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Statistical Test of the Existence of a Turning Point

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ABSTRACT

A method for testing monotonicity versus unimodality is presented. One specification of the problem is treated in detail. It is also discussed how transformations and combinations can be used to get solutions for other specifications. A maximum likelihood ratio test based on non-parametric regression estimates is derived. A test with an upper limit for the size is presented. The power of the test is examined by a simulation study.

Keywords: TURNING POINT; LIKELIHOOD RATIO; NON-PARAMETRIC; MONOTONIC REGRESSION; UNIMODAL REGRESSION.

1. Introduction

In several areas of science we can find relations between two variables, which are considered to include a turning point. It could be situations where the relations consist of a down-phase followed by an up-phase or the opposite. The aim of this work is to develop methods, which are useful in such cases. We are going to deal with problems in which both the null and alternative hypotheses impose order restrictions. For simplicity we focus on a single explaining variable but adjustment for other factors can be made.

In Section 2, a family of statistical models is described. Most notations and specifications are given in this section. In Section 3, a maximum likelihood ratio test is derived. Some properties of the test statistic are discussed and some statements about the distribution of the test statistic are made. In Section 4, a conservative test is constructed and in Section 5, the power of this test is examined. In Section 6, the problem of making inference about the monotonicity properties of a continuous curve from information at discrete design points is discussed. In Section 7, some concluding remarks are given.

1.1 Some applications

An example of a case where it is of interest to verify a turning point is the relation between the daily consumption of alcohol and health. Earlier it was assumed that the risk of bad health increases monotonically with the alcohol consumption. Now, when more information is available (Power, Rodgers, & Hope, 1998), it is assumed that the risk is decreasing with increasing amount of alcohol up to some consumption value. Consumption, larger than this value, then increases the risk of bad health. The question whether the regression includes a down-phase followed by an up-phase could be answered by the test given here. Another example is the relation between the risk a child having Down's syndrome and the age of the woman in confinement. One has earlier considered that the risk that a child has Down's syndrome increases with the age of the mother. Lately one has begun to suspect that also very young women have increased risk to bear children with Down's syndrome. The shape of the relation between the probability of the syndrome and the age of the mother could be examined by means of the test described here.

In a trial, cancer patients are treated with radiotherapy regimes with the aim to reduce pain as long as possible. There are several patterns of response. Some patients have a quick reduction of pain, some, get the relief later. For some patients the relapse is early for others it is late. All of them have a unimodal response curve. For some, the relief might be permanent and the response curve is monotonic. It is of interest to classify patients according to the monotonic or unimodal pattern.

Relations in the economic area are often considered to include a turning point. Examples of such relations are marginal productivity against the quantity of labour, and demand of inferior goods against household income. Also the turning points of business cycles are of great interest (Andersson, 1999).

These examples indicate that there is a need for a statistical test for the existence of a turning point.

1.2 Earlier work

When investigating a potentially unimodal relationship a common approach is to split the axis for the explaining variable into intervals and to plot the average of the response for each interval. This is often done for several potential splittings. It thus contains arbitrariness and is no base for formal statistical analysis.

Another common approach is to fit a more or less flexible parametric regression function. The most frequently used approach might be to fit a quadratic function and then test if the parameter corresponding to the non-linearity is significantly different from zero. This was done in (Samuelsson, Wilhelmsen, Pennert, Wedel, & Berglund, 1990).

A more flexible function consisting of two quadratic parts was suggested in (Goetghebeur & Pocock, 1995), where several tests based on this model are suggested. It is pointed out that the power of this kind of tests is much lower than expected.

Confidence limits for both the level and the position of the turning point based on the estimates in (Frisén, 1986) are given in (Dahlbom, 1994).

2. Models, notations and specifications

In this work the class of problem where the relation between the variables is unimodal and perhaps monotonic is treated.

The situation is either experimental or non-experimental. If the situation is experimental, we choose levels for the independent variable, according to an experimental design. The chosen levels of the independent variable are called the design points. In the non-experimental case we might condition on the observed random values of the independent variable. Thus the design points could be regarded as non-random in both cases.

All observations are assumed independent. The normal distribution is considered to be a good approximation for the distribution of the dependent variable in each design point. For the design points i = 1, 2, ..., k, we have the vectors of parameters $\mu = \{\mu_1, \mu_2, ..., \mu_k\}$ of expected values and $\sigma^2 = \{\sigma_1^2, \sigma_2^2, ..., \sigma_k^2\}$ of variances. The means μ_i are unknown, but the variances σ_i^2 are assumed known. We have n_i observations at design point i, Y_{ij} is the *j*:th observation of Y_i , $j = 1, 2, ..., n_i$, and \overline{Y}_i the mean of those observations. \overline{Y}_i is normally distributed with unknown mean μ_i and known variance of the mean, which is used as an index of information $w_i = n_i \sigma_i^{-2}$.

Some notations for order restrictions, which will be used, will now be introduced.

Definition 2.1: The regression is unimodal if $\exists m; \mu_1 \geq ... \geq \mu_m$ and $\mu_m \leq ... \leq \mu_k$ or $\exists m; \mu_1 \leq ... \leq \mu_m$ and $\mu_m \geq ... \geq \mu_k$.

Definition 2.2: The regression is U-shaped if $\exists m; \mu_1 \geq ... \geq \mu_m$ and $\mu_m \leq ... \leq \mu_k$.

Definition 2.3: The regression is inversely U-shaped if $\exists m; \mu_1 \leq ... \leq \mu_m$ and $\mu_m \geq ... \geq \mu_k$.

Definition 2.4: The regression is monotonic if $\mu_1 \leq ... \leq \mu_k$ or $\mu_1 \geq ... \geq \mu_k$.

Definition 2.5: The regression is increasing if $\mu_1 \leq ... \leq \mu_k$.

Definition 2.6: The regression is decreasing if $\mu_1 \ge ... \ge \mu_k$.

Definition 2.7: The regression has a turning point if it is not monotonic.

Observe that the Definitions 2.2-2.6 all are special cases of unimodality. Some examples of unimodal, in some cases also monotonic, regressions are illustrated in Figure 2.1.



