3) are frequently used. Therefore, based on the study on the critical value, $R^2_0$, a guideline can be established as follows:

When a trend function has $R^2 > 0.20$, we may safely say that the trend function is statistically useful at $\alpha = 5\%$ regardless the trend function is formed by polynomial of order 1 or order 2. Hence, trend removal is necessary and the residuals obtained should be used for further analyses in applications. Or else, trend removal is not necessary.
3.0 The Effect on Trend Removal: A Parametric Study

It is noted that when trend removal is not performed on a data set where trend is shown to be significant, larger variability will be reflected in the statistical parameters such as standard deviation, coefficient of variation (COV) and scale of fluctuation. Hence, a certain amount of error would occur in these statistical parameters that are obtained from the raw data compare to the statistical parameters obtained from the data set where proper trend removal is done.

However, a question is raised here: how large is the error that would occur? If the error can still be tolerated and ignored, then necessity on trend removal is not very high. Or else, proper trend removal should be performed and further analyses are to be done using the residuals.

Again, the significance of the trend that exhibits in the data set is represented by $R^2$ of the trend function. Hence, the necessity of trend removal would depend on how significance of the trend (i.e. how large is the $R^2$ of the trend function) and how large of the error that can be tolerated and ignored. Hence, these two elements are studied in this section by using numerous data sets generated from different scenarios.

3.1 Soil Profile with different Slopes

It is learned that the definition of $R^2$ can be written as

$$R^2 = \frac{SST - SSE}{SST} = \frac{\sum_{i=1}^{n} (y_i - \bar{y})^2 - \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}, \quad (7)$$

where $\bar{y}$, $y_i$ and $\hat{y}_i$ refers to the sample mean, $i$-th observed value and $i$-th predicted value, respectively.

Taking an example of soil property in vertical direction, when trend is not significant in the profile, the soil property exhibits a constant profile along depth. Figure 3 gives an example of soil property exhibiting constant profile with sample mean = 10.
In this situation, the sample mean would be best used to predict any value along the depth. Therefore, we may say that \( \hat{y}_i = \bar{y} \). Considering \( \hat{y}_i = \bar{y} \) in Equation (7), we can obtain \( R^2 = 0 \).

In another word, when trend is truly not significant (possessing constant profile), \( R^2 = 0 \). Hence, a larger value of \( R^2 \) (any \( R^2 > 0 \)) is expected when trend exists in the soil profile. Hence, a linear trend that is represented by a straight-line with slope would have \( R^2 > 0 \). Figure 3 presents examples of soil property having linear trend with different slopes (slope = 0.06, 0.2, 0.4).

![Figure 3: Soil property in vertical direction: data set with constant profile where its sample mean = 10; data sets having linear trend with different slopes (slope = 0.06, 0.2, 0.4)](image-url)
3.2 The Characteristics of the Simulated Data

In this study, numerous data sets are generated. The data sets have COV ranging from 0.05 to 0.3. COV is obtained by normalizing the standard deviation with respect to the mean of the observations, that is \( \text{COV} = \frac{\text{standard deviation}}{\text{mean}} \). COV is a dimensionless quantity and perceived as an almost universal parameter in representing the variability of soil property. It is noted that if the variable resembles the theoretical normal distribution, a COV of 0.3 implies that the variable can take values that are 90 – 100% lower or higher than the mean value (Lacasse and Nadim, 1996). The variability presents in the data where its values covering this range is considerably very large. Hence, COV of 0.3 is chosen as the largest COV for the data sets in this study.

The following data sets (with sample size of \( n = 50 \)) representing constant profile are first generated from normal random numbers:

(i) \( \text{COV} = 0.05, \text{mean} = 10, \text{standard deviation} = 0.5 \)
(ii) \( \text{COV} = 0.1, \text{mean} = 10, \text{standard deviation} = 1 \)
(iii) \( \text{COV} = 0.2, \text{mean} = 10, \text{standard deviation} = 2 \)
(iv) \( \text{COV} = 0.3, \text{mean} = 10, \text{standard deviation} = 3 \)

As discussed in Section 3.1, a data set with constant profile (trend is truly not significant) has \( R^2 = 0 \) while a larger value of \( R^2 \) (any \( R^2 > 0 \)) is expected when trend exists in the data set. In this study, the effect of different values of \( R^2 \) is of interest. Hence, data sets with linear trend of different slopes are further generated.

From each of the 4 generated constant profiles (i – iv), different slopes are imposed on these data in order to obtain data sets with linear trend of different slopes. Hence, data sets with linear trend \( t(x) = \beta_0 + \beta_1 x \) are generated, where \( \beta_0 = 10 \) but various values are assigned to \( \beta_1 \). Some examples of data sets having linear trend with different slopes (\( \beta_1 \)) is shown in Figure 2. We can see that data set with larger magnitude of slope possessing a trend that is more obvious and can be observed through eyes. Hence, the effect of this trend should not be neglected.
3.3 The Relationship between the Slope of Trend Line and $R^2$

A graph showing the relationship between the slope of linear trend line and $R^2$ is given in Figure 4. It is observed that, a trend line having a larger magnitude of slope would have larger $R^2$. For example, in the data sets where COV = 0.05, the trend line with slope of 0.03 has $R^2 = 0.2$ while the trend line with slope of 0.06 has larger $R^2$, that is $R^2 = 0.5$ (Figure 4). Furthermore, a larger magnitude in the slope would directly imply that the inclined angle for the linear trend line is bigger and hence the trend becomes ‘considerably obvious’ (Figure 5). Figure 5 showing the cases for COV = 0.05 and COV = 0.3.

