2. How to Properly Test for U- and S-Shaped Relationships?

2.1. Testing for U

As mentioned, many hypotheses in tourism and hospitality focus on U (or inverted U)-shaped relationships (e.g. Park and Lee, 2009; Jang and Tang, 2009; Chen et al. 2012; Chen and Lin, 2015, among others). Theorizing a U-shaped relationship simple requires that "the dependent variable Y first decreases with the independent variable X at a decreasing rate to reach a minimum, after which Y increases at an increasing rate as X continues to rise" (Hans et al. 2016, p. 1178). The opposite is true for the inverted U.

Unfortunately, most studies in tourism and hospitality do not properly test for U (or inverted U) -shaped relationships. The common trend, for instance, is to estimate a model like:

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 \tag{4}$$

where the independent variables include both X and its square. For β_2 that is negative and significant, studies tend to accept an inverted U-shaped relationship between X and for β_2 that is positive and significant studies tend to accept a U-shaped relationship.

Unfortunately, we argue that while this is important, it is never sufficient for accepting a U (or inverted U) -shaped relationships (Lind and Mehlum, 2010; Hans et al. 2016). For instance, the sign and significance of β_2 is only one of the three steps required to confirm a U (or inverted U) -shaped relationships. For proper testing, one also needs the slope to be steep enough at both tails of the data range (Hans et al. 2016). For instance, the marginal effect (ME) for the model in (4) is:

$$ME = \frac{\partial Y}{\partial X} = \beta_1 + 2\beta_2 X \tag{5}$$

and the turning point of the curve:

$$\frac{\partial Y}{\partial X} = 0 \Rightarrow X^* = -\frac{\beta_1}{2\beta_2} \tag{7}$$

If β_1 or β_2 are insignificant there could be no optimum (U-shaped or inverted U-shaped relationships)[1]. To have a U-shaped relationship we need: $\beta_2 > 0$, and also :

$$X_L < X^* < X_U \tag{8}$$

[1] If β_2 is insignificant we have a problem as the denominator is zero and b1/b2 follows asymptotically a Cauchy distribution

where X_L and X_U are the lower and upper end of the X -range. For a proper testing for a U (or inverted U) -shaped relationships one also needs to test whether the slope at both X_L and X_U is significant. For instance, using (8) we have:

$$X_L < -\frac{\beta_1}{2\beta_2} < X_U \Leftrightarrow 2\beta_2 X_L < -\beta_1 < 2\beta_2 X_U \Leftrightarrow -2\beta_2 X_L > \beta_1 > -2\beta_2 X_U$$

or

$$\beta_1 + 2\beta_2 X_L < 0 \tag{9}$$

$$\beta_1 + 2\beta_2 X_U > 0 \tag{10}$$

Hence, the left hand side of both (9) and (10) need also to be significant. The same process for the inverted-U. We need $\beta_2 < 0$, and also:

$$\beta_1 + 2\beta_2 X_L > 0 \tag{11}$$

$$\beta_1 + 2\beta_2 X_U < 0 \tag{12}$$

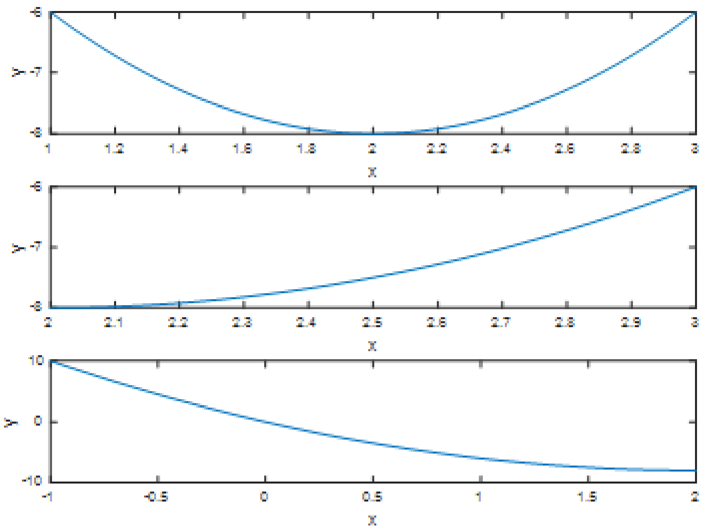
Finally, along with above, we also need to confirm that $-\frac{\beta_1}{2\beta_2}$ is within the range of the data. The same applies for inverted-U-shape. Hence, to sum up, to confirm a U-shape relationship, we need $\beta_2 > 0$, (9) and (10) to be significant, and $-\frac{\beta_1}{2\beta_2}$ within the range of the data. To confirm an inverted U-shape, we need $\beta_2 < 0$, the left hand side of (11) and (12) to be significant, and $-\frac{\beta_1}{2\beta_2}$ within the range of the data. To confirm that $-\frac{\beta_1}{2\beta_2}$ is within the range of data, one can construct a confidence interval for this term, and check whether this confidence interval is within the data range.

We show in Figure 1 an example of a true U-shaped relationship. The second and third graph of this Figure show a failed U-shaped when the domain of the data is to the right and left of the minimum, respectively. We truly recommend drawing the $X - Y$ relationship over the relevant range of X to clearly illustrate and confirm the shape the relationship. Hans et al. (2016) further recommended further important robustness checks to confirm the quadratic shape of the model in (4). For example, one can split the data on the turning point and estimate two separate regressions, and then validate whether the slope of these regressions are consistent with the U (or inverted U) shape of the curve. For example, the regression on the data before the turning point should provide a negative relationship between X and Y, and the one after the turning point should provide a positive relationship between X and Y [2].

[2] This procedure does not however guarantee statistical efficiency and one needs to have a large sample.

Some other robustness check may include confirming the existence of the U-shaped relationship using flexible methods such as non-parametric regression prior to estimating the traditional regression in (3). We also recommend conducting the proper specification tests to confirm the non-linear shape of the model in (4)[3]. Finally, it is also important to check for the endogeneity problem due the potential reverse causality problem between X and Y, which may lead to spurious regression and incorrect conclusion about the true shape of the relationship between X and Y. We discuss this issue in more detail in later sections of the paper.

Figure 1. Different Cases of a U-Shaped Relationship



2.2. Testing for S

Many studies go beyond the traditional U-shaped relationship and test for S-shaped relationship between X and Y (Lu and Beamish, 2004). This can be done by adding the cubic term of X to the model in (4).