Figure 2.1: Examples of unimodal, in some cases also monotonic regression. All regressions are unimodal according to Definition 2.1. The regressions in (a), (b), (c), (d), (g), (h) and (i) are U-shaped according to Definition 2.2. The regressions in (a), (b), (c), (c), (e), (f), (g), (h) and (i) are inversely U-shaped according to Definition 2.3. The regressions in (a), (b), (c), (g), (h) and (i) are monotonic according to Definition 2.4. The regressions in (a), (g), (h) and (i) are increasing according to Definition 2.5. The regressions in (a), (b) and (c) are decreasing according to Definition 2.6.

We treat now the case there the monotonicity of one part of the curve is known, while uncertainty is prevailing only for the other part. Information is here available according to one of the four following descriptions.

- Case i: We are sure about the final part of the curve. The relation there is increasing.However, we are uncertain if also the first part of the curve is increasing or if the relation, in this part, is decreasing but not constant.
- *Case ii:* We know that the first part of the curve is decreasing, but we are not sure about the following part. Either the shape of the curve continues to be decreasing or it turns up, being increasing but not constant.
- *Case iii:* We are sure about the final part of the curve. The relation there is decreasing. However, we are uncertain if also the first part of the curve is decreasing or if the relation, in this part, is increasing but not constant.
- *Case iv:* We know that the first part of the shape of the curve is increasing, but we are not sure about the following part. Either the shape of the curve continues to be increasing or it turns down, being decreasing but not constant.



Figure 2.2: The four principal cases where the curve might include a turning point. The bold lines represent the part with known monotonicity while the dotted lines represent parts under question.

The following four combinations of hypotheses correspond to the cases described above and are of interest in turning point problems:

- Case i: H_0 : The regression is increasing H_1 : The regression is U-shaped but not increasing
- Case ii: H_0 : The regression is decreasing H_1 : The regression is U-shaped but not decreasing
- Case iii: H_0 : The regression is decreasing H_1 : The regression is inversely U-shaped but not decreasing
- Case iv: H_0 : The regression is increasing H_1 : The regression is inversely U-shaped but not increasing

We treat *Case i* in detail, but the other three cases can easily be analysed in an analogous way. The hypotheses in *Case ii* are identical with the hypotheses in *Case i* for the random variable $Y'_i = Y_{k+l-i}$. The hypotheses in *Case iii* are identical with the hypotheses in *Case i* for the random variable $Y''_i = -Y_i$ and the hypotheses in *Case iv* are identical with the hypotheses in *Case i* for the random variable $Y''_i = -Y_i$ and the hypotheses in *Case iv* are identical with the hypotheses in *Case i* for the random variable $Y''_i = -Y_i$.

When there is uncertainty about the whole curve, combinations of the hypotheses treated here can be used. The theory of multiple testing can be used to handle this.

3. The maximum likelihood ratio test statistic

In this section we derive and discuss the maximum likelihood ratio test statistic for the model specified in *Case i* in Section 2 for testing H_0 : *The regression is increasing* versus H_1 : *The regression is U-shaped but not increasing*. As was demonstrated at the end of Section 2 the results can easily be used for the other cases.

The hypotheses are not simple but composite. Thus, a full likelihood ratio test cannot be achieved. The way chosen here to handle the nuisance parameters is to construct the maximum likelihood ratio test.

As the information about the shape of the curve is limited to order-restricted relations only, no parameters of some assumed function has to be estimated. Hence the analysis method will be based on non-parametric regression analysis. Let ${}_{0}\hat{\mu}_{i}$ be the maximum likelihood estimate of μ_{i} under H_{0} . The maximum likelihood estimator under the restriction that the regression is increasing is given in e.g. (Barlow, Bartholomew, & Brunk, 1972). It is not possible to express the estimator explicitly. The "Pool-Adjacent-Violators" algorithm described by e.g. (Robertson, Wright, & Dykstra, 1988) groups the adjacent design points into "level sets". For each level set the common estimator is the weighted mean of the observations corresponding to the set.

Further let $\hat{\mu}_i$ be the maximum likelihood estimate of μ_i under $H_0 \cup H_1$. The maximum likelihood estimator under the restriction that the regression is U-shaped is given in (Frisén, 1986). The likelihood for each of the finite number of partitions in one decreasing phase followed by an increasing one can be determined. The maximum of these values corresponds to the maximum likelihood estimator.

Theorem 3.1: The maximum likelihood ratio test of H_0 versus H_1 rejects H_0 for large values of the statistic, $T = \sum_{i=1}^k w_i (\overline{Y}_i - _0 \hat{\mu}_i)^2 - \sum_{i=1}^k w_i (\overline{Y}_i - \hat{\mu}_i)^2$.

Proof: The specifications in Section 2 implies that the likelihood function, $L(\mu)$, is

$$\prod_{i=l}^{k} \frac{1}{(\sqrt{2\pi} \sigma_{i})^{n_{i}}} exp\left\{\sum_{j=l}^{n_{i}} -\frac{(y_{ij} - \mu_{i})^{2}}{2\sigma_{i}^{2}}\right\}.$$

$$Let \Lambda = \frac{sup_{\mu \in (H_{0} \cup H_{1})}L(\mu)}{sup_{\mu \in H_{0}}L(\mu)} . Then \Lambda = \frac{\prod_{i=l}^{k} \frac{1}{(\sqrt{2\pi} \sigma_{i})^{n_{i}}} exp\left\{\sum_{j=l}^{n_{i}} -\frac{(y_{ij} - \hat{\mu}_{i})^{2}}{2\sigma_{i}^{2}}\right\}}{\prod_{i=l}^{k} \frac{1}{(\sqrt{2\pi} \sigma_{i})^{n_{i}}} exp\left\{\sum_{j=l}^{n_{i}} -\frac{(y_{ij} - \hat{\mu}_{i})^{2}}{2\sigma_{i}^{2}}\right\}} = \frac{1}{1}$$

$$=\frac{\prod_{i=l}^{k} exp\left\{-\frac{1}{2\sigma_{i}^{2}}\left(\sum_{j=l}^{n_{i}} y_{ij}^{2}+n_{i}\hat{\mu}_{i}^{2}-2\hat{\mu}_{i}\sum_{j=l}^{n_{i}} y_{ij}\right)\right\}}{\prod_{i=l}^{k} exp\left\{-\frac{1}{2\sigma_{i}^{2}}\left(\sum_{j=l}^{n_{i}} y_{ij}^{2}+n_{i-0}\hat{\mu}_{i}^{2}-2_{-0}\hat{\mu}_{i}\sum_{j=l}^{n_{i}} y_{ij}\right)\right\}}=$$