From the relationship between the slope of linear trend and $R^2$, we can see that a larger $R^2$ could imply that the data set having a ‘considerably obvious’ trend (larger magnitude of slope). The effect of this ‘considerably obvious’ trend should be taken into account and the necessity of trend removal should be studied. In the following section, the effect of trend removal will be evaluated quantitatively based on the error produced in standard deviation of the data set.

![Graph of slope of linear trend line versus $R^2$.](image)

Note: $p$-value from $F$-test:

- $p$-value $> 0.05$
- $p$-value $< 0.05$
Figure 5: Graph of inclined angle versus $R^2$ for (a) COV = 0.05, (b) COV = 0.3 and (c) an example showing linear trend line with inclined angle = 3.4° and 11°
3.4 Relative Error of Standard Deviation versus $R^2$

When linear trend ($t(x) = \beta_0 + \beta_1 x$) exists in the data set, proper trend removal should be performed. The linear trend function should be fitted to the data using regression analysis based on the method of ordinary least squares (OLS). Then, the residuals ($u(x)$) as given in $z(x) = t(x) + u(x)$ (Equation 1) are obtained. The standard deviation of the residuals ($s_0$) is used to reflect the variability of the data set.

However, many people might neglect the importance of proper trend removal. Hence, in the case where trend removal is not done, the standard deviation of the raw data set ($s$) is used. The magnitude of $s$ is usually larger than $s_0$.

In order to evaluate the error in standard deviation that is produced from the case where trend removal was not done, the relative error of standard deviation is defined as $\frac{s - s_0}{s_0} \times 100\%$.

In addition, the $R^2$ associated with the trend line is produced. A graph of the relative error of standard deviation versus $R^2$ is given in Figure 5.

It is observed that small amount of error in standard deviation is occurred when the $R^2$ of the trend line is small. However, the error becomes larger when $R^2$ increases. As discussed in Section 3.3, a large $R^2$ implies that the data set having a ‘considerably obvious’ trend. Therefore, when the ‘considerably obvious’ trend is not removed, a large error would occur in the standard deviation obtained from data where trend removal is not performed. In this case, the said standard deviation would not reflect the true variability of the property that is of interest.

In general, the relationship between the relative error in standard deviation and $R^2$ is quite consistent regardless of different values of COV, as shown in Figure 6.
Figure 6: Graph of relative error of standard deviation versus $R^2$
From Figure 6, the general relationship between the relative error in standard deviation and $R^2$ of linear trend line is tabulated in Table 3.

Table 3: The relationship between the relative error in standard deviation and $R^2$ of linear trend line

<table>
<thead>
<tr>
<th>$R^2$</th>
<th>Relative error in standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>5%</td>
</tr>
<tr>
<td>0.2</td>
<td>10%</td>
</tr>
<tr>
<td>0.3</td>
<td>20%</td>
</tr>
<tr>
<td>0.4</td>
<td>30%</td>
</tr>
<tr>
<td>0.5</td>
<td>40%</td>
</tr>
</tbody>
</table>

We can see that 5% of error occurred in standard deviation when the linear trend line with $R^2 = 0.1$ is not removed. The error increases to 10% when the linear trend line with $R^2 = 0.2$ is not removed. The error keeps on increase for larger $R^2$.

In addition, the standard deviation obtained from data set where trend removal is not performed is always larger than the actual standard deviation that is reflected in residuals. Therefore, the probability density distribution (p.d.f.) for the data set for the larger standard deviation always has longer tails than the p.d.f. for the residuals. Figure 7 shows the comparison between the p.d.f. of these data sets where trend removal is not performed and the p.d.f. of the residuals. For comparison purpose, the p.d.f. are superimposed and aligned at mean.

Based on the general relationship between the relative error in standard deviation and $R^2$ of linear trend line, if 10% is the largest tolerated or acceptable error in practice, the following conclusion is obtained:

Trend removal should be performed on data set having linear trend line with $R^2$ higher than 0.2. In another word, linear trend line with $R^2 > 0.2$ is considered significant enough to bring large effect on the statistical parameter such as standard deviation.
COV = 0.2

Figure 7: Comparison between the p.d.f. of data sets where trend removal is not performed and the p.d.f. of the residuals

4.0 Conclusion

In this paper, a guideline on using $R^2$ to evaluate the necessity of trend removal is established. Furthermore, the effect on trend removal is also discussed using a parametric study. These could serve as reference for readers when dealing with data with trend.

References