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 \tag{13}$$

Most studies test for S-Shape (e.g. Lu and Beamish, 2004) by checking whether the relationship is negative at low level of X (i.e. $\beta_1 < 0$), positive at medium level of X (i.e. $\beta_2 > 0$), and negative again at high level of X ($\beta_3 < 0$). However, we argue that such approach has its limitations. For a more complete and accurate testing, one would need to follow the same approach described in 2.1. To illustrate, the marginal effect for the model in (13) is:

$$ME = \frac{\partial Y}{\partial X} = \beta_1 + 2\beta_2 X + 3\beta_3 X^2 \tag{14}$$

[3] For details, see Assaf and Tsionas (2019).

and the curvature is:

$$\frac{\partial^2 Y}{\partial X^2} = 2\beta_2 + 6\beta_3 X \tag{15}$$

Setting (14) to zero and solving for X, in order to have S-shape we need two distinct roots. The discriminant of this quadratic is:

$$\Delta = 4\beta_2^2 - 12\beta_1\beta_3 = 4\left(\beta_2^2 - 3\beta_1\beta_3\right) \tag{16}$$

If $\beta_2^2 - 3\beta_1\beta_3 = 0$ is true, then we do not have two distinct roots. If $\Delta < 0$, then we do not have any root at all. So, we recommend a confidence interval for $\beta_2^2 - 3\beta_1\beta_3$. Suppose now that $\Delta < 0$, so there is a possibility of S-shape.

The roots are:

$$X_{1,2}^* = \frac{-\beta_2 \pm \sqrt{\beta_2^2 - 3\beta_1\beta_3}}{3\beta_3} \tag{17}$$

$$\left.\frac{\partial^2 y}{\partial X^2}\right|_{X = X_1^*} = 2\left(\beta_2 + 3\beta_3 X_1^*\right) \tag{18}$$

$$\left.\frac{\partial y}{\partial X^2}\right|_{X = X_2^*} = 2\left(\beta_2 + 3\beta_3 X_2^*\right) \tag{19}$$

Suppose that $X_1^* < X_2^*$ so that we have a minimum at X_1^* and a maximum at X_2^*. So, we need:

i) First, $\beta_2^2 - 3\beta_1\beta_3 > 0$ so that we have two distinct roots.

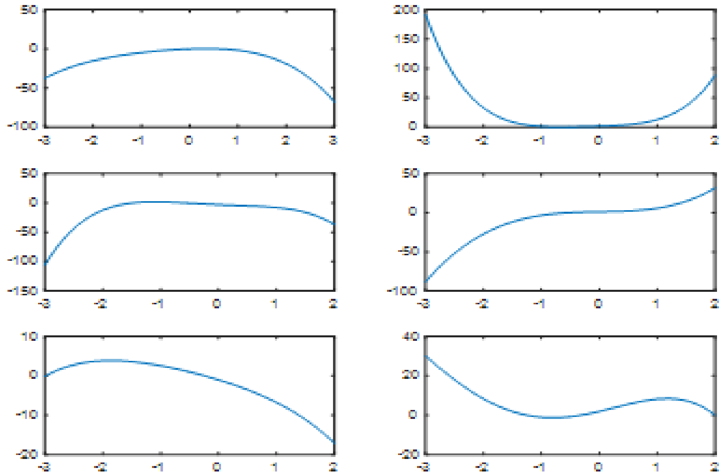
ii) Evaluating $\frac{\partial^2 y}{\partial X^2}$ at the two roots we obtain: $2\left(\beta_2 + 3\beta_3 X^*\right)$. Manipulating the expression for the two roots we have: $\beta_2 + 3\beta_3 X^* = \pm 2\sqrt{\beta_2^2 - 3\beta_1\beta_3}$ so, the second derivative is positive at X_1^* and negative at X_2^*, giving us a minimum and maximum respectively.

iii) The difference between the two roots is $X_2^* - X_1^* = \frac{-2\sqrt{\beta_2^2 - 3\beta_1\beta_3}}{3\beta_3} > 0 \Leftrightarrow \beta_3 < 0.$

iv) So, the idea of simply having $\beta_3 < 0$ and $\beta_1 > 0$ is not sufficient and more restrictive than necessary. In reality however, we need $\beta_3 < 0$ and $\beta_2^2 > 3\beta_1\beta_3$. If $\beta_1 > 0$ this will certainly happen but, in fact, it can happen even with $\beta_1 < 0$ provided $\beta_2^2 > 3\beta_1\beta_3$.

Therefore, for S-shape, we need $\beta_3 < 0$, $\beta_2^2 > 3\beta_1\beta_3$, $X_1^* \geq X_L, X_2^* \leq X_U$. These place nonlinear restrictions among the coefficients which are hard to test. Figure 2, for example, presents various example of a S-relationship. Only the last case of this figure represents a true S relationship while the others fail some of the conditions discussed above.

Figure 2. Different Cases of a S-Shaped Relationship



3. Testing for Moderating Effects with U and S

3.1. Moderating with a U-shaped Relationship

As mentioned, the use of moderating variables is highly common in tourism and hospitality research. However, it is astonishing that most studies do not properly test for moderation in the presence of non-linear relationships such as U or S. For instance, let us assume we have the following U-shaped relationship:

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 Z + \beta_4 XZ + \beta_5 X^2 Z \qquad (20)$$

where the model is similar to (4) but now we have one moderator Z that affects the relationship between X and Y. Also note that the moderator in (20) is multiplied by both by X and its square term. In the presence of a U-shaped relationship, we argue that this is the correct and more complete thing to do.

Studies in the field seem to be taking one of these three different approaches to handle moderation with non-linear effect (i.e. U or S):

1- Testing for shape and moderation separately. For instance, estimating a model like (4) to test for a U (or inverted U)-shaped relationship between X and Y, and then a separate model like : $Y = \beta_0 + \beta_1 X + \beta_3 Z + \beta_4 XZ$ to test for moderating effect.

2- Estimating a simplified version of model in (20) through excluding the term $X^2 Z$ from the model. Hence, using a model such as: $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 Z + \beta_4 XZ$.

3- Estimating the model in (20), but not fully exploiting the moderating effect of Z. For instance, it is common for studies to state that Z affects the curvilinear relationship between X and Y without providing any insight about the nature of this moderation.