$$=\prod_{i=l}^{k} exp\left\{-\frac{1}{2\sigma_{i}^{2}}\left(\sum_{j=l}^{n_{i}} y_{ij}^{2}+n_{i}\hat{\mu}_{i}^{2}-2\hat{\mu}_{i}\sum_{j=l}^{n_{i}} y_{ij}-\sum_{j=l}^{n_{i}} y_{ij}^{2}-n_{i}\hat{\mu}_{i}\hat{\mu}_{i}^{2}+2\hat{\mu}_{i}\hat{\mu}_{i}\sum_{j=l}^{n_{i}} y_{ij}\right)\right\}=$$

$$= \prod_{i=l}^{k} exp \left\{ -\frac{1}{2\sigma_{i}^{2}} \left(n_{i}\hat{\mu}_{i}^{2} - 2\hat{\mu}_{i}n_{i}\overline{y}_{i} - n_{i} {}_{0}\hat{\mu}_{i}^{2} + 2 {}_{0}\hat{\mu}_{i}n_{i}\overline{y}_{i} \right) \right\} =$$

$$= \prod_{i=l}^{k} exp \left\{ -\frac{n_{i}}{2\sigma_{i}^{2}} \left(\overline{y}_{i}^{2} + \hat{\mu}_{i}^{2} - 2\hat{\mu}_{i}\overline{y}_{i} - \overline{y}_{i}^{2} - {}_{0}\hat{\mu}_{i}^{2} + 2 {}_{0}\hat{\mu}_{i}\overline{y}_{i} \right) \right\} =$$

$$= \prod_{i=l}^{k} exp \left\{ -\frac{n_{i}}{2\sigma_{i}^{2}} \left[(\overline{y}_{i} - \hat{\mu}_{i})^{2} - (\overline{y}_{i} - {}_{0}\hat{\mu}_{i})^{2} \right] \right\}$$

 $H_0 \text{ will be rejected for large values of } T = 2\ln\Lambda = -\sum_{i=1}^k w_i \left[\left(\overline{Y}_i - \hat{\mu}_i \right)^2 - \left(\overline{Y}_i - _0 \hat{\mu}_i \right)^2 \right] = \sum_{i=1}^k w_i (\overline{Y}_i - _0 \hat{\mu}_i)^2 - \sum_{i=1}^k w_i (\overline{Y}_i - \hat{\mu}_i)^2 .$

Now we will look at the test statistic under the family of linear transformations of Y_i .

Theorem 3.2: T is invariant under the family of linear transformations of Y_i , $Y'_i = a + bY_i$, if b > 0.

Proof:
$$T' = \sum_{i=1}^{k} w'_i (\overline{Y}'_i - {}_0 \hat{\mu}'_i)^2 - \sum_{i=1}^{k} w'_i (\overline{Y}'_i - \hat{\mu}'_i)^2$$

By $Y'_i = a + bY_i$, Lemma 3.2.2 and Lemma 3.2.3 we have
 $T' = \sum_{i=1}^{k} \frac{n_i}{b^2 \sigma_i^2} (a + b\overline{Y}_i - a - b_0 \hat{\mu}_i)^2 - \sum_{i=1}^{k} \frac{n_i}{b^2 \sigma_i^2} (a + b\overline{Y}_i - a - b \hat{\mu}_i)^2 =$
 $= \sum_{i=1}^{k} \frac{n_i}{b^2 \sigma_i^2} b^2 (\overline{Y}_i - {}_0 \hat{\mu}_i)^2 - \sum_{i=1}^{k} \frac{n_i}{b^2 \sigma_i^2} b^2 (\overline{Y}_i - \hat{\mu}_i)^2 = \sum_{i=1}^{k} w_i (\overline{Y}_i - {}_0 \hat{\mu}_i)^2 - \sum_{i=1}^{k} w_i (\overline{Y}_i - {}_0 \hat{\mu}_i)^2 = T$

Lemma 3.2.1: Linear transformations of Y_i , $Y'_i = a + bY_i$, b > 0, do not change the level sets determining the ML-estimator under H_0 .

Proof: If the level sets determining ${}_{0}\hat{\mu}$ are A_{s} , s=1,2,...,t, then ${}_{0}\hat{\mu}_{i} = \frac{\sum_{i \in A_{s}} w_{i}\overline{Y}_{i}}{\sum_{i \in A_{s}} w_{i}}$ and if the

level sets determining $_{0}\hat{\mu}'$ are A'_{s} , s=1,2,...,t', then $_{0}\hat{\mu}'_{i} = \frac{\sum_{i \in A'_{s}} w'_{i}\overline{Y}'}{\sum_{i \in A'_{s}} w'_{i}}$.

We study the subset $\{c-1,c,c+1\}$ of the set $\{1,...,c-1,c,c+1,...,k\}$ of k design points. Let $P_{c-1} = \left(\overline{Y}_{c-1}, \sum_{i=1}^{c-1} w_i\right)$, $P_c = \left(\overline{Y}_c, \sum_{i=1}^{c} w_i\right)$ and $P_{c+1} = \left(\overline{Y}_{c+1}, \sum_{i=1}^{c+1} w_i\right)$. According to the "Pool-Adjacent-Violators" algorithm (Robertson et al., 1988) the design point c is a

violator if the slope between P_{c-1} and P_c is stronger than the slope between P_c and P_{c+1}

or equivalently if
$$\frac{\overline{Y}_{c} - \overline{Y}_{c-l}}{\sum_{i=l}^{c} w_{i} - \sum_{i=l}^{c-l} w_{i}} > \frac{\overline{Y}_{c+l} - \overline{Y}_{c}}{\sum_{i=l}^{c+l} w_{i} - \sum_{i=l}^{c} w_{i}} \Leftrightarrow \frac{\overline{Y}_{c} - \overline{Y}_{c-l}}{w_{c}} > \frac{\overline{Y}_{c+l} - \overline{Y}_{c}}{w_{c+l}}.$$

Now, consider the linear transformation $Y'_i = a + bY_i$, and the same subset of design points. Then, c is a violator if $\frac{a + b\overline{Y}_c - (a + b\overline{Y}_{c-1})}{\sum_{i=1}^c \frac{w_i}{b^2} - \sum_{i=1}^{c-l} \frac{w_i}{b^2}} > \frac{a + b\overline{Y}_{c+1} - (a + b\overline{Y}_c)}{\sum_{i=1}^c \frac{w_i}{b^2} - \sum_{i=1}^{c-l} \frac{w_i}{b^2}} \Leftrightarrow \frac{b^3(\overline{Y}_c - \overline{Y}_{c-1})}{w_c} > \frac{b^3(\overline{Y}_{c+1} - \overline{Y}_c)}{w_{c+1}}.$

Thus, if b > 0 then m' = m and $A'_s = A_s \quad \forall s = 1, 2, ..., t$.

