8 Quadratic models

It is frequently necessary to work with non-linear models. The maximum of a linear function is obtained at the boundary of the area of the x-variables. In case we need to find the optimal response, it is natural to work with quadratic models. The major disadvantage of working with quadratic models is that many parameters are needed to estimate the model. And according to the H-principle each parameter has a price. If the model is large a big price may have to be paid for estimating the parameters. Let us consider this situation closer. Suppose that the theoretical model is given by

$$y_i = \boldsymbol{\beta}_i'\mathbf{x} + \mathbf{x}'\,\mathbf{C}_i\,\mathbf{x} + \text{residual}, \quad i = 1,2, \ldots M. \tag{22}$$

Here $\mathbf{x}$ is a K-vector. If K is equal to 100 we are talking about a model of medium size compared to the ones we meet in practice. In that case the number of elements in each set ($\boldsymbol{\beta}_i$, $\mathbf{C}_i$) are 100+100*101/2=5150. For the case of three response variables, M=3, there will be 15450 parameters that need to be estimated. In such cases it is not feasible to estimate the parameters ($\boldsymbol{\beta}_i$, $\mathbf{C}_i$) directly. Instead we seek to determine directions or components that more adequately can identify the surface that describes the response values.

It is appropriate to illustrate the situation closer, where we seek a second order surface of lower order than the original proposed model. Consider the mathematical model

$$y = 0.95\,x_1 + 2.01\,x_2 + 0.5\,x_1^2 + 2\,x_1\,x_2 + 2\,x_2^2 + \text{residual}$$

$$= (x_1 + 2\,x_2) + 0.5\,(x_1 + 2\,x_2)^2 + (-0.05\,x_1 + 0.01\,x_2) + \text{residual}$$

$$= t_1 + 0.5\,t_1^2 + t_2 + \text{residual},$$

where

$$t_1 = x_1 + 2\,x_2 \qquad \text{and} \qquad t_2 = -0.05\,x_1 + 0.01\,x_2.$$

From mathematical point of view we can equally well work with the t-variables as the x-variables. It can happen that the residual values are so large that the component t_2 is not worth keeping, because the sum of t_2-values and the residual values are of the same size as the residual values alone. One can state that in this case the component t_1 alone appropriately identifies the surface, in which case we

can state that data are appropriately described by a parable in the direction of t_1. Predictions based only on t_1 may be more precise than if we want to base them on both t_1 and t_2.

We can insert the transformation (20), $\mathbf{x}=\mathbf{PDt}$ into (22). Using $\mathbf{RP'D}=\mathbf{I}$, we get

$$(23) \qquad y_i = \boldsymbol{\beta}_i' \mathbf{x} + \mathbf{x}' \mathbf{C}_i \mathbf{x} = \boldsymbol{\beta}_i' \mathbf{D P R}' \mathbf{x} + \mathbf{x}' \mathbf{R P}' \mathbf{D C}_i \mathbf{D P R}' \mathbf{x}$$

$$= (\mathbf{P'D}\boldsymbol{\beta}_i)' (\mathbf{R'x}) + (\mathbf{R'x}) (\mathbf{P'DC}_i\mathbf{DP}) (\mathbf{R'x}) = \boldsymbol{\alpha}_i'\mathbf{t} + \mathbf{t}' \mathbf{G}_i \mathbf{t},$$

where

$$\boldsymbol{\alpha}_i = \mathbf{P'D}\, \boldsymbol{\beta}_i \qquad \text{and} \qquad \mathbf{G}_i = \mathbf{P'D}\, \mathbf{C}_i\mathbf{D}\, \mathbf{P}.$$

If all K components are selected, there is a one-to-one relationship between $\mathbf{t}$ and $\mathbf{x}$. But in practical applications not all components are normally selected. This means that $\mathbf{P}$ and $\mathbf{R}$ only have A columns, $\mathbf{P}=\mathbf{P}_A$ and $\mathbf{R}=\mathbf{R}_A$. Note that $\mathbf{t}$ here will be an *A* vector.

