GÖTEBORG UNIVERSITY

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RESEARCH REPORT 1994:10
ISSN 0349-8034

A NOTE ON ROTATABILITY

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1994

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Abstract

The need of a measure of rotatability is discussed and exemplified through some examples. The examples also shows the difficulties with measuring rotatability. A graphical technique for exploring the variance function is discussed.

Keywords: Measure of Rotatability, Graphical Approach.

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Introduction

When constructing designs, rotatability is one property that has to be considered. A design is said to be rotatable if there exist a point $\mathbf{x}_0$ (the designs center point) such that the variance of a predicted value in a point $\mathbf{x}$, $\mathrm{Var}(\hat{y}(\mathbf{x}))$, only depends on the distance between $\mathbf{x}_0$ and $\mathbf{x}$, and of course on the experimental error. See Box and Draper [1987].

For some classes of models, rotatable designs can always be constructed. Especially this is true for polynomial models (Box and Draper [1987]). For other types of models, or when blocked designs are used, it may not be possible to find an exact rotatable design. Another situation when a rotatable designs not can be found is when the experimenter cannot afford to run the number of experiments that are required.

This leads us to the problem of measuring rotatability. This is a fairly new topic in the theory of construction of designs and has its origin in two articles from 1988, Khuri [1988] and Draper and Guttman [1988]. These two articles deals with single number measures of rotatability. A design's departure from a rotatable design can take many forms. Also is the departure different at different distances from the design center. This complexity makes it impossible, which is also mentioned by Draper and Guttman[1988], to describe the degree of/lack of rotatability with a single number. Giovanitti-Jensen and Myers [1989] suggest a graphical method of assessing the degree of/lack of rotatability, using what they call a variance dispersion graph.

In next section we will study an example to emphasize the complexity of rotatability. Thereafter is the graphical method presented together with an alternative method for constructing such graphs. The last section includes a brief discussion of the problem with measuring rotatability, and some words about a related property to rotatability, but by no means not so well understood or examined.

An Example of a Non-Rotatable Design

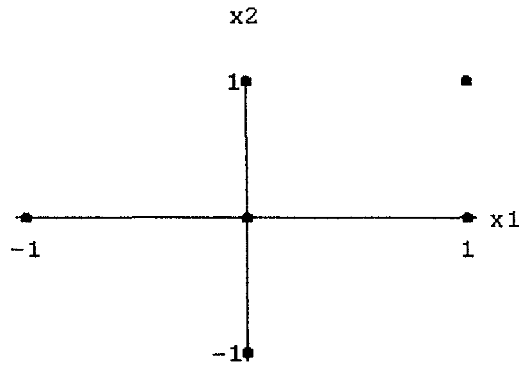
Consider following situation. We have a response variable Y and two explanatory variables x_1 and x_2. Over a well defined region we want to determine the functional relationship between the response variable and the explanatory variables. The usual assumptions of i.i.d. normally distributed measurement errors are assumed. We know that the relationship is on one of the two forms;

$$\text{(i)}\quad E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$\text{(ii)}\quad E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2$$

Now assume that the collection of data is of such nature that changing the levels of the explanatory variables and the preparations for a set of runs are connected with great costs. Because of this we like to perform only one set of runs, minimum of six observations to be able to estimate model (ii), and to use as few levels as possible. One possible design meeting these criteria's is the design with design matrix

$$\mathbf{D} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 1 & 1 \end{pmatrix}.$$

What this design looks like is shown in next figure. As seen, the design has an



asymmetrical pattern, and we would not expect it to be rotatable. Intuitively one would guess that the variance of the predictions is lower when both x_1 and x_2 are greater than zero, compared with other points at the same distance from the origin. The variance of a predicted value in any point **x**, can be shown to be

$$\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t (\mathbf{X}^t\mathbf{X})^{-1} \mathbf{x}\, \sigma^2$$

where **X** is the designs **X**-matrix and σ^2 is the variance of the experimental error and $\hat{y}(\cdot)$ is the fitted model.