Lemma 3.2.2: Linear transformations of Y_i , $Y'_i = a + bY_i$, b > 0, implies ${}_0 \hat{\mu}'_i = a + b_0 \hat{\mu}_i$.

Proof: By Lemma 3.2.1 we have $A'_s = A_s \forall s=1,2,...,t$ and thus:

$${}_{0}\hat{\mu}'_{i} = \frac{\displaystyle\sum_{i \in A'_{s}} w'_{i}\overline{Y'}}{\displaystyle\sum_{i \in A_{s}} w'_{i}} = \frac{\displaystyle\sum_{i \in A_{s}} \frac{w_{i}(a+b\overline{Y}_{i})}{b^{2}}}{\displaystyle\sum_{i \in A_{s}} \frac{w_{i}}{b^{2}}} = \frac{\frac{a}{b^{2}} \displaystyle\sum_{i \in A_{s}} \frac{n_{i}}{\sigma_{i}^{2}} + \frac{b}{b^{2}} \displaystyle\sum_{i \in A_{s}} \frac{n_{i}\overline{Y}_{i}}{\sigma_{i}^{2}}}{\frac{l}{b^{2}} \displaystyle\sum_{i \in A_{s}} \frac{n_{i}}{\sigma_{i}^{2}}}.$$

Multiplying numerator and denominator with $\frac{b^2}{\sum_{i \in A_r} \sigma_i^2}$ gives

$${}_{\scriptscriptstyle 0}\hat{\mu}'_{\scriptscriptstyle i} = a + b \frac{\displaystyle\sum_{i \in A_s} w_i \overline{Y}_i}{\displaystyle\sum_{i \in A_s} w_i} = a + b {}_{\scriptscriptstyle 0}\hat{\mu}_i$$

Lemma 3.2.3: Linear transformations of Y_i , $Y'_i = a + bY_i$, b > 0, implies $\hat{\mu}'_i = a + b\hat{\mu}_i$.

Proof: As the unimodal regression estimator is constructed by a choice of combinations of independent monotonic parts, it follows by Lemma 3.2.2 that $\hat{\mu}'_i = a + b\hat{\mu}_i$ since all the monotonic parts are transformed in that way.

4. A test with an upper limit for the size

With the aim to construct a conservative test, we elucidate the least favourable configuration under H_0 for the test statistic $T = \sum_{i=1}^{k} w_i (\overline{Y}_i - {}_0 \hat{\mu}_i)^2 - \sum_{i=1}^{k} w_i (\overline{Y}_i - \hat{\mu}_i)^2$, which was derived in Theorem 3.1.

Theorem 4.1: Using the critical value t_{α} , from the distribution of T, when $\mu_i = \mu$, i=1,2,...,k, makes the test conservative for all other members of H_0 .

Proof: We introduce the notations ${}_{0}Q = \sum_{i=1}^{k} w_{i} (\overline{Y}_{i} - {}_{0}\hat{\mu})^{2}$ and $Q = \sum_{i=1}^{k} w_{i} (\overline{Y}_{i} - \hat{\mu})^{2}$. $T = {}_{0}Q - Q$ is stochastically increasing with μ_{l} since

1) $_{0}Q$ is stochastically increasing with μ_{1} by Lemma 4.1.1.

2) Q is stochastically decreasing with increasing μ_l given $Q \neq_0 Q$ by Lemma 4.1.2.

3) $Pr(Q=_{0}Q)$ decreases with increasing μ_{l} by Lemma 4.1.3.

The largest possible value of μ_l under H_0 is μ_k which implies $\mu_i = \mu_k$, i=1,...,k-1. Thus $Pr(T > t_{\alpha} \mid H_0) \le Pr(T > t_{\alpha} \mid \mu_i = \mu, i = 1, 2, ..., k)$.

Lemma 4.1.1: $_{0}Q$ is stochastically increasing with μ_{l} .

Proof: In this lemma we use the notations ${}_{0}Q^{k} = \sum_{i=1}^{k} {}_{0}Q_{i}^{k} = \sum_{i=1}^{k} w_{i}(\overline{Y}_{i} - {}_{0}\hat{\mu}_{i}^{k})^{2}$ and $Q^{k} = \sum_{i=1}^{k} Q_{i}^{k} = \sum_{i=1}^{k} w_{i}(\overline{Y}_{i} - {}_{0}\hat{\mu}_{i}^{k})^{2}$, where the super-index k denotes that the statistic is based

on the design points 1,2,...,k. Corresponding notations with super-index k-1 denote that the statistic is based on the k-1 design points 2,3,...,k.

If
$${}_{\scriptscriptstyle 0}\hat{\mu}^k_{\scriptscriptstyle I} = \overline{Y}_{\scriptscriptstyle I}$$
 then ${}_{\scriptscriptstyle 0}Q^k_{\scriptscriptstyle I} = 0$ and ${}_{\scriptscriptstyle 0}Q^k = {}_{\scriptscriptstyle 0}Q^{k-1}$.