The criterion of selecting 'quadratic' components

I shall now present a criterion for determining 'quadratic' components. This theory is presented in the univariate case in [3] and in the multivariate case in [1]. Here only the numerical criterion will be presented.

When the *a*th component t_a is added to the model, there are in fact being added (a+1) variables to the model, namely t_a, t_a^2, t_at_1,t_at_2, ... ,t_at_{a-1}. In order to simplify the notation let $\otimes$ denote the elementwise product of two vectors, e.g.

$$\mathbf{t}_1 \otimes \mathbf{t}_2 = (t_{i1} \times t_{i2}) = (t_{11} \times t_{12},\ t_{21} \times t_{22},\ t_{31} \times t_{32},\ \ldots\ ,\ t_{N1} \times t_{N2}).$$

Using this notation, the following matrices are computed

$$\mathbf{V}_k = \mathbf{Y} \otimes \mathbf{t}_k = (y_{ij} \times t_{ik}), \quad k = 1, \ldots , a\text{-}1.$$

$$\mathbf{H} = \mathbf{X}' (\mathbf{YY}' + \mathbf{V}_1 \mathbf{V}_1' + \ldots + \mathbf{V}_{a-1} \mathbf{V}_{a-1}') \mathbf{X}$$

$$\mathbf{G}_j = \mathbf{X}' \operatorname{Diag}(\mathbf{y}_j) \mathbf{X}, \qquad j=1, \ldots , M.$$

Here Diag($\mathbf{y}_j$) is the diagonal matrix with $\mathbf{y}_j$ in its diagonal. The numerical task is

(24) maximize $\mathbf{w}' \mathbf{H} \mathbf{w} + \Sigma_j [\mathbf{w}' \mathbf{G}_j \mathbf{w}]^2$ for $|\mathbf{w}|=1$

This is a nonlinear expression in $\mathbf{w}$. It is solved by considering the Lagrangian function

$$f(\mathbf{w}) = \mathbf{w}' \mathbf{H} \mathbf{w} + \Sigma_j [\mathbf{w}' \mathbf{G}_j \mathbf{w}]^2 - \lambda (\mathbf{w}'\mathbf{w} - 1)$$

Differentiating f($\mathbf{w}$) we get

$$f'(\mathbf{w}) = 2 \mathbf{H} \mathbf{w} + \Sigma_j [2 (\mathbf{w}' \mathbf{G}_j \mathbf{w}) \mathbf{G}_j \mathbf{w}] - \lambda 2 \mathbf{w}$$

This shows that a stationary point, f '($\mathbf{w}$)=0, is given by

(25) $$\mathbf{w} = [\mathbf{H} \mathbf{w} + \Sigma_j(\mathbf{w}' \mathbf{G}_j \mathbf{w}) \mathbf{G}_j \mathbf{w}]/[\mathbf{w}' \mathbf{H} \mathbf{w} + \Sigma_j(\mathbf{w}' \mathbf{G}_j \mathbf{w})^2]$$

Thus (24) is solved by iterating (25) in the same way as in the case of the power method of determining the largest eigenvalue and associated vector. Good initial values can be obtained by computing first the largest eigen value and associated eigen vector for $\mathbf{H}$ and use the eigen vector as a starting vector in the right-hand side of (25). Numerical experience on several examples, large and small, has shown that convergence is arrived at with the same speed as the normal power method of computing eigen values/vectors. I.e. convergence is normally arrived at within 10 to 30 iterations of (25).