We are now interested in studying $\mathrm{Var}(\hat{y}(\cdot))$ at fixed distances from the origin. To do this, introduce polar coordinates

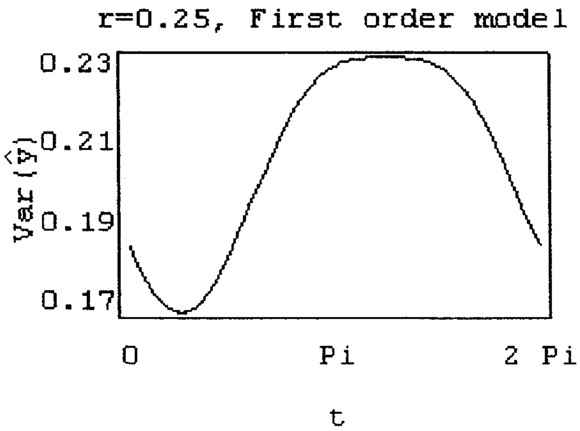
$$\begin{cases} x_1 = r\cos(t) \\ x_2 = r\sin(t) \end{cases}$$

where $r \in (0,\infty)$ and $t \in (0,2\pi)$. Now, hold r fixed and let t go from 0 to 2π. By constructing graphs for some different values of r, we will get a good picture of how $\mathrm{Var}(\hat{y}(\cdot))$ behaves in different directions and how this behavior depends on r.

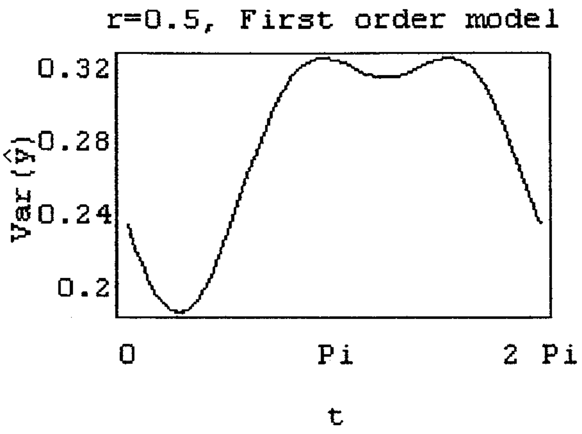
Let us now examine model (i) and model (ii) one by one.

Examination of the first order model

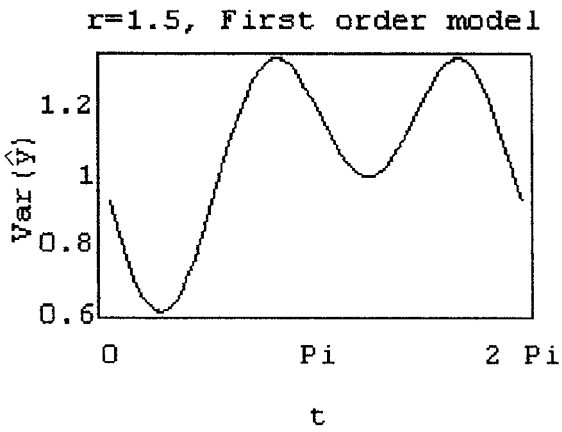
For r = 0.25 we obtain the following graph. Not surprisingly, the best predictions are