Else,
$$_{0}\hat{\mu}_{1}^{k} = \frac{\sum_{i=l}^{r} w_{i}\overline{Y}_{i}}{\sum_{i=l}^{r} w_{i}}$$
, where $r > 1$ and $\overline{Y}_{l} >_{0}\hat{\mu}_{l}^{k}$

We then write ${}_{0}Q^{k} = {}_{0}Q_{1}^{k} + \left[\sum_{i=2}^{k} {}_{0}Q_{i}^{k} - \sum_{i=2}^{k} {}_{0}Q_{i}^{k-1}\right] + {}_{0}Q^{k-1}$. The first term has its minimum zero when ${}_{0}\hat{\mu}_{1}^{k} - \overline{Y}_{1}$ is zero and is increasing with this difference when it is negative. The same is true for the middle term since $\sum_{i=2}^{k} {}_{0}Q_{i}^{k-1}$ is the minimum deviance based on k-1 design points and the larger \overline{Y}_{1} the larger deviation from this minimum. The last term is independent of \overline{Y}_{1} . Thus, ${}_{0}Q^{k}$ is stochastically increasing with μ_{1} .

Lemma 4.1.2: Q is stochastically decreasing with increasing μ_l given that $Q \neq_0 Q$.

Proof: Let ${}_{m}Q$ be the quadratic deviation when the maximum likelihood estimation is done under the restriction " $\mu_{1} \ge ... \ge \mu_{m}$ and $\mu_{m} \le ... \le \mu_{k}$ ", where ${}_{l}Q \equiv_{0}Q$. By the same technique as in Lemma 4.1.1 it can be proved that the deviation ${}_{m}Q$ is stochastically decreasing with increasing μ_{l} if m > 1. Given that $Q \neq_{0}Q$ we have $Q = \min_{m>l} {}_{0}Q$. Since each ${}_{m}Q$, m > 1, decreases with μ_{l} also the minimum decreases. Thus, Q is stochastically decreasing with increasing μ_{l} given that $Q \neq_{m}Q$.

Lemma 4.1.3: $Pr(Q=_{0}Q)$ decreases with increasing μ_{I} .

Proof: $Pr(Q=_{0}Q) = Pr(\min_{m=1,2,...,k} Q=_{0}Q)$, where $_{m}Q$ is defined in Lemma 4.1.2, is decreasing with increasing μ_{I} , since $_{0}Q$ is stochastically increasing with μ_{I} , while $_{m}Q$, m>1 is decreasing with increasing μ_{I} .

Theorem 4.1 is valid for all vectors **w**. However, the distribution of *T* depends on how uneven information we have at different design points. From now on we only treat the case of equal information in all design points, that is $w_i = w$ for all *i*.

4.1 The distribution of the test statistic for the worst case under H_0

For the worst case with equal expected values and for the case of equal information in all design points the distribution of T under H_0 does not depend on any parameters besides the number, k, of design points. The distribution has been studied by means of simulation for this situation. The cumulative density function is illustrated for k = 5 and k = 20 in Figure 4.1.1.



Figure 4.1.1: The distribution for k=5 *and* k=20, *respectively.*

The distribution of the test statistic is mixed. It consist of a discreet part where T=0 and a continuous part, where T>0.

Theorem 4.1.1: When $\mu_i = \mu$, i=1,2,...,k we have: for k=2,3, Pr(T=0)=1/k, for larger values of k we have Pr(T=0)<1/k.

Proof: T=0 if and only if the maximum likelihood estimates are equal under the two restrictions, that is $_{0}\hat{\mu} = \hat{\mu}$. This can happen only when the first design point has the least observed value.

For k=2 and 3, the estimators are equal if the first design point has the least observed value. The probability of this is 1/k. Thus Pr(T=0)=1/k for k=2 and 3.

For k>3, there are other possibilities, with probability larger than zero, than that the two estimators are equal, when the first design point has the least observed value. Thus Pr(T=0)<1/k.



Figure 4.1.2: Comparison of Pr(T=0) estimated by simulations (symbol \times) and 1/k (symbol \circ).

By simulations, critical values that guarantee that the size of the test is less than 0.05 and 0.01, respectively, have been estimated and the results are presented in Table 4.2.1 and Figure 4.2.1.

The critical values given in Table 4.2.1 are percentiles in the empirical distribution of 100 000 replicates of T for each situation. Thus, an approximate 95% confidence interval for the true value of α at the nominal value $\alpha=0.05$ is 0.05 ± 0.00136 . The corresponding confidence interval at the nominal value $\alpha=0.01$ is 0.01 ± 0.00062 .

Table 4.2.1: Critical values, T_{α} *such that* $Pr(T > T_{\alpha}) \le \alpha$

k	$\alpha = 0.05$	$\alpha = 0.01$	k	$\alpha = 0.05$	<i>α</i> = 0.01
2	2.70018	5.38288	18	11.5505	16.0376
3	4.21823	7.33161	19	11.7670	16.4073
4	5.25369	8.58753	20	11.9503	16.5436
5	6.13142	9.54701	21	12.2048	16.9065
6	6.80475	10.2967	22	12.3617	17.0355
7	7.38956	11.2040	23	12.5750	17.2640
8	7.97443	11.7000	24	12.8106	17.3623
9	8.48308	12.2560	25	12.8652	17.7199
10	8.85470	12.6842	26	13.1571	17.9440
11	9.18725	13.1183	27	13.3429	18.0701
12	9.58137	13.6551	28	13.4254	18.1562
13	9.96327	14.1130	29	13.5763	18.1734
14	10.3419	14.5143	30	13.7376	18.5098
15	10.6497	14.9969	50	16.0418	21.0389
16	10.9210	15.2197	100	19.3402	24.5410
17	11.2215	15.6325			



Figure 4.2.1: The relation between T_{α} and k for $\alpha=0.05$ (symbol \times) and $\alpha=0.01$ (symbol \circ).

5. The power of the test

In this section the power of the test is estimated for some examples of the alternative hypothesis. The estimation is done by simulations. Critical values for the least favourable configuration for the test statistic under H_0 are used. As for the determination of critical values in Section 4, only the case of equal information, w, at all design points is treated.

The shape of the regression can be expressed by the successive differences, $\mu_{i+1} - \mu_i$, i=1,2,...,k-1. When these differences are standardised we have $\gamma_i = w(\mu_{i+1} - \mu_i)$, i=1,2,...,k-1. The vector $\gamma = \{\gamma_1,...,\gamma_{k-1}\}$ thus contains all necessary information. The location of the turning point is important and is determined by *m*, where $\gamma_1,...,\gamma_{m-1} \leq 0$ and $\gamma_m,...,\gamma_{k-1} \geq 0$. At least one of the inequalities for $\gamma_1,...,\gamma_{m-1}$ is strict. Under H_1 the value of *m* can be any value between 2 to *k*.