As mentioned above, introducing a new component t_a means that there are being added (a+1) new variables in the model, namely t_a, t_a^2, t_at_1, t_at_2, ... ,t_at_{a-1}. Usually not all of these variables are wanted in the model, because the 'price' may be too high. It is important to look at the results and check which ones should be eliminated. In the practical applications (16) is used to check the components. The inequality (16) is checked for each numerical component, i.e. for $\mathbf{t}=\mathbf{t}_a$, $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_a$, $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_1$, $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_2$, ..., $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_{a-1}$. In case the inequality (16) is not satisfied for any response variable, the corresponding term is excluded in the criterion above. E.g., if (16) is not satisfied for $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_1$, the term $\mathbf{X}' (\mathbf{V}_1 \mathbf{V}_1') \mathbf{X}$ is excluded in the computation of $\mathbf{H}$. Then (25) is used to iterate a new value $\mathbf{w}$, where the terms in the expression corresponding to the variables that were not found significant are excluded. There are situations, where (16) is not satisfied for $\mathbf{t}=\mathbf{t}_a$, or for $\mathbf{t}=\mathbf{t}_a\otimes\mathbf{t}_a$, but the linear and the squared terms are not excluded. There are cases where these terms are needed in order to get a working solution. See closer the example below on finding the optimal response.

The weight vector **w** can be determined from all of **X**, from $\mathbf{X}_i$ or any other part of **X**. Usually we use the partition (8) to determine which part of **X** that should be used. This would mean that the first choices are linear models on, say, $\mathbf{X}_1$, $\mathbf{X}_2$ and $\mathbf{X}_3$, followed by a quadratic model involving $\mathbf{X}_4$, and then again a linear one and so on.

The advantage of the criterion (24) is that if all quadratic variables are not found significant, the criterion reduces to the PLS criterion (1). Thus we can always check if quadratic components are needed when analyzing a block of **X**. But we should be careful in these applications. As mentioned above, many variables are available, when we ask for a quadratic surface. The criterion (16) may be satisfied for some of them although the surface is not quadratic, because there are so many choices to select among.

The traditional approach to quadratic modeling is to work with the original variables and estimate the parameters in the model (22). Usually, this approach is not satisfactory. The reason is that so many variables are needed to adequately identify the surface. This will be illustrated by an example below. These examples generally show that the present approach is preferable, even in small models.

9 Some basic variational considerations

There are some basic issues of variational type that are important to be aware of, when carrying out experimentation with the purpose of displaying the behaviour of response variables. It is concerning the different types of variation that is involved in the experimentation. I shall discuss them closer.

In agronomic practice the response value is the actual observation. The agronomic people look at the observation in a following way:

Observation = Design effect + Treatment effect + Experimental error
+ Measurement error

The '*design effect*' is the effect on the observational unit due to the specific design. One field may be more fertile than another, there may be fertility gradients due to the sun, slope of the field, dampness of the soil, there may be boundary effects

(plants on the boundary may get more sun and wind), there may effects from the instruments used in carrying out the cultivation and so on. It is important to be aware of that there may be different conditions that may give the final observational result. *Treatment effect* is the one that we usually want to get hold on. Often there are many ways to specify the treatment effects. They are the 'factors' that we think influence the response value. *Experimental error* is the variation from one 'plant' to a neighbouring one in the agronomic language. *Measurement error* is the variation that we get when we actually carry out the measurement.

In the analysis of data it is important to be aware of these different type of variations. When we have an effect it is not always correct to compare the variation of this effect to the residual variation. Consider a trivial example. Suppose that we have treated 30 patients by some treatments and we measure the variation of the patients by their temperature. Now suppose that the temperature has been measured by three types of thermometers. Then we have 90 measurements of the temperature. Here the variation in the temperature for a given patient is of no interest, because it is only a measurement error. Probably the best we can do is to take the average of the three temperature measurements and work further with the average values.

10 Approaches to experimental design

The literature on experimental design is extensive, see e.g., [4]. Also fine program packages like SAS, MODDE and others have been developed for experimental design. In the literature there are some different approaches to experimental design that have become a tradition in certain types of areas. There are basically three types of considerations, that we shall consider closer.