We argue that each of the three approaches above is potentially problematic. The first approach, for instance, is contradicting the theoretical proposition that X and Y follow a U (or inverted U)-shaped relationship. In other words, if a U-shaped has been theoretically supported in the model, then the moderating effect needs to also to be present in the full model in (20).

The second approach is also missing some important moderating effects. For example, β_4 only represents the moderating effect on the marginal effect of X. For example, using $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 Z + \beta_4 XZ$, the marginal effect is $\frac{\partial Y}{\partial X} = \beta_1 + 2\beta_2 X + \beta_4 Z$, and the moderating effect is $\frac{\partial^2 y}{\partial X \partial Z} = \beta_4$, which is simply a constant. The decision to remove the term $X^2 Z$ should be theoretically and empirically supported (e.g. the term is not significant).

The third approach is certainly the most complete, but simply stating that the moderator affects the curvilinear relationship is vague and not sufficient. One needs for instance to hypothesize and test the nature of this moderation, which can be due to two effects. For example, is this moderation due to a shift of the turning point of the U-shaped relationship, or it due to flattening or steepening of the curve? Each of these moderations is theoretically and empirically different (Hans et al. 2016).

Unfortunately, it is rare to see any study in tourism and hospitality hypothesizing any of these of these two moderation effects. Other fields of study such as strategy have more common mentioning of these effects (e.g. Henderson et al. 2006; Mihalache et al. 2012). For example, one can write a hypothesis like the following to state a steepening effect on the U-Shaped relationship:

H1: *The performance gap steepens the U-shaped relationship between learning and customer dissatisfaction*

or a hypothesis like the following to indicate a shift of the turning point:

H2: the negative impact of learning on customer dissatisfaction will occur earlier for luxury hotels than for economy hotels

To illustrate how to test for these two different moderating effects, we start with the marginal effect $\frac{\partial Y}{\partial X}$ for the model in (20), which can be written as:

$$\frac{\partial Y}{\partial X}=\beta_1+2\left(\beta_2+\beta_5 Z\right)X+\beta_4 Z \tag{21}$$

Setting $\frac{\partial y}{\partial X}=0$, and solving for X, we can obtain the turning point of the curve:

$$X^*=-\frac{\beta_1+\beta_4 Z}{2\left(\beta_2+\beta_5 Z\right)} \tag{22}$$

To test for U-shape in the presence of the moderator Z, the same process applies here, as described in 2.1. We need X^* to be a minimum which in the presence of the moderator implies: $\beta_2+\beta_5 Z>0$. For Inverted U-Shape, we need: $\beta_2+\beta_5 Z<0$. We must also have: $X_L<X^*<X_U$, i.e. $X_L<\frac{\beta_1+\beta_4 Z}{2\left(\beta_2+\beta_5 Z\right)}<X_U$. This condition yields, after some algebra:

$\beta_1+2\beta_2+(\beta_4+2\beta_5 X_U)Z>0,\ \beta_1-2\beta_2+(\beta_4-2\beta_5 X_L)Z>0.$ This condition should be easy to check at specific values of Z. What we need is to test the joint hypothesis:

$$\theta_1\equiv X_L+\frac{\beta_1+\beta_4 Z}{2\left(\beta_2+\beta_5 Z\right)}<0 \tag{23}$$

$$\theta_2\equiv X_U+\frac{\beta_1+\beta_4 Z}{2\left(\beta_2+\beta_5 Z\right)}>0$$ [4]

Turning Point Moderation

To test a hypothesis like H2, we need to examine how the turning point in (22) changes with the moderator Z. This can be done by taking the derivative of X^* with respect to Z :

$$\frac{\partial X^*}{\partial Z}=-\frac{1}{2}\frac{\partial}{\partial Z}\left(\frac{\beta_1+\beta_4 Z}{\beta_2+\beta_5 Z}\right) \tag{24}$$

Therefore, we have:

[4] Again, we have nonlinearities in the parameters, but an important point is that we need a joint confidence interval for θ_1 and θ_2 to test whether $\theta_1<0$, $\theta_2>0$. We can perhaps draw a large number of draws from the asymptotically normal distribution of β_1,β_2,β_4, β_5, evaluate θ_1 and θ_2 for each draw and present contours of their implied bivariate distribution.

$$\frac{\partial X^*}{\partial Z} = -\frac{1}{2}\frac{\beta_4\left(\beta_2+\beta_5 Z\right)-\beta_5\left(\beta_1+\beta_4 Z\right)}{\left(\beta_2+\beta_5 Z\right)^2}$$
$$= -\frac{1}{2}\frac{\beta_2\beta_4-\beta_1\beta_5}{\left(\beta_2+\beta_5 Z\right)^2} \tag{25}$$

So $\frac{\partial X^*}{\partial Z} > 0 \Leftrightarrow \beta_2\beta_4 - \beta_1\beta_5 < 0$ (26)

So when $\beta_2\beta_4 - \beta_1\beta_5 < 0$, as Z increases, the turning point X^* moves to the right, and when $\beta_2\beta_4 - \beta_1\beta_5 > 0$, the turning point will move to the left as Z increases.

As $\theta = \beta_2\beta_4 - \beta_1\beta_5$ is a single parameter we can use a confidence interval to see whether an increase in Z_1 moves the curve to the right or left, respectively.

Figure 4, for example, provides an example of a turning point moderation, where the upper panel different cases of U-shape or inverted-U shape as the moderating variable changes. We can see clearly that as the value of the moderator Z is increasing the turning point is moving to the right [5].

Flattening or Steepening Moderation

To examine a hypothesis like H1, which involves flattening or steepening moderation, Hans et al. (2016) recommended comparing the slope at two different turning points (X_1^* and X_2^*) for two specific values of the moderator $Z = Z_1$ and $Z = Z_2$, where $Z_1 < Z_2$ [6]. However, one can obtain their results in a far simpler way by deriving the curvature:

$$\frac{\partial^2 Y}{\partial X^2} = 2\left(\beta_2 + \beta_5 Z\right) \tag{27}$$

and then taking the partial derivative of (27) with respect to Z:

$$\frac{\partial}{\partial Z}\left(\frac{\partial^2 Y}{\partial X^2}\right) = 2\beta_5 \tag{28}$$

Therefore, for steepening, we simple need the coefficient of X^2Z, $\beta_5 < 0$, and for flattening, we need $\beta_5 > 0$ [7].