We want to make statements on how the following factors influence the power:

- the total number of design points
- the number of design points corresponding to the part under question and the part with known monotonicity, respectively
- the slope of the regression in the part under question and the part with known monotonicity, respectively

By means of some examples we now investigate how the factors above influence the power. The examples come from the class of problems where $\gamma_1, ..., \gamma_{m-1} = \gamma'$ and $\gamma_m, ..., \gamma_{k-1} = \gamma''$. We start by examining the case where $|\gamma'| = \gamma'' = \gamma > 0$, k is odd and $m = \frac{k+1}{2}$. In this class of problems, the first half part of the regression in the design points is linearly decreasing and the following half part is linearly increasing. The results from the simulation study for this first case are presented in Table 5.1 for different values of γ in the interval 0.26 - 1.00 and different number of design points. The value $\gamma = 0.26$ is a relevant value in studies of business cycles (Andersson, 1999).

γ	k	α=0.05	α=0.01	γ	<u>k</u>	α=0.05	α=0.01
0.26*	19	0.60258	0.33389	0.65**	9	0.4779	0.2435
	21	0.72668	0.46495		11	0.7232	0.4808
	23	0.84549	0.62183		13	0.8964	0.7380
	25	0.93327	0.76722		15	0.9829	0.9256
	27	0.97677	0.88935		17	0.9985	0.9903
	29	0.99441	0.96195		19	1.0000	0.9998
0.30**	17	0.5966	0.3340	0.70**	9	0.5392	0.2902
	19	0.7255	0.4663		11	0.7851	0.5638
	21	0.8575	0.6393		13	0.9376	0.8164
	23	0.9385	0.7900		15	0.9920	0.9631
	25	0.9862	0.9136		17	0.9996	0.9976
	27	0.9961	0.9736				
0.35**	15	0.5759	0.3143	0.75**	9	0.5982	0.3467
	17	0.7314	0.4846		11	0.8382	0.6404
	19	0.8574	0.6452		13	0.9647	0.8766
	21	0.9472	0.8160		15	0.9973	0.9835
	23	0.9781	0.8994		17	1.0000	0.9992
	25	0.9989	0.9875				
0.40**	13	0 5026	0 2553	0 80**	7	0 3782	0 1620
0.40	15	0.5020	0.2333	0.00	<u>,</u>	0.5782	0.1029
	13	0.0920	0.4346		9	0.0307	0.4010
	17	0.0430	0.0300		11	0.0033	0.7142
	19	0.9378	0.8007		15	0.9814	0.9208
	21	0.9800	0.9313		15	0.9993	0.9918
	23	0.9986	0.9843				
	25	1.0000	0.9991				
0.45**	13	0.5983	0.3436	0.85**	7	0.4153	0.1876
	15	0.7917	0.5620		9	0.7030	0.4610
	17	0.9189	0.7685		11	0.9180	0.7788
	19	0.9798	0.9078		13	0.9910	0.9551
	21	0.9972	0.9810		15	0.9998	0.9974
	23	0.9999	0.9986				
0.50**	11	0.4995	0.2608	0.90**	7	0.4529	0.2178
	13	0.6946	0.4420		9	0.7530	0.5262
	15	0.8704	0.6825		11	0.9482	0.8358
	17	0.9635	0.8733		13	0.9958	0.9768
	19	0.9938	0.9642		15	1.0000	0.9992
	21	0.9994	0.9958				
0 55**	11	0 5795	0 3270	0 92**	7	0 4013	0 2497
0.55	13	0.3793	0.5446	0.75	ó	0.7062	0.5877
	15	0.7789	0.3440		11	0.7902	0.3877
	17	0.9279	0.7841		12	0.9040	0.8800
	10	0.9032	0.2374		15	0.7701	0.7000
	17	0.7707	0.7075				
0.60**	11	0.6518	0.4005	1.00*	7	0.53642	0.28239
	13	0.8473	0.6427		9	0.83407	0.63459
	15	0.9631	0.8703		11	0.97865	0.91851
	17	0.9954	0.9738		13	0.99912	0.99441
	19	0.9999	0.9973		15	1.00000	0.99940
	21	1 0000	0 9998				

Table 5.1: The power of the test when $|\gamma'| = \gamma'' = \gamma > 0$, k is odd and $m = \frac{k+1}{2}$.

*The power is estimated from 100 000 replicates of T** The power is estimated from 10 000 replicates of T

In Figure 5.1 the results are illustrated for $\gamma=0.26$, $\gamma=0.50$, $\gamma=0.75$ and $\gamma=1.00$. The results show how, given γ , the power increases with the number, k, of design points.



 $\alpha = 0.05$



 $\alpha = 0.01$

Figure 5.1: The power as a function of the number of design points, for $\gamma = 0.26$ (symbol \Box), $\gamma = 0.50$ (symbol \triangle), $\gamma = 0.75$ (symbol \bigcirc) and $\gamma = 1.00$ (symbol \times).

Further conclusion is that the stronger slope the fewer design points are needed to receive great power. However, even for the weakest slope exemplified, 0.26, the test is quite useful. For that case, about twelve points on each side of the turning point give an acceptable power. In Figure 5.2, combinations of γ and the least value of k, of those values given in Table 5.1, which guarantees power >0.65 and >0.90 are presented. Another conclusion from Table 5.1 and Figure 5.1 is that the stronger slope the greater is the effect of the number of design points on the power. In other words, the stronger slope the steeper power curve.

Intuitively, the part where it is uncertainty about the monotonicity of the curve has great effect on the power. A strong slope in this part increases the probability that data supports H_1 . However, in these examples, the slope is the same also in the increasing part of the regression, which mainly are design points corresponding to the part of the curve with known monotonicity. A strong slope in the part with known monotonicity will give slightly less power since the probability of a false indication of turn in that part decreases, but the impact of the slope in the unknown part dominates the effect on the power and this influence will now be examined.



 $\alpha = 0.05$



 $\alpha = 0.01$

Figure 5.2: Combinations of k and γ that guarantee power >0.65 (symbol \times) and >0.90 (symbol \circ).