1^{o} **Based on extension of X-data**
Here the design considerations are based on the variation that is present in the **X**-data. A representative for this approach is [5]. The numerical variables are typically scaled so that the data used in the analysis are just few values (see the examples). The basic considerations are

- specification of center values and extreme values of the variables
- replicates (multiple measurements) are carried out at center of data
- mathematical properties are sought for (rotatable, D-optimal etc)

2^{o} **Taguchi design**
The Taguchi design were developed in engineering environments, where there were many variables and ‘one experimental run’ relatively expensive or difficult to carry out. A representative for this approach is [6]. The basic considerations were

- many variables, few levels, few runs
- orthogonal design
- at most two level interactions

These designs were developed quality design environments.

3° **Analysis of variance (Agricultural experiments)**

Experimental design has a long tradition in agriculture and animal breeding. [4] is a good representative for this approach. The main design considerations are

- Specification of gradients of 'yields' in terms of blocks, plots and subplots.
- Many levels of each variable and many interactions (Large design matrix)
- Different types of statistical tests.

A very extensive literature exists on these topics.

The H-principle suggests modeling to be carried out in steps. Experimental design should also be carried out sequentially, where a new step should utilize the information obtained at previous steps. Thus we have a fourth approach to experimental design:

4° **H-principle**

The methodology of the H-principle and the associated algorithm suggests a following procedure for carrying out the experimental design.

- Iterative procedure: First a pilot study, then a new data design and so on.
- Identify the 'noise level' (measurement or experimental variation)
- Priorities on effects and factors.

These four approaches to experimental design are considered closer in the following, where the approaches are illustrated by small examples. First it is shown, how the design matrix X is generated from the model for given data values.

Central composite experimental design. The factorial and star design can be combined into one design. Such designs are often called central composite experimental design. The design considerations are of three kind:

1. A factorial design for the first part. The design can be full factorial or fractional factorial design or other special types of factorial design (lattice, simplex etc).
2. A certain amount of center points
3. Positive and negative extremes of each variable.

The first consideration is based on what main effects and interactions are needed. The last two are based on getting a reliable model to work with. An example of such a design is the following one:

Run	x1	x2	x3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1.682	0	0
10	1.682	0	0
11	0	-1.682	0
12	0	1.682	0
13	0	0	-1.682
14	0	0	1.682
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

Table 13. An example of a central composite design

The first eight runs will give us estimate of the main effects and interactions. The last six ones give us information on the variation of the response variable. And runs nine to fourteen will make the model more stable.

Example. Yield of snap beans.
We shall consider closer the data studied by [5], Khuri et al., pp 188. They use a central composite design to investigate the effects of three fertilizer ingredients on the yield of snap beans under field conditions. The fertilizer ingredients were nitrogen (N), phosphoric acid (P_2O_5) and potash (K_2O). The coded variables are

$$x_1=(N - 3.62)/1.59, \quad x_2=(P_2O_5 - 1.78)/0.71, \; x_3=(K_2O - 2.42)/1.07.$$

The design in Table 13 was used in the field experiment. For the values of the yield see Khuri et al, p 190. For these data we are interested in estimating the optimal yield of snap beans. There is a clear curvature in data (seen e.g. by plotting the first PLS component against the yield). Therefore a quadratic model is a natural one to work with. Several standard program are available to analyze this quadratic model. I have chosen here to apply the RSREG procedure in the SAS system. The results are shown in Table 14.