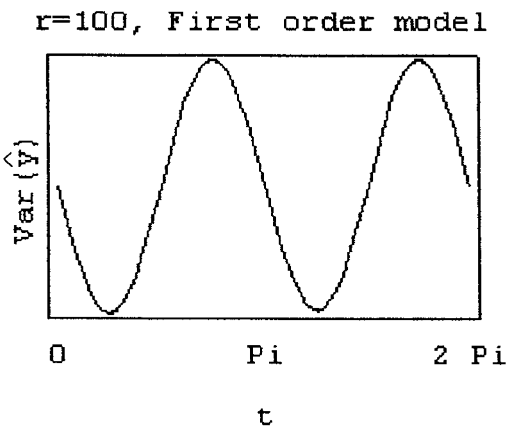


made in the direction $t = \pi/4$, i.e. in the direction towards the "extra" design point $(1,1)$. The worst prediction are made in the opposite direction, $t = 5\pi/4$. When r = 0.5, next graph, $\mathrm{Var}(\hat{y}(\cdot))$ looks somewhat different. The best predictions are still made in the direction of $t = \pi/4$. However, the worst predictions are now made in two new directions, $t = 5\pi/4 \pm t_r, r = 0.5$. When r gets large, t_r tends to $\pi/2$.



From a practical point of view it is of interest to study Var($\hat{y}(\cdot)$) for moderate values of r (r not much larger than the distance from the design center to the outermost design point), but from a theoretical viewpoint also larger values of r are of interest. The two following graphs shows the behavior of Var($\hat{y}(\cdot)$) when r = 1.5 and r = 100.



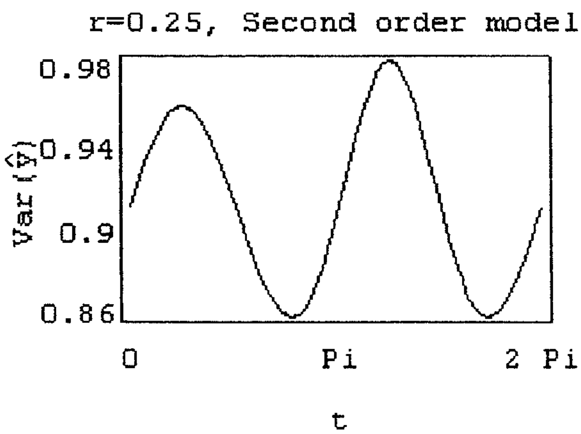


The last graph, $r = 100$, does not show the values of $\mathrm{Var}(\hat{y}(\cdot))$. What is interesting is the shape of $\mathrm{Var}(\hat{y}(\cdot))$. The best predictions are made in the two directions $t = \pi / 4$ and $t = 5\pi / 4$, for large r, and the worst predictions are made in the two directions $t = 3\pi / 4$ and $t = 7\pi / 4$. Notice that for small values of r, $t = 5\pi / 4$ is the worst direction for predictions, but as r gets larger the predictions are better and better (relative other directions) and asymptotically it is the best direction together with $t = \pi / 4$.

We have seen that even for the simplest of models, the degree of/lack of rotatability will not be easily described. Let us now examine the second order model.

Examination of the second order model

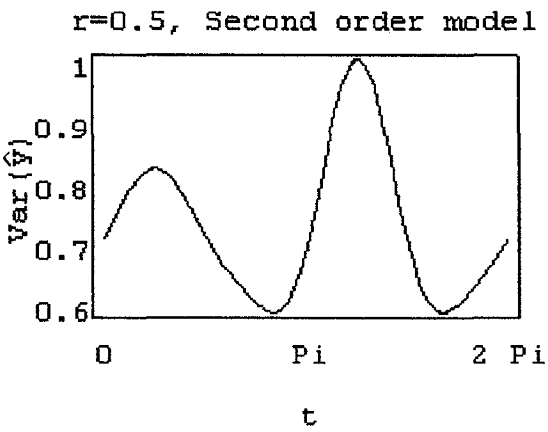
This model is somewhat more complicated than the first order model. Still, intuitively, it is reasonable to believe that predictions are made with greater accuracy in the direction $t = \pi / 4$. By studying the graph of $\mathrm{Var}(\hat{y}(\cdot))$ when $r = 0.25$ we see that this is not true,