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[5] Of course, it is important to have the optimum in the range of the data.

[6] Specifically, Haans et al. (2016) proposed to compare the slopes S_1 and S_2 at points $X_1^* - h$ and $X_2^* - h$, where X_1^*, X_2^* correspond to the solutions when $Z = Z_1$ and $Z = Z_2$, and $h > 0$. If $S_2 > S_1$ then the inverted-U shape is steepening, and if $S_2 < S_1$ the inverted-U shape is flattening. As shown in their (A4.5) (p. 1195), this depends only on β_5 as we have shown in our equation (28) using a much simpler argument.

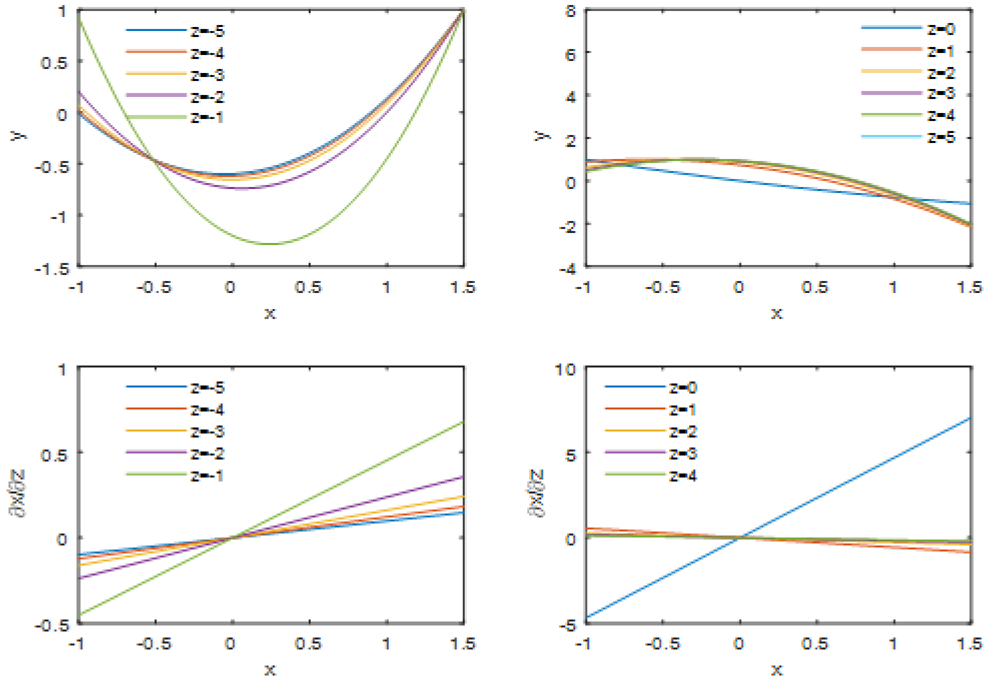
[7] Appendix 1 provides more details about using the curvature for flattening and steepening.

As an alternative approach one can also check whether:

$$\left.\frac{\partial^2 Y}{\partial X^2}\right|_{\substack{X=X_1^* \\ Z=Z_1}} > \left.\frac{\partial^2 Y}{\partial X^2}\right|_{\substack{X=X_2^* \\ Z=Z_2}} \qquad (29)$$

The argument is based on the rate of change of the first derivative which is much slower when $Z = Z_1$ compared to $Z = Z_2$.

Figure 4. Turning Point Moderation with U and Inverted U



3.2. Moderating with a S-shaped Relationship

When a study is hypothesizing a moderating effect on the S-relationship between X and Y, the model can be written as follows:

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \beta_4 X^2 + \beta_5 X^2 Z + \beta_6 X^3 + \beta_7 X^3 Z \tag{30}$$

In the case of S, we recommend interacting the moderator Z with both X^2 (as discussed in 3.1) and X^3. Again, any specification that is different from (30) require theoretical and empirical justification. For instance, the paper by Lu and Beamish (2004) tested a model of the following form: $Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \beta_4 X^2 + \beta_5 X^3$. Hence, they had the S-relationship but they only interacted the moderator with X. As discussed in Section 3.1, this only represents the moderating effect on the marginal effect of X. For instance, the marginal effect is $\frac{\partial Y}{\partial X} = \beta_1 + \beta_3 Z + 2\beta_4 X + 3\beta_5 X^2$, and the moderating effect is $\frac{\partial^2 y}{\partial X \partial Z} = \beta_3$, which is simply a constant[8].

To test for the presence of S-relationship in a model like (30) we follow the same approach as in Section 2.2. For instance, the marginal effect is:

$$\frac{\partial Y}{\partial X} = 3X^2\left(\beta_6 + \beta_7 Z\right) + 2X\left(\beta_4 + \beta_5 Z\right)X + \left(\beta_1 + \beta_3 Z\right) \tag{31}$$

For S-Shape (such as the las case of Figure 2) we need two roots of $\frac{\partial Y}{\partial X} = 0$. The discriminant of the second-order polynomial is:

$$\Delta = 4\left(\beta_4 + \beta_5 Z\right)^2 - 12\left(\beta_6 + \beta_7 Z\right)\left(\beta_1 + \beta_3 Z\right) \tag{32}$$

And we have two roots:

$$X^*_{1,2} = \frac{-\left(\beta_4 + \beta_5 Z\right) \pm \sqrt{\Delta_0}}{3\left(\beta_6 + \beta_7 Z\right)} \tag{33}$$

where $\Delta_0 = \frac{\Delta}{4} = \left(\beta_4 + \beta_5 Z\right)^2 - 3\left(\beta_6 + \beta_7 Z\right)\left(\beta_1 + \beta_3 Z\right)$

For $\Delta_0 > 0$ (so we can have two real roots) we expand the expression of Δ_0:

$$\begin{aligned}\Delta_0 &= \beta_4^2 + \beta_5^2 Z^2 + 2\beta_4\beta_5 Z - 3\beta_1\beta_6 - 3\beta_3\beta_6 Z - 3\beta_1\beta_7 Z - 3\beta_3\beta_6 Z^2 \\ &= Z^2\left(\beta_5^2 - 3\beta_3\beta_6\right) + Z\left(2\beta_4\beta_5 - 3\beta_3\beta_6 - 3\beta_1\beta_7\right) + \beta_4^2 - 3\beta_1\beta_6\end{aligned} \tag{34}$$

[8] Note that the moderating effect with respect to (31) is $3\beta_7 X^2 + 2\beta_5 X + \beta_3$. Given the discriminant $\wp = 4\left(\beta_5^2 - 3\beta_3\beta_7\right)$ this is positive if $\beta_5^2 - 3\beta_3\beta_7 < 0$ and $\beta_7 > 0$, and negative if $\beta_5^2 - 3\beta_3\beta_7 < 0$ and $\beta_7 > 0$.