Parameter	Degrees of Freedom	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob > |T|
INTERCEPT	1	10.462	0.406	25.756	0.0000
X1	1	-0.574	0.270	-2.129	0.0591
X2	1	0.183	0.270	0.680	0.5117
X3	1	0.455	0.270	1.690	0.1219
X1*X1	1	-0.676	0.262	-2.578	0.0275
X2*X1	1	-0.678	0.352	-1.924	0.0833
X2*X2	1	0.563	0.262	2.145	0.0576
X3*X1	1	1.183	0.352	3.358	0.0073
X3*X2	1	0.233	0.352	0.660	0.5240
X3*X3	1	-0.273	0.262	-1.042	0.3218

Table 14. Results from the RSREG procedure in SAS

The root mean square error, s, is computed as $s=\sqrt{s^2}$, with

$$s^2 = \Sigma (y_i - \_i)^2/(20-10) = 0.99196.$$

The R^2-value is 78.61%. It is not very high, but common in field experiments. The criterion (16) for redundancy of a variable, or equivalently a t-value of 1.41, is not satisfied for three variables in the analysis, x_2, $x_2 \times x_3$ and x_3^2. Thus these three variables create more modeling variation than the variation they explain of the yield. Also, besides the mean level, only two variables are significant at the 5% level of significance. Therefore, the estimated model has a high degree of overfitting, which makes the optimal solution unstable. The estimated model is $y=\mathbf{a'x}+\mathbf{x'Ax}$. The optimal sample is obtained by differentiating the estimated model, giving $\mathbf{a}+2\mathbf{Ax}=\mathbf{0}$. This gives the optimal solution $\mathbf{x}_{opt}$=(-0.394,-0.364, -0.175), which is a saddle point. The associated optimum is y_{opt}=10.502.

It is important to see if the approach in section 8 is able to give a more stable estimate of the optimal solution and associated response value. The procedure is that first we determine the parable, $a+b_1 t_1 + c_{11} t_1^2$. Then **X** is adjusted for t_1 and **Y** is adjusted for the variation due to t_1 and t_1^2. At the next step we estimate the model,

$b_2\ t_2 + c_{22}\ t_2^2 + c_{12}\ t_1\ t_2$. And again **X** is adjusted for t_2 and **Y** is adjusted for t_2, t_2^2 and $t_1 t_2$. Finally, we estimate the parameters in the model $b_3\ t_3 + c_{33}\ t_3^2 + c_{13}\ t_1\ t_3 + c_{23}\ t_2\ t_3$. The variation obtained is as follows.

i	t_i	t_i^2 and $t_i \times t_j$		
1	6.5600	13.7013	0.1278	0.0137
2	1.1103	0.1278	11.9499	0.0038
3	0.1180	0.0137	0.0033	0.3718

Table 15. Variation explained by linear, squared and cross product terms

The variation explained is $(\mathbf{y't})^2/(\mathbf{t't})$ for $\mathbf{t}=\mathbf{t}_1$, $\mathbf{t}=\mathbf{t}_1^2$ etc. The requirement for not doing overfitting is that the variation explained by a variable should be at least $2\times0.99196 = 1.98392$ (see (16)). Only three terms satisfy this, t_1 t_1^2 and t_2^2. Thus a proper second order surface that the yield projects onto is a parable in t_1 and also in t_2. It is proper to suppress these cross product terms, $t_i t_j$, when estimating the second order model in the score variables. This means that we do not use the corresponding terms in the expression (24). If we do that we get the following table.

i	t_i	t_i^2 and $t_i \times t_j$		
1	6.3068	13.7618	0	0
2	1.3159	0	11.9499	0
3	0.1655	0	0	0.3716

Table 16. Variation explained by linear and squared terms

The term t_3 is included in order to get a one-to-one relationship between the sample and score values. The term t_3^2 is included in order to get a unique optimum.

i	t_i	t_i^2 and $t_i \times t_j$		
1	0.6795	-1.1678	0	0
2	-0.3104	0	0.6508	0
3	0.1101	0	0	0.1298

Table 17. Regression coefficients of linear and squared terms

When we similarly solve $\mathbf{b}+2\mathbf{C}\mathbf{t}=\mathbf{0}$, we get the optimal solution for the score vector as $\mathbf{t}_{opt}$=(0.2909, 0.2385, -0.4241). With the constant term in the model equal 10.4624 the optimal response value is y_{opt}=10.5709, which is somewhat larger than the first optimum. The transformation matrix (**PD**) that transforms score vector to sample vector is

$$\mathbf{PD} = \begin{matrix} -0.8054 & 0.2719 & 0.5267 \\ -0.2000 & -0.9611 & 0.1903 \\ 0.5579 & 0.0479 & 0.8285 \end{matrix}$$