The slope of the regression is an important factor for the power. We now investigate separately how the slope of the regression influences the power in the class of problems where $\gamma_1, ..., \gamma_{m-1} = \gamma'$, $\gamma_m, ..., \gamma_{k-1} = \gamma'' = 1$, k=9 and $m = \frac{k+1}{2} = 5$.

Keeping the slope in the increasing part of the regression constant we study the power for some slopes of the decreasing but not constant part. In Table 5.2 results are presented for $\gamma' = -0.01$, which gives a configuration under H_1 very close to H_0 , to $\gamma' = -2.00$, which gives a configuration under H_1 far from H_0 .



Figure 5.3: The configurations of the regression in the design points for $\gamma' = -0.01$ and $\gamma' = -2.00$, k=9, m=5 and $\gamma'' = 1$

Table 5.2: The power for different values of γ' , when k=9, m=5 and $\gamma''=1$

γ	α = 0.05	α = 0.01
-0.01	0.0197	0.0036
-0.25	0.0787	0.0182
-0.50	0.2531	0.0974
-0.75	0.5580	0.3139
-1.00	0.83407	0.63459
-1.25	0.9677	0.8906
-1.50	0.9975	0.9842
-1.75	0.9999	0.9992
-2.00	1.0000	1.0000

The result confirms the earlier statement. Stronger slope in the decreasing but not constant part consisting mainly of design points corresponding to the uncertainty part of the curve gives great power. Figure 5.4 illustrates the result.



Figure 5.4: The power as a function of $|\gamma|$, when k=9, m=5 and $\gamma''=1$, for $\alpha=0.05$ (symbol \circ) and $\alpha=0.01$ (symbol \times).

Finally, we study how the number of design points corresponding to the decreasing part in proportion to the number of design points in the increasing part effects the power for $\gamma = 1$ and k=9. In Table 5.3 the results for different values of *m*, from m=2, which gives a configuration under H_1 very close to H_0 , to m=9, which gives a configuration under H_1 far from H_0 are presented.



Figure 5.5: The configurations of the regression in the design points for m=2 and m=9, k=9 and $\gamma=1$.

The conclusion is that many design points in the decreasing but not constant part gives great power. In other words, design points corresponding to the uncertainty part of the curve give great power.

Table 5.3: The power for different values of m, k=9, $\gamma=1$.

т	α=0.05	α=0.01
2	0.0176	0.0044
- 3	0.1340	0.0451
4	0.4545	0.2368
5	0.83407	0.63459
6	0.9831	0.9360
7	0.9996	0.9968
8	1.0000	1.0000
9	1.0000	1.0000



Figure 5.6: The power as a function of m, k=9, $\gamma = 1$, $\alpha = 0.05$ (symbol \circ), $\alpha = 0.01$ (symbol \times)

6. The choice of design

We make statements about the relation between the independent variable and the expected values of the dependent variable, only in the design points. A turning point exists if the configuration of the regression in the design points is in accordance with the alternative hypothesis.

In this section we discuss the choice of design for *Case i*. Of course, corresponding statements can be made for the other three cases.

For understanding that the restriction under the alternative hypothesis implies that the curve includes a turning point, we must have in mind our prior knowledge about the shape of the curve. We are uncertain about the first part and certain about the final part of the curve. Example 6.1 illustrates that a turning point must exist if H_1 is true, but also how the choice of design points affects the possibility to indicate an existing turning point.

Example 6.1: Suppose that the information about the shape of the curve can be illustrated as in Figure 6.1.1.



Figure 6.1.1: The prior information about the shape of the curve implies uncertainty about the first part and certainty about the final part of the curve.

Let us now study five examples of three-points-designs for testing H_0 : The regression is increasing versus H_1 : The regression is U-shaped but not increasing. Important is that the hypotheses refer to the regression in the design points and not the curve.

If the curve includes a turning point, choosing three design points, the following four principal cases can arise:



Figure 6.1.2: The design points are chosen from the interval of the independent variable corresponding to the increasing part of the curve. The curve includes a turning point, but choosing design points corresponding to the part of the curve with known monotonicity always implies that H_1 is false.



Figure 6.1.3: The design points are chosen from the interval of the independent variable corresponding to the turning point part of the curve. The curve includes a turning point, but the design points are chosen in such a way that H_1 is false.



Figure 6.1.4: The design points are chosen from the interval of the independent variable corresponding to the turning point part of the curve. The curve includes a turning point and the design points are chosen in such a way that H_1 is true.



Figure 6.1.5: The design points are chosen from the interval of the independent variable corresponding to the decreasing part of the curve. Choosing design points corresponding to the part of the curve under question, when the curve includes a turning point, always implies that H_1 is true. The regression in the design points is certainly monotonic, but, bearing the prior information about the curve in mind, a decreasing regression in the design points implies that the curve must include a turning point.

If the curve is increasing and then not includes a turning point, choosing three design points, only one principal case can arise:



Figure 6.1.6: It does not matter which design points we are chosen from the independent variable. If the curve does not include a turning point H_1 can never be true.

If the curve includes a turning point, we then have to choose design points so that the configuration of the regression in the design points is in accordance with H_I . In other words, we have to choose a design not missing that a turning point in fact exist. If all design points are chosen in the curve's up-phase, then we miss it. If the design points are chosen in the turning point interval of the curve, then we might miss it. If all design points are chosen in the curve's down-phase, then we never miss it.

So then, if the curve includes a turning point, the design can miss it. However, H_I can never be true if the curve does not include a turning point. Thus, the size of the test still holds.

The discussion so far points to choose the design points in the down-phase of the curve, to eliminate the risk of missing the turning point of the curve. The results in Table 5.3 and Figure 5.6 illustrates that the power of the test is greatest when a large proportion of the design points corresponds to the down phase. We then have two good reasons to choose design points in the down-phase of the curve.

However, we must also have in mind a reason for another design choice strategy. If we chose all design points in the down-phase of the curve we do not get a validation of the curve's up-phase. Maybe it does not even exist an up-phase. Perhaps the curve is non-increasing but not constant. The validation of the 'knowledge' we have about the shape of the curve requires design points even in the up-phase of the curve.