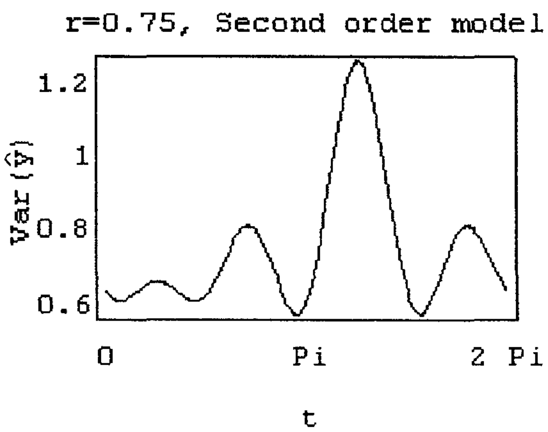


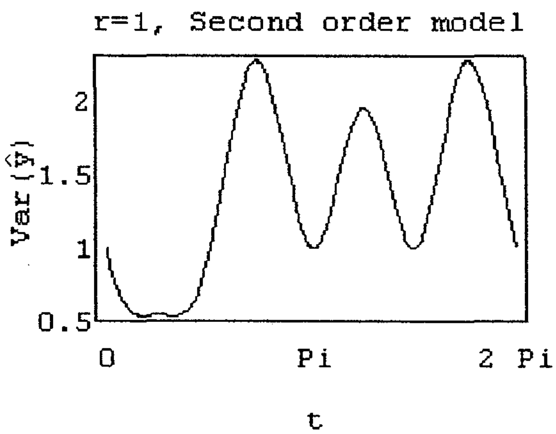
for small values of r. In fact, the best predictions are made in the directions $t = 5\pi / 4 \pm t_r, r = 0.25$. When r tends to zero, it can be shown that t_r tends to $\pi / 2$. Further, when r is small, $\mathrm{Var}(\hat{y}(t = \pi / 4)) \approx \mathrm{Var}(\hat{y}(t = 5\pi / 4))$, and $t = \pi / 4$ and $t = 5\pi / 4$ are the worst directions of predictions. So compared with the first order model is the situation very different.

By introducing polar coordinates, and then study $\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{x}\,\sigma^2$, for small values of r, one will gain a mathematical understanding of the behavior of $\mathrm{Var}(\hat{y}(\cdot))$ close to the origin. However, it is not easy to see intuitively why $\mathrm{Var}(\hat{y}(\cdot))$ behaves as it does in the graph above. So even in this trivial example with a simple design and a well understood model, the behavior of $Var(\hat{y}(\cdot))$ at fixed distances from the design center is not easy to grasp.

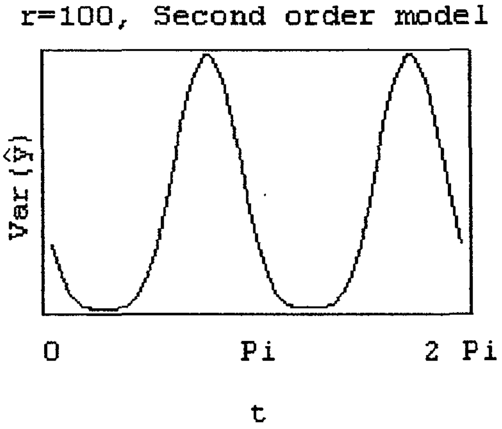
What follows is a sequence of graphs for some different values of r, namely $r = 0.5$, $r = 0.75$ and $r = 1$. The purpose is to show how different $Var(\hat{y}(\cdot))$ looks at different distances, and also to show the complexity of $Var(\hat{y}(\cdot))$ at some fix distances.







The shape of $Var(\hat{y}(\cdot))$ for the second order model, remains more and more of the shape of the corresponding function for the first order model, when r gets large. This is verified by studying $Var(\hat{y}(\cdot))$ when $r = 100$. One can see that the curves of $Var(\hat{y}(\cdot))$, $r = 100$, for the first order model and the second order model have the same characteristics, even if they not are exactly identical.