For Δ_0 we need the discriminant of (34) :

$$D = \left(2\beta_4\beta_5 - 3\left[\beta_3\beta_6 + \beta_1\beta_7\right]\right)^2 - 4\left(\beta_5^2 - 3\beta_3\beta_6\right)\left(\beta_4^2 - 3\beta_1\beta_6\right) \tag{35}$$

to be < 0 and also $\beta_5^2 - 3\beta_3\beta_7 > 0$.

So, we need (35) to hold, $\Delta_0 > 0$ and the roots in (33) to always exist. One roots correspond to minimum and the other to maximum so that $X_1^* < X_2^*$, with X_1^* being the minimum and X_2^* being the maximum and also within the range of the data[9].

To make sure $X_1^* < X_2^*$ we have

$$X_1^* - X_2^* = \frac{2\sqrt{\Delta_0}}{3\left(\beta_6 + \beta_7 Z\right)} < 0 \Leftrightarrow \beta_6 + \beta_7 Z < 0 \tag{36}$$

Turning Point Moderation

To obtain how the moderator affects the turning, we need again to derive $\frac{\partial X^*}{\partial Z}$. We start with (31) which this can be expressed as:

$$\beta_1 + \beta_3 Z + 2\beta_4 X^* + 2\beta_5 X^* Z + 3\beta_6 X^{*2} + 3\beta_7 X^{*2} Z \tag{37}$$

where X^* is either X_1^* or X_2^*.

Differentiating this turning point with respect to the moderator Z, we obtain:

$$\frac{\partial X^*}{\partial Z} = -\frac{\beta_3 + 2\beta_5 X^* + 3\beta_7 X^{*2}}{2\left[\left(\beta_4 + \beta_5 Z\right) + 3X^*\left(\beta_6 + \beta_7 Z\right)\right]} \tag{38}$$

The denominator is > 0 at $X = X_1^*$ and < 0 at $X = X_2^*$ by (). Therefore:

$$\text{At } X^* = X^{*1}, \frac{\partial X^*}{\partial Z} > 0 \Leftrightarrow \beta_3 + 2\beta_5 X^* + 3\beta_7 X^{*1} < 0 \tag{39}$$

$$\text{At } X^* = X^{*2}, \frac{\partial X^*}{\partial Z} < 0 \Leftrightarrow \beta_3 + 2\beta_5 X^* + 3\beta_7 X^{*2} < 0 \tag{40}$$

Therefore, the critical expression is : $\beta_3 + 2\beta_5 X^* + 3\beta_7 X^*$[10].

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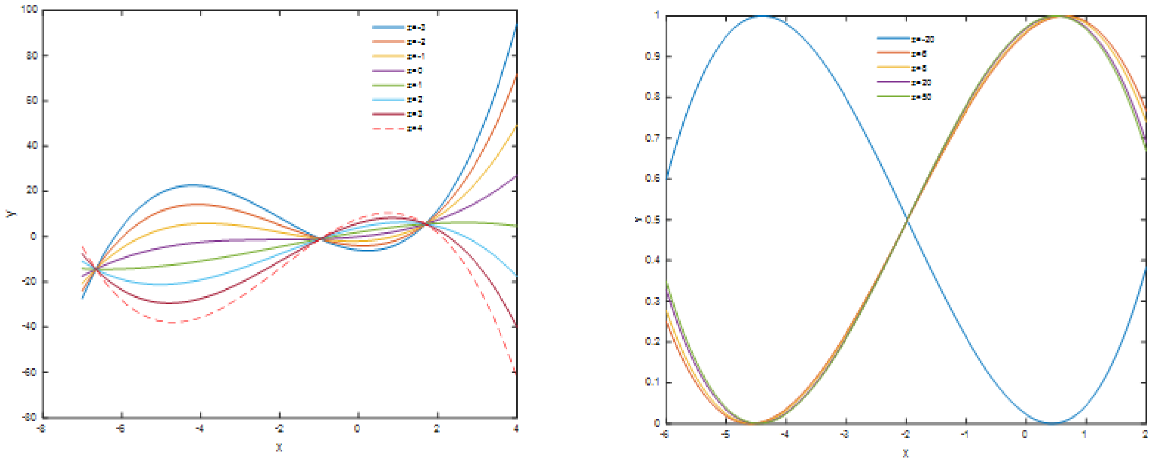
[9] Notice that if $\beta_6 = \beta_7 = 0$ (i.e. U-Shape) then () has only one solution as it becomes a linear equation.

[10] We present in Figure 5 an illustration on how the turning point shift with the moderator. For instance, it is clear from the first case that the turning point is moving to the left when the value of the moderator

Figure 5. Turning Point Moderation with the S-Curve



Flattening or Steepening Moderation

To derive the flattening/steepening moderation we again use the curvature and take its partial derivative which respect to Z. The curvature can be expressed as:

$$\frac{\partial^2 Y}{\partial X^2} = 2\beta_4 + 6\beta_6 X + 2\beta_5 Z + 6\beta_7 XZ \tag{41}$$

And the partial derivative of (32) with respect to Z is:

$$\frac{\partial}{\partial Z}\left(\frac{\partial^2 Y}{\partial X^2}\right) = 2\left(\beta_5 + 3\beta_7 X\right) \tag{42}$$

Based on these results we have the following propositions:

Proposition 1: Suppose that $D < 0$, $\beta_5^2 - 3\beta_3\beta_7 > 0$ as in () and $\beta_6 + \beta_7 Z < 0$ as in (). For flattening near the maximum we need $\beta_5 + 3\beta_7 X_2^* > 0$. For steepening we need $\beta_5 + 3\beta_7 X_2^* < 0$. For flattening near the minimum we need $\beta_5 + 3\beta_7 X_2^* < 0$, and for steepening we need $\beta_5 + 3\beta_7 X_2^* > 0$.

increases. In the second case however (Z =6,8,20) we do get the S-shape although it appears that the maxima and minima are not very different corresponding to different values of z.