Furthermore, we must remember that perhaps we do not know where the possible turning point is located, and by that we cannot securely choose a design point in a given phase of the curve.

According to (Goetghebeur & Pocock, 1995), there are many more data points to the right of the turning point than to the left in most medical examples. In many applications one can expect to have much information on one part but less on the other.

In Example 6.2 an important aspect of the choice of design is illustrated.

Example 6.2: Suppose that the curve is shaped as in Figure 6.2.1 (a), a linear downphase followed by a linear up-phase.

In Figure 6.2.1 (b), (c) and (d) three-points-designs are illustrated. In all designs the design points are chosen equidistant from the independent variable. In (b), the first two design points are chosen corresponding to the curve's down-phase and the last point is chosen corresponding to the curve's up-phase. In (c), the design points are chosen from an over lapping, but of the same width, interval as in (b). However, all design points are chosen corresponding to the curve's down-phase. In (d), all design points are chosen corresponding to the curve is down-phase. In (d), all design points are chosen corresponding to the curve is down-phase. In (d), all design points are chosen corresponding to the down-phase of the curve, but from a wider interval compared to (c).



Figure 6.2.1: Examples of three-points-designs. In (b) the values 7, 9 and 11, in (c) the values 5, 7 and 9 and in (d) the values 2, 6 and 10 are chosen from the dependent variable.

According to the simulation results, d) gives greater power than c), which gives greater power than b). The conclusion is then, given the number of design points, that great power is received if all design points are chosen from a wide interval of the downphase, that is the uncertainty part, of the curve.

Another important aspect of the choice of design is illustrated in Example 6.3. Expanding a design with additional design points may change the slope of the regression in the design points.

Example 6.3: Suppose that the curve is shaped as in Figure 6.3.1 (a), a linear downphase followed by a linear up-phase. Figure 6.3.1 (b) shows a three-points-design where the design points are chosen equidistantly from the interval of the independent variable corresponding to the curves down-phase. Figures 6.3.1 (c) and (d) show examples of five-points-designs. Both designs include the points in (a) and two more points. In (c) the design points are chosen equidistantly from a wider interval of the independent variable, corresponding to the curves down-phase, than in (b).

The slopes of the regressions are then the same in (b) and (c). In (d) the design points are chosen in the same interval as in (b), equidistant but closer. Therefore the slope of the regression in (d) is weaker compared to (b) and (c).



Figure 6.3.1: One three-points-design and two five-points-designs. In (b) the values 5, 7 and 9, in (c) the values 1, 3, 5, 7 and 9 and in (d) the values 5, 6, 7, 8 and 9 are chosen from the independent variable.

The conclusion is then that when expanding the design with additional design points, the choice of points will affect the slope of the regression in the design points. This is important when using Table 5.1, for example.

7. Concluding remarks

Situations with limited information about the shape of the curve have been treated. Only information in terms of order-restricted relations is used. No parametric regression function is assumed. In this respect the estimation and test are non-parametric. However, the residuals around the regression function are assumed to have the normal distribution. In this distributional respect, the test is not non-parametric. Interesting for future investigations is the robustness of the test for other distributions than the normal one.

The test statistic has been derived for one of four principal combinations of hypotheses, but the other three cases can simply be handled by transforming the data and formulating the hypotheses for the new data. The aim of the transformations is of course to make use of the results from *Case i*, presented in this work. The transformations presented in Section 3 imply how we change from the actual *Case ii*, *iii* or *iv* to *Case i*. Observe that the whole problem is described in new way and that we also test other hypotheses, namely the hypotheses in *Case i*. An alternative to the transformations is to derive the likelihood ratio test in an analogous way as in *Case i*.

When the hypotheses cannot be expressed as any of the four cases above, but as a combination of these like "monotonicity versus existence of a turning point" we can handle this by standard methods for multiple inference.

The test is invariant under linear transformations as long as the scale parameter b is positive. By that the test statistic has two important properties. For all levels, a, of the independent variable the data can be transformed $y'_{ij} = y_{ij} - a$ without making any change of the value of the test statistic. Choosing $a = y_{11}$, for example, the differences $y_{ij} - y_{11}$ are enough besides the information vector calculating the test statistic. Further, it does not matter in which scale the variable is expressed. Transforming the data from metre to the centimetre, for example, does not affect the value of the test statistic

A linear transformation, where the sign of b is negative always implies a change between two cases. As mentioned in Section 3, for a=0 and b=-1, the hypotheses in

Case iii for the original data describes the same problem as the hypotheses in *Case i*, for the transformed data.

A conservative test has been constructed using the least favourable configuration of the regression for the test statistic under H_0 . In the class of problems with equal information in all design points the distribution of the test statistic depends on the number of design points only. Equal information in all design points implies that the maximum likelihood estimates for each level set are un-weighted means of the observations corresponding to the set. The amount of information does not influence the distribution of the test statistic under the "worst case" of H_0 . Thus one table of critical values is enough. Interesting for future investigation is the robustness of the test for divergence from equal information in all design points.

The power of the test has been estimated for some examples of configurations under H_1 . The results are that the test has high enough power to be useful.

An important factor, influencing the power, is the configuration of the regression in the design points. In this work, the class of problems where the regression is linear both in the down-phase as in the up-phase has been studied and the configuration has been expressed and discussed in terms of the slope of the regression in the design points. The slope depends on two factors, the shape of the curve and the chosen design points. The conclusion from the simulation study is that, for design points chosen in the part of uncertainty of the curve, strong slope gives great power. This result is the expected one.

Given the amount of information in the design points, great power is received with many design points and in so wide an interval as possible in the part of the curve where uncertainty about the shape is prevailing.

For a fixed interval of the curve, increasing the number of design points, which means that the design points are chosen closer, gives values of $\gamma_i = w(\mu_{i+1} - \mu_i)$, which are closer to zero. However, the power will still be greater because of an increasing number of design points gives greater power. In other words, it is no loss of power increasing the amount of information. This is what should be expected by a fair test.

An argument against designs where all points are chosen in the part of uncertainty is that it will be no validation about the certainty part of the curve. Perhaps we are testing the wrong class of hypotheses. However, if the analysis is confirmative, enough knowledge about the problem may be available for using designs giving great power before validation of the model.

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