Mathematical examination of the variance functions

As seen, the form of $Var(\hat{y}(\cdot))$ can be very complex at some distances and will not be easily expressed in mathematical terms. When r tends to zero or infinity the expression of $Var(\hat{y}(\cdot))$ is simplified, and it is worthwhile to study these special cases to learn more about the behavior of the function.

Let V_1 denote $Var(\hat{y}(\cdot))$ in the first order case, and V_2 the same function in the second order case. The following results are easily verified.

$$
\begin{aligned}
&V_1 \to a_1 + a_1' \ \sin(t+\pi/4) \quad \text{as} \quad r \to 0,\\
&V_1 \to b_1 + b_1' \ \sin(2t) \quad \text{as} \quad r \to \infty,\\
&V_2 \to a_2 + a_2' \ \sin(2t) \quad \text{as} \quad r \to 0,\\
&V_2 \to b_2 + b_2' \ \sin(2t)\ (1-\sin(2t)/2) \quad \text{as} \quad r \to \infty
\end{aligned}
$$

This explains why V_2 is so flat when 2t is close to $\pi / 4$ and $5\pi / 4$ for large r in the second order model. To see this, let $u = 2t$. A Taylor expansion of sin(u) around $u = \pi / 4$ (the case $u = 5\pi / 4$ is similar), gives $\sin(u) \approx 1 - (u - \pi / 4)^2 / 2$. Therefore is $\sin(u)\ (1 - \sin(u) / 2) \approx 1 / 2 - (u - \pi / 4)^4 / 8$. That is, in a neighborhood of $u = \pi / 4$ can the function be approximated with a fourth order polynomial function with multiple roots in $\pi / 4$.

The Variance Dispersion Graph Approach

A design is said to be rotatable if $Var(\hat{y}(\cdot))$ is constant on spheres of radius r, all $r > 0$, centered at the designs center. This means that a non-rotatable design is not constant on spheres, and a natural way of measuring the departure from rotatability is to find $\max\{Var(\hat{y}(\cdot))\}$ and $\min\{Var(\hat{y}(\cdot))\}$ on the spheres.

We can now construct a variance dispersion graph by plotting $(\max\{Var(\hat{y}(\cdot))\}, \min\{Var(\hat{y}(\cdot))\})$ against r for some appropriate chosen values of r.

The problem is to find $\max\{Var(\hat{y}(\cdot))\}$ and $\min\{Var(\hat{y}(\cdot))\}$, for a given r. We have seen in the previous section, that even in a simple situation, $Var(\hat{y}(\cdot))$ can have a rather complex form.

Giovanitti-Jensen and Myers [1988] suggest two different solutions depending on if the model is of first order or second order. In the first order case it can be shown that $\max\{Var(\hat{y}(\cdot))\} = (1/N + \lambda_{max} r^2)\sigma^2$ and $\min\{Var(\hat{y}(\cdot))\} = (1/N + \lambda_{min} r^2)\sigma^2$ where λ_{max} and λ_{min} are the largest and the smallest eigenvalues of $(\mathbf{X}^t\mathbf{X})^{-1}$. In the second order case they use a search algorithm (not described in the paper) to find an optimum. The problem with using such algorithm is commented upon by the authors in their paper and their reflection of this problem is partly reproduced in the following quotation.

> "In many situations, multiple locations exist for the maximum value of the variance on a particular sphere. As in the case of many optimization routines in which one has nonlinear equality constraints and the objective function is this complex, there is no guarantee of finding the global optimum."