Proposition 2: Flattening or steepening are not the only possibilities. When $\Delta_0 > 0$ at some $Z = Z_1$ but $\Delta_0 = 0$ at some $Z = Z_2$ or even $\Delta_0 < 0$ at some $Z = Z_3$, then we move from two roots $X^*_{1,2}$ to a single root X^*, and then to no real roots at all.

The condition for $\Delta_0 < 0$ is $D < 0$ and $\beta_5^2 - 3\beta_3\beta_6 < 0$, and for $\Delta_0 = 0$ (i.e. single root), we need $\beta_5^2 - 3\beta_3\beta_6 = 0$, and the single root can be expressed as: $-\dfrac{\beta_4^2 - 3\beta_4\beta_6}{2\beta_4\beta_5 - 3(\beta_3\beta_6 + \beta_1\beta_7)}$, which may or may not belong to the range of the data. So, the value of $\beta_5^2 - 3\beta_3\beta_6$ appears to be very important, and it is a parameter that we should always check in the context of S-Shape models. If $\beta_3 = 0$ and for $\beta_6 = 0$ no issue for criticality (should we define criticality?) arises (why?).

Another situation arises when we do not have always have $D < 0$ as in (35). Remember that

D depends on the parameters (β). For example, when $\beta_5^2 - 3\beta_3\beta_6 \le 0$ (i.e. the criticality parameters) then $D \ge 0$, and the equation $\Delta_0 = 0$ has at least one real root (and two in general). So, the roots $X^*_{1,2}$ in (33) may or may not exist depending on the particular value of Z.

4. Deviation from an arbitrary point

Here we re-examine all previous models when the data for explanatory variables are expressed as deviations from an arbitrary point x_0, z_0. The deviations are $X - x_0$, $Z - z_0$. The dependent variable y is kept the same. We show that we have vast simplifications in terms of analysing marginal effects, moderation effects, flattening, steepening, etc.

U-Shape:

We can write (20) as:

$$y = \beta_1 x + \beta_2 z + \beta_3 zx + \beta_4 x^2 + \beta_5 x^2 z \tag{43}$$

Choosing an arbitrary point, say:

$x = x_0$, $z = z_0$

We will use the deviations:

$X = x - x_0$, $Z = z - z_0$

We can write the model as follows:

$$\begin{aligned} y = {} & \beta_0 + \beta_1(X + x_0) + \beta_2(Z + z_0) + \beta_3(Z + z_0)(X + x_0) + \beta_4(X + x_0)^2 \\ & + \beta_5(X + x_0)^2(Z + z_0) \end{aligned} \tag{44}$$

Our intention is to regress y on the variables X, Z, XZ, X^2, X^2Z. We will show that considerable simplification is possible if we do so. Marginal and moderation effects will be simpler to analyse and the same will be for the case for the examination of flattening or steepening.

We can write (44) as:

$$y = \beta_0 + \beta_1 X + \beta_1 x_0 + \beta_2 Z + \beta_2 z_0 + \beta_3 \left(XZ + Xz_0 + x_0 Z + x_0 z_0\right) + \beta_4 \left(X^2 + x_0^2 + 2x_0 X\right)$$
$$+ \beta_5 \left(X^2 Z + x_0^2 Z + 2x_0 XZ + z_0 X^2 + x_0^2 z_0 + 2x_0 z_0 X\right)$$

Or:

$$\begin{aligned} y = {} & X\left(\beta_1 + 2\beta_4 x_0 + 2\beta_5 x_0 z_0 + \beta_3 z_0\right) + Z\left(\beta_2 + \beta_3 x_0 + \beta_5 x_0^2\right) + XZ\left(\beta_3 + 2\beta_5 x_0\right) \\ & + X^2\left(\beta_4 + \beta_5 z_0\right) + X^2 Z\left(\beta_5\right) + \left(\beta_0 + \beta_1 x_0 + \beta_2 z_0 + \beta_3 x_0 z_0 + \beta_4 x_0^2 + \beta_5 x_0^2 z_0\right) \end{aligned} \tag{45}$$

So, when the point of approximation is $x = x_0$ and $z = z_0$, the deviations form in (45) has the same functional form as (43) but the coefficients are different.

So, if we write the model in () as :

$$y = \gamma_0 + \gamma_1 X + \gamma_2 Z + \gamma_3 XZ + \gamma_4 X^2 + \gamma_5 X^2 Z, \tag{46}$$

where the $\gamma' s$ are the same as the complicated expression of the coefficients in (45).

We see that:

$$\frac{\partial y}{\partial X} = \gamma_1 + \gamma_3 Z + 2\gamma_4 X + 2\gamma_5 XZ \tag{47}$$

which is simply $= \gamma_1$ at $X = Z = 0$

The moderation with respect to the marginal effect is:

$$\frac{\partial^2 y}{\partial X} = 2\gamma_4 + 2\gamma_5 Z = 2\gamma_4 \text{ at } Z = 0 \tag{48}$$

Turning Point Moderation:

For the derivation of the turning point , we again set the marginal effect in (47) to 0 zero and solve for X . We obtain the following:

$$X^* = -\frac{\gamma_1 + \gamma_3 Z}{2\left(\gamma_4 + \gamma_5 Z\right)} \tag{49}$$

To see how the turning point changes with the moderator Z , we take the derivative of (49) with respect to Z :

$$\frac{\partial X^*}{\partial Z} = \frac{\gamma_5\gamma_1 - \gamma_3\gamma_4}{2\gamma_4^2} \tag{50}$$

This is a non-linear function of the parameters which we can plot along with $\pm$ 2 standard errors as function of x_0 (given z_0) or as a function of z_0 (given x_0).