The optimal sample value is now $\mathbf{x}_{opt}= (\mathbf{PD})\mathbf{t}_{opt} = (-0.3928, -0.3681, -0.1776)'$. This optimal sample value is close to the one found by the first approach. There is a rather large variation in the data, which is the main reason for that there is so little difference between these two approaches. Note that we are working with slight overfitting in order to get a unique relationship between sample and score values. Figures 4 and 5 show a clear quadratic relationship between the response value and the respective score values. Figure 6 shows the relationship between the third score vector and the adjusted response values. There is a sign of curvature in data, which justifies that we use the third component, although there is a large variation around the estimated curve.

This example is a small one, but it shows how we work. The transformation **R** is here equal to (**PD**) because the matrix **X** has orthogonal columns. If the present design is extended with a new sample, the new score vector can be computed as $\mathbf{t}=\mathbf{R}'\mathbf{x}$. For large design this approach gives more stable solution. But often, like in this example, we allow some redundant variables in order to get the advantage of a one-to-one transformation or a unique optimal solution.

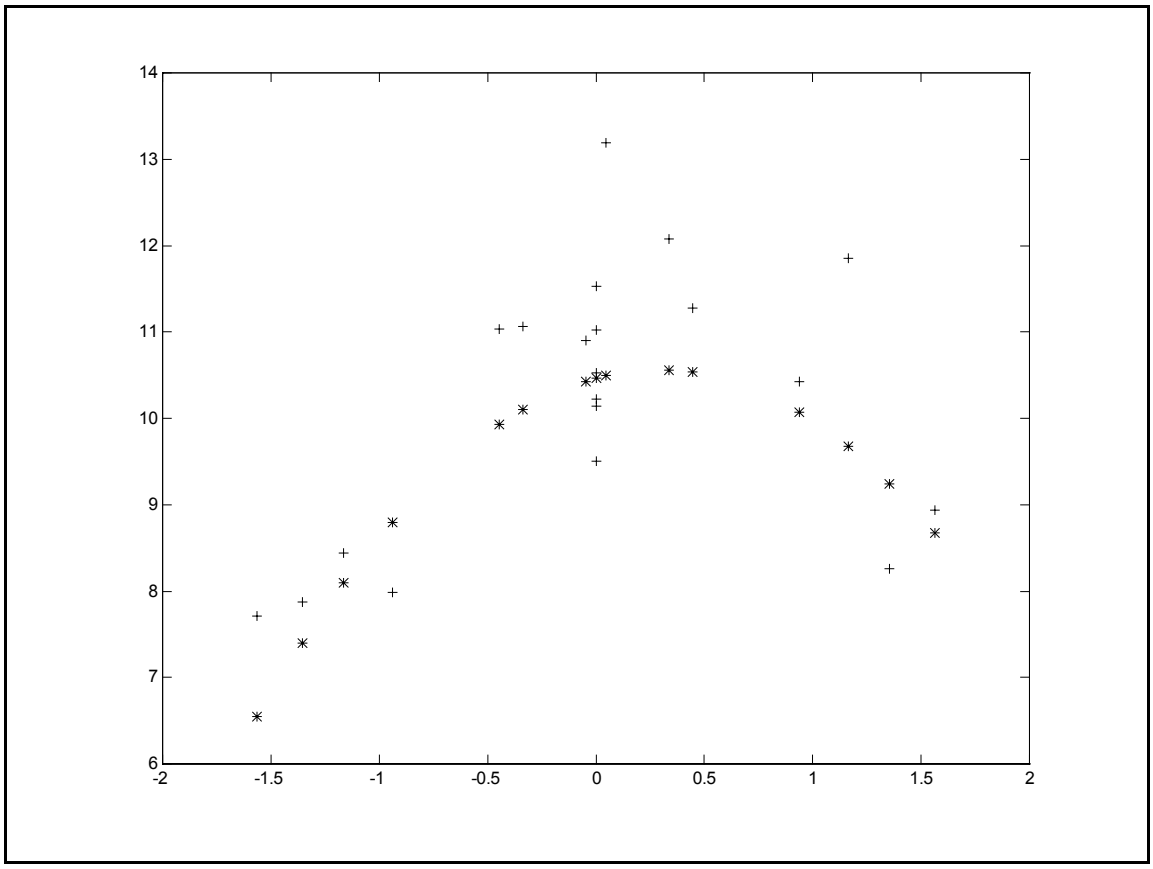

Figure 4. Plot of the response value vs the first component

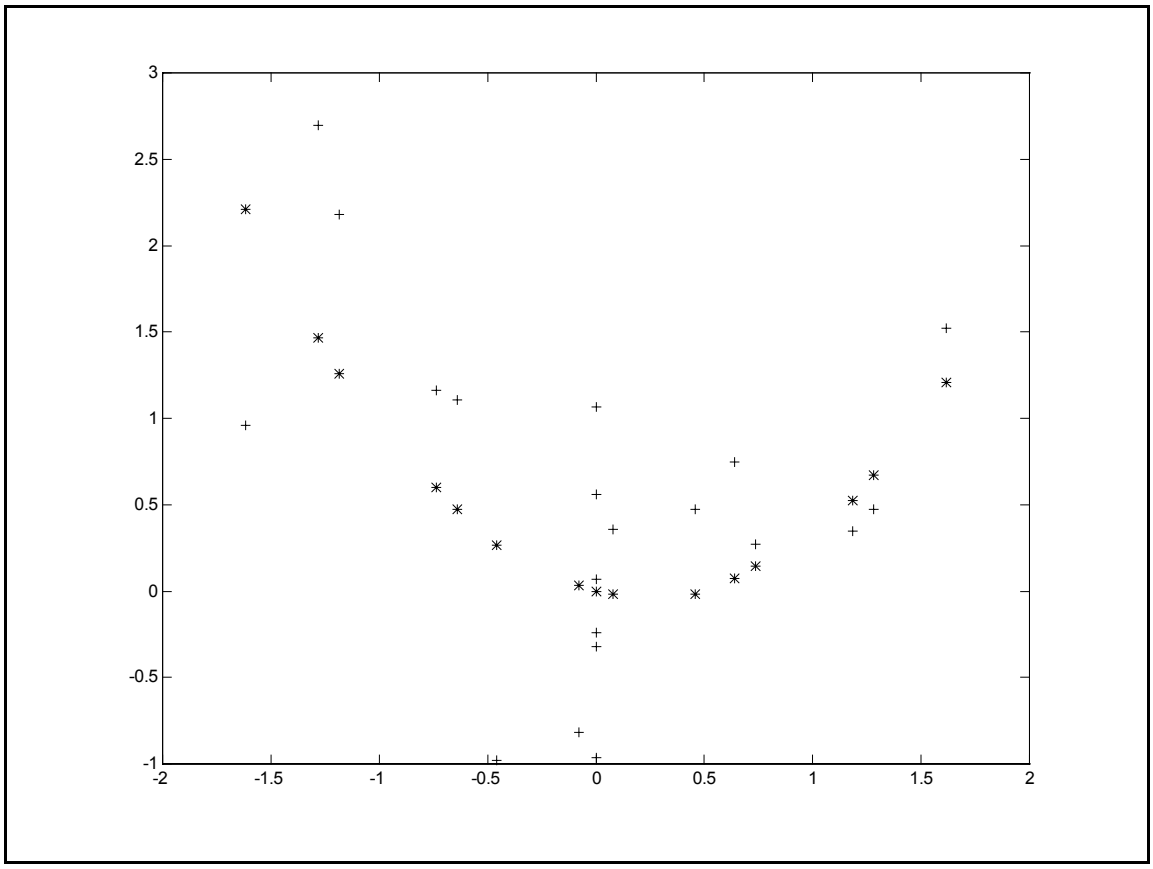

Figure 5. Plot of adjusted (for t_1) response value vs the second component

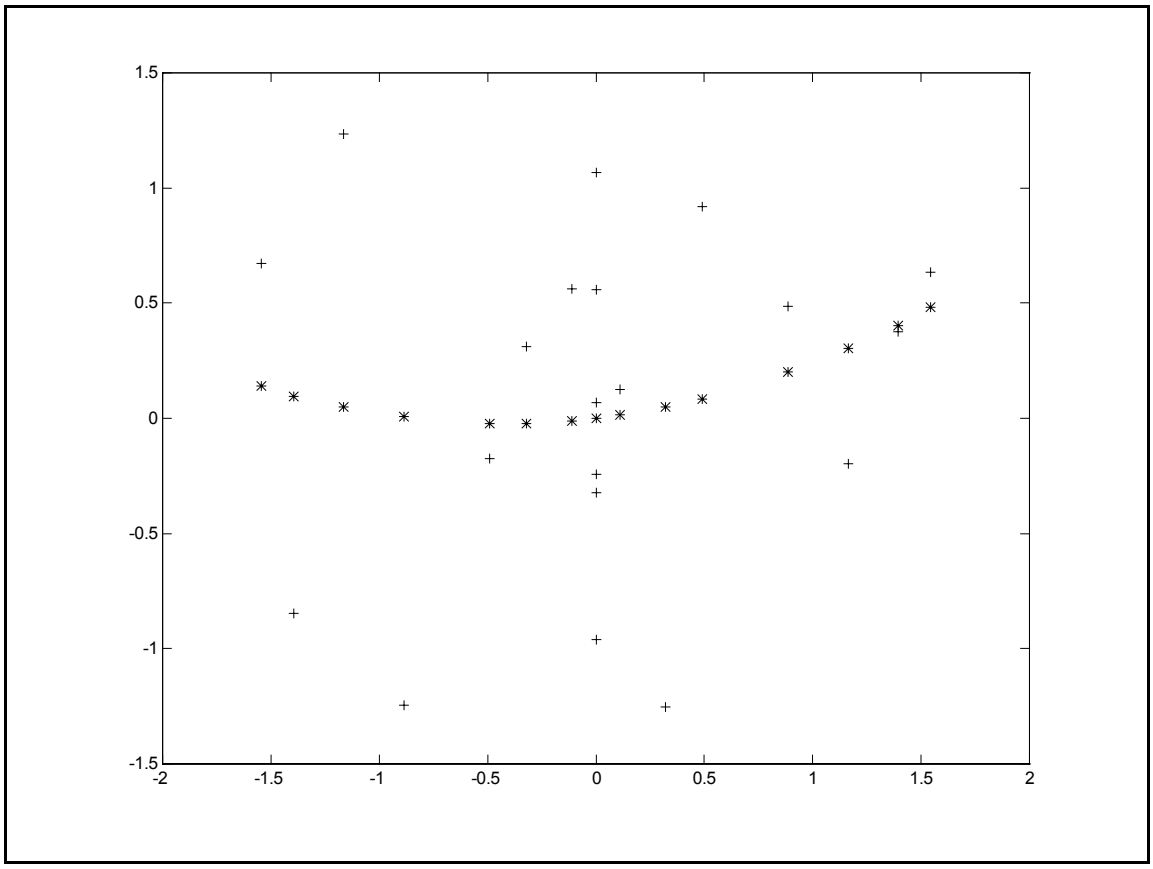

Figure 6. Plot of adjusted (for t_1 and t_2) response value vs the third component