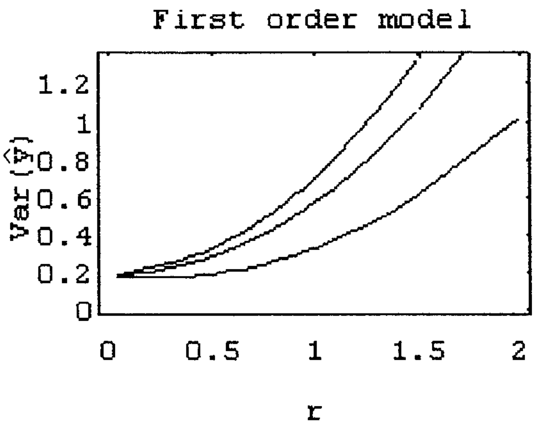
This is a problem that not should be underestimated. Consider the graph of the second order model when $r = 1$. There is local optimum at the point $t = \pi / 4$. If the value of $Var(\hat{y}(\cdot))$ in this point is reported as $\max\{Var(\hat{y}(\cdot))\}$, this will of course affect the variance dispersion graph negative.

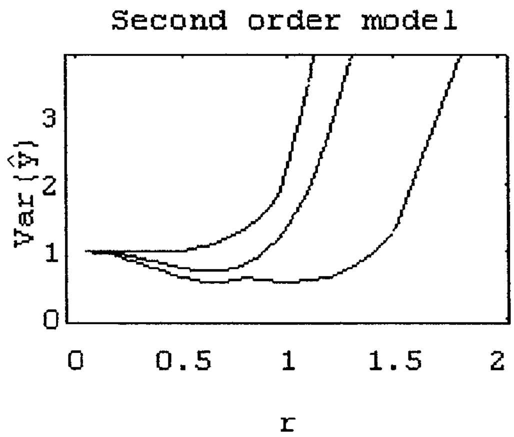
What we need to do is to find all local maxima and minima on the sphere and then find out which ones are the global ones. This can be done using Lagrange multiplicator. After solving the nonlinear equation system

$$\frac{\partial L}{\partial x_1} = 0$$
$$\vdots$$
$$\frac{\partial L}{\partial x_k} = 0$$
$$\frac{\partial L}{\partial \lambda} = 0$$

where $L = Var(\hat{y}(x)) - \lambda(\sum_{i=1}^{k} x_i^2 - r^2)$, it is easily verified which of the optimum values that are global.

It is also useful in the variance dispersion graph, for each r, plot the mean of $Var(\hat{y}(\cdot))$ on the sphere. If ψ_r is the surface area of the sphere U_r at distance r, the mean is found as $\psi_r^{-1}\int_{U_r} Var(\hat{y}(x))\,dx$. Below is shown what this graph looks like for the two examples in the previous section.





For studying the characteristics of a design, with respect to rotatability, the variance dispersion graph is useful. When coming to a situation when a visual examination of the graphs not is enough for discriminating between several designs, one need a measure of the degree of/lack of rotatability to be able to pick one of the proposed designs. A measure close related to the variance dispersion graphs is the area between the upper and the lower curve. The smaller the better and an area equals zero means that the design is rotatable.

Discussion

Rotatability is a property which is important when predictions in all directions are of equal interest. In many situations it is not possible to construct an exact rotatable design, but it shows that in many situations you can often find an almost rotatable design, without suffering (to much) from other nice properties of the design. It is therefore of interest to learn how to compare designs with respect to rotatability, and learn how to construct almost rotatable designs in different situations.

The examples shows the difficulties in understanding the behavior of $\mathrm{Var}(\hat{y}(\cdot))$. Also one can understand the difficulties in measuring the degree of/lack of rotatability with a single value. In a rotatable design is $\mathrm{Var}(\hat{y}(\cdot))$ constant for each fixed value of r, i.e. the graphs in section 2 had been straight lines parallel to the x-axis. It is not hard to imagine that the departure from rotatability can take many forms.

Rotatability implies constant variance on spheres centered at the design center. Taking this one step further, one would wish constant variance on all spheres. That is, constant variance over the whole region of interest. Is it possible to construct such designs? This is a problem that has not been discussed in the literature.

A rotatable design is represented as a single curve in the variance dispersion graphs. A design with constant variance over the whole region of interest, would be represented as a line parallel to the x-axis. With this knowledge, one can construct measures of how close a design is to meet the condition of a "constant variance design", and this is a first step in the search of designs with this desired property.

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