Flattening or Steepening Moderation:

For flattening or steepening moderation, we again find the the curvature point:

$$\frac{\partial^2 y}{\partial X^2} = 2\gamma_4 + 2\gamma_5 Z = 2\gamma_4 \text{ at } Z = 0 \tag{51}$$

The partial derivative of (51) with respect to Z is:

$$\frac{\partial}{\partial Z}\left(\frac{\partial^2 y}{\partial X^2}\right) = 2\gamma_5 \tag{52}$$

Hence, all the above expressions are quite simple and can be obtained by:

I. Choosing a point of approximation (x_0, z_0)
II. Expressing the variables in terms of deviations $X = x - x_0, Z = z - z_0$.
III. Estimating () by OLS and obtain estimates of $\gamma' s$
IV. Change the point of approximation (x_0, z_0) and go to II.

We also recommend to plot the estimates of $\gamma' s$ and their standard errors to trace out the various effects discussed above.

S-Shape:

$$y = \beta_1 x + \beta_2 z + \beta_3 xz + \beta_4 x^2 + \beta_5 x^2 z + \beta_6 x^3 + \beta_7 x^3 z \tag{53}$$

Again if we chose:

$x = x_0$, $z = z_0$, and express the model in terms of: $X = x - x_0, Z = z - z_0$:

$$\begin{aligned} y &= \beta_1 (X + x_0) + \beta_2 (Z + z_0) + \beta_3 (X + x_0)(Z + z_0) + \beta_4 (X + x_0)^2 \\ &+ \beta_5 (X + x_0)^2 (Z + z_0) + \beta_6 (X + x_0)^3 + \beta_7 (X + x_0)^3 (Z + z_0) \end{aligned}$$

with some algebra we can show that :

$$
\begin{aligned}
y = X &\left(\beta_1 + \beta_3 z_0 + 2\beta_4 x_0 + 2\beta_5 x_0 z_0 + 3\beta_6 x_0^2 + 3\beta_7 x_0^2 z_0\right) + \\
&Z\left(\beta_2 + \beta_3 x_0 + \beta_5 x_0^2 + \beta_7 x_0^3\right) + XZ\left(\beta_3 + 2\beta_5 x_0 + 3\beta_7 x_0^2\right) + \\
&X^2\left(\beta_4 + \beta_5 z_0 + 3\beta_6 x_0 + 3\beta_7 x_0 z_0\right) + X^2 Z\left(\beta_5 + 3\beta_7 x_0\right) + \\
&X^3\left(\beta_6 + \beta_7 z_0\right) + X^3 Z\left(\beta_7\right) + \left(\beta_1 x_0 + \beta_2 z_0 + \beta_4 x_0^2 + \beta_5 x_0^2 z_0 + \beta_6 x_0^3 + \beta_7 x_0^3 z_0\right)
\end{aligned} \tag{54}
$$

Suppose we write the model on (54) as follows:

$$
y = \gamma_0 + \gamma_1 X + \gamma_2 Z + \gamma_3 XZ + \gamma_4 X^2 + \gamma_5 X^2 Z + \gamma_6 X^3 + \gamma_7 X^3 Z, \tag{55}
$$

where the $\gamma's$ are the coefficients in (54) which depend on x_0, z_0 . We obtain:

$$
\frac{\partial y}{\partial X} = \gamma_1 + \gamma_3 Z + 2\gamma_4 X + 2\gamma_5 XZ + 3\gamma_6 X^2 + 3\gamma_7 X^2 Z = \gamma_1, \text{ at } X = Z = 0 \tag{56}
$$

$$
\frac{\partial^2 (y)}{\partial X \partial Z} = \gamma_3 + 2\gamma_5 X + 3\gamma_7 X^2 = \gamma_3, \text{ at } X = Z = 0 \tag{57}
$$

Flattening or Steepening:

Contribution of Z to curvature:

$$
\frac{\partial}{\partial Z}\left(\frac{\partial^2 E(y \mid X, Z)}{\partial X^2}\right) = 2\gamma_5 + 6\gamma_7 X = 2\gamma_5, \; X = Z = 0.
$$

The Case of Limited Dependent Variables (LDV)

Suppose $y = \Phi(F)$, where $F = F(x, z)$ is an arbitrary functional form, and $\Phi(.)$ is a cumulative density function (CDF) with density $\varphi(.)$. In the case where:

$$
F(x, z) = \gamma_0 + \gamma_1 x + \gamma_2 z + \gamma_3 xz + \gamma_4 x^2 + \gamma_5 x^2 z + \gamma_6 x^3 + \gamma_7 x^3 z \tag{58}
$$

We have the following

Proposition: For the probit model, the marginal effect is:

$$
\frac{\partial E(y \mid x, z)}{\partial x} = \gamma_1 \tag{59}
$$

The moderation effect is:

$$
\frac{\partial E(y \mid x, z)}{\partial x \partial z} = \varphi(\gamma_0)(\gamma_3 - \gamma_0 \gamma_1 \gamma_3) \tag{60}
$$

The curvature is:

$$\frac{\partial^2 E(y|x,z)}{\partial x^2} = 2\gamma_4 , \tag{61}$$

And the contribution of z to the curvature is:

$$\frac{\partial}{\partial z}\left[\frac{\partial^2 E(y|x,z)}{\partial x^2}\right] = -\varphi(\gamma_0)\left\{\left(1-\gamma_0^2\right)\gamma_1^2\gamma_2 + 2\gamma_0\left(\gamma_1\gamma_3+\gamma_2\gamma_4\right) - 2\gamma_5\right\} \tag{62}$$

Proof: The proof relies on the general function form $F = F(x,z)$. We have:

$$\frac{\partial E(y|x,z)}{\partial x} = \varphi(F)F_x$$

$$\frac{\partial E(y|x,z)}{\partial x \partial z} = \varphi^{'}(F)F_xF_z + \varphi(F)F_{xz}$$

$$\frac{\partial^2 E(y|x,z)}{\partial x^2} = \varphi^{'}(F)F_x^2 + \varphi(F)F_{xx},$$

Where the subscripts indicate differentiation. Moreover,

$$\frac{\partial}{\partial z}\left[\frac{\partial^2 E(y|x,z)}{\partial x^2}\right] = \varphi^{''}(F)F_x^2F_z + 2\varphi^{'}(F)F_xF_{xz} + \varphi^{'}(F)F_zF_{xx} + \varphi(F)F_{xxz}$$

After some algebra, we get:

$$\frac{\partial}{\partial z}\left[\frac{\partial^2 E(y|x,z)}{\partial x^2}\right] = \left\{\frac{\varphi^{''}(F)}{\varphi(F)}F_x^2F_z + \frac{\varphi^{'}(F)}{\varphi(F)}\left[2F_xF_{xz} + F_zF_{xx}\right] + F_{xxz}\right\}$$

In the case of probit we have:

$\varphi(z) = (2\pi)^{-1/2} e^{-z^2/2}, \dfrac{\varphi^{'}(z)}{\varphi(z)} = -z$, and

$$\frac{\varphi^{''}(z)}{\varphi(z)} = -\left(1-z^2\right), \forall z \in \mathbb{R}.$$

We obtain the following derivatives:

$$F_x = \gamma_1 + \gamma_3 z + 2\gamma_4 x + 2\gamma_5 xz + 3\gamma_6 x^2 + 3\gamma_7 x^2 z,$$

$$F_{xz} = \gamma_3 + 2\gamma_5 x + 3\gamma_7 x^2,$$

$$F_{xx} = 2\left(\gamma_4 + \gamma_5 z + 3\gamma_6 x + 3\gamma_7 xz\right),$$

$F_{xxz} = 6\gamma_7$.

Setting $x = z = 0$, we obtain:

$\frac{\partial E\left(y \mid x, z\right)}{\partial x} = \gamma_1$, The moderation effect is :

$\frac{\partial E\left(y \mid x, z\right)}{\partial x \partial z} = \varphi\left(\gamma_0\right)\left(\gamma_3 - \gamma_0\gamma_1\gamma_3\right)$, and $\frac{\partial}{\partial z}\left[\frac{\partial^2 E\left(y \mid x, z\right)}{\partial x^2}\right]$ as stated in the proposition.

At a local extrema, we have $\gamma_1 = 0$, and this is maximum (minimum) if $\gamma_4 < 0\left(> 0\right)$. The contribution of z to the curvature at this point is:

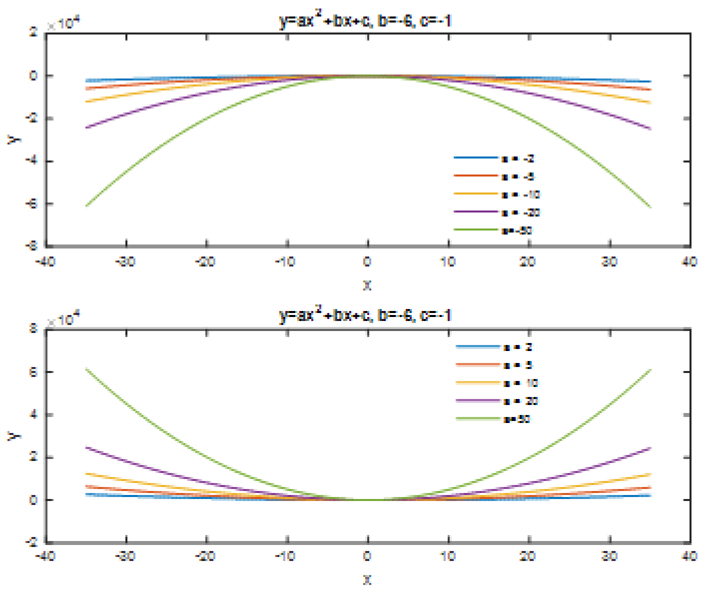
$\frac{\partial}{\partial z}\left[\frac{\partial^2 E\left(y \mid x, z\right)}{\partial x^2}\right] = -2\varphi\left(\gamma_0\right)\left\{\gamma_0\gamma_2\gamma_4 - \gamma_5\right\}$. Notice that the moderation effect does not depend exclusively on γ_3 as in linear models but on $\gamma_0, \gamma_1, \gamma_2$ as well.

Appendix 1: The Flattening and Steepening Concepts

To illustrate our new concept of steepening / flattening based on the curvature, we use a second-order polynomial: $y = f(x) = ax^2 + bx + c$. The second derivative is $f''(x) = 2a$ so, steepening / flattening should depend on the magnitude of a. The alternative in the literature is to examine how the root of $f'(x^*) = 2ax^* + b = 0 \Rightarrow x^* = -\frac{b}{2a}$ changes with a moderator Z, i.e. examine $\frac{dx^*}{dZ}$. As both a and b can depend on Z, this can become quite complicated.

For example, if we have inverted-U shape, so that $a < 0$, the function can be thought of as a log-likelihood in terms of "parameter" x. The variance of the "parameter" is given by minus the inverse of the second derivative, the well-known Fisher information: $I = -\frac{1}{f''(x)} = -\frac{1}{2a}$. Flattening corresponds to larger variance and, therefore, corresponds to higher values of a. With U-shape curves, higher values of a will produce steepening, as we show in Figure A.1. Moreover, in terms of the absolute value of a, we can state that as $|a|$ increases we have steepening and as $|a|$ decreases we have flattening, in a neighbourhood of x.

Figure A.1. Flattening and Steepening



As an example, consider the model:

$$Y = f(X) = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \tfrac{1}{2}\beta_4 X^2 + \tfrac{1}{2}\beta_5 X^2 Z \tag{A.1}$$

We obtain the following derivatives:

$$\frac{\partial Y}{\partial X} = \beta_1 + \beta_3 Z + \left(\beta_4 + \beta_5 z\right) X \tag{A.2}$$

$$\frac{\partial^2 Y}{\partial X^2} = \beta_4 + \beta_5 Z \tag{A.3}$$

Clearly, the contribution of z to the curvature is: $\frac{\partial}{\partial Z}\left(\frac{\partial^2 Y}{\partial X^2}\right) = \beta_5$, so we can see immediately that as $|\beta_5|$ increases we have more curvature and, therefore, flattening.

The argument based on slopes would be far more complicated with cubic effects (S-shape). For example, if we have

$$Y = \beta_0 + \beta_1 X + \beta_2 Z + \beta_3 XZ + \tfrac{1}{2}\beta_4 X^2 + \tfrac{1}{2}\beta_5 X^2 Z + \tfrac{1}{3}\beta_6 X^3 + \tfrac{1}{3}\beta_7 X^3 Z \tag{A.4}$$

it is easy to show that:

$$\frac{\partial}{\partial Z}\left(\frac{\partial^2 Y}{\partial X^2}\right) = \beta_5 + 2\beta_7 X \tag{A.5}$$

and, therefore, the contribution of Z to curvature depends on X.