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Non-linearity measures: a case-study

by

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Eindhoven, August 1974

Non-linearity measures: a case-study

by H.N. Linssen *

0. Summary

A frequently encountered problem is the fitting of a data-vector by means of a model function with a number of parameters, whose ^{values} are unknown. Minimizing the residual sum of squares delivers the least squares estimates. The problem of their precision is only solved in the linear case. We discuss and illustrate the quality of approximate (though asymptotically exact) confidence statements.

1. Definitions and Notations

The regression equation is:

$$\underline{y} = f(\beta) + \underline{e} ,$$

where $\underline{y}$ is the data vector, f the vector valued model function, $\underline{e}$ the error term (all three size n), and β the parameter vector (size p).

The residual sum of squares is:

$$S(\beta) := \|\underline{y} - f(\beta)\|^2 .$$

The l.s. estimates of β are denoted by $\hat{\beta}$. Furthermore

$$s^2 := S(\hat{\beta})/(n-p) .$$

In sample space we define the solution locus:

$$\theta := \{\underline{y} \mid \exists_{\beta} \underline{y} = f(\beta)\} .$$

Linear approximation of f in $\hat{\beta}$ will be called linearization.

The linearized solution locus is:

$$\tau := \{\underline{y} \mid \exists_{\beta} \underline{y} = f(\hat{\beta}) + \frac{\partial f}{\partial \beta} (\beta - \hat{\beta})\} ,$$

where

$$\frac{\partial f}{\partial \beta} = \left(\frac{\partial f_i}{\partial \beta_j} \Big|_{\hat{\beta}} \right) .$$

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2. A measure of non-linearity

2.1. Definition

$\theta \equiv \tau$ holds in the linear case. As a measure of non-linearity we might use:

$$\|f(\beta) - \tau(\beta)\|^2.$$

This measure is unstandardized, depending as it is on the choice of β .

Because of

$$\|f(\beta) - \tau(\beta)\| = O(\|\beta - \hat{\beta}\|^2) \quad \text{and} \quad \|f(\hat{\beta}) - \tau(\beta)\| = O(\|\beta - \hat{\beta}\|),$$

$$\|f(\beta) - \tau(\beta)\|^2 / \|f(\hat{\beta}) - \tau(\beta)\|^4$$

can be considered to be a standardized measure. Its denominator has dimension observation squared and the nominator observation to the fourth. So at last:

$$M := ps^2 \|f(\beta) - \tau(\beta)\|^2 / \|f(\hat{\beta}) - \tau(\beta)\|^4$$

is a standardized and dimensionless measure of non-linearity. p is added for reasons of simplicity.

2.2. Interpretation

We assume $\underline{e} \sim N(0, \sigma^2 I)$, s^2 is then an estimate of σ^2 and the linearized confidence ellipsoid (confidence $1-\alpha$) is given by

$$\left\| \frac{\partial f}{\partial \beta} (\beta - \hat{\beta}) \right\|^2 \leq ps^2 F_{n-p}^p(\alpha).$$

To compute M β is taken on the ellipsoids contour. Then:

$$\left\| \frac{\partial f}{\partial \beta} (\beta - \hat{\beta}) \right\|^2 = \|\tau(\beta) - f(\hat{\beta})\|^2 = d^2 = ps^2 F_{n-p}^p(\alpha) \quad (\text{fig.1}).$$

So:

$$M = ps^2 \epsilon^2 d^2 / d^4 = \epsilon^2 / F_{n-p}^p(\alpha).$$

- (1) If $\epsilon < .1$ (say) or equivalently $M < .01/F_{n-p}^p(\alpha)$ the model is nearly linear, else if $\epsilon < 1$ or equivalently $M < 1/F_{n-p}^p(\alpha)$ it can be said to be moderately linear, else it is severely non-linear.

Mind. Beale introduced several non-linearity measures. Among them one similar to M , but with $\|f(\hat{\beta}) - f(\beta)\|^4$ in the denominator. Call this measure N then it is easy to see:

$$\epsilon \ll 1 \rightarrow N \approx M$$

and

$$\epsilon \gg 1 \rightarrow M = O(\epsilon^2) \quad \text{and} \quad N = O(1/\epsilon^2),$$

so when ϵ is large N is small and the rule of thumb (1) does not apply for N .

2.3. Example

A model for the viscosity of lubricants in dependence of pressure and temperature was developed by Witt. It goes:

$$f(\beta) = \frac{\beta_1}{\beta_2 + t} + \beta_3 d + \beta_4 d^2 + \beta_5 d^3 + (\beta_6 d + \beta_7 d^3) \cdot \exp\left(-\frac{t}{\beta_8 + \beta_9 d^2}\right),$$

where d = excess pressure (bar), t = temperature ($^{\circ}\text{C}$), $n = 54$ and $p = 9$.
 The observational error is *independent, homogeneous and normally distributed*.
 To make M as insensitive as possible to the choice of β , a number of points β_w ($w = 1, \dots, W$) was chosen, namely all the endpoints of the principal axes of the 50% linearized confidence ellipsoid. The adjusted measure is denoted by M^* and equals:

$$M^* = ps^2 \sum_{w=1}^W \|f(\beta_w) - \tau(\beta_w)\|^2 / \sum_{w=1}^W \|f(\hat{\beta}) - \tau(\beta_w)\|^4 .$$

M^* was computed for two lubricants (lubricant 1, with model (5) and lubricant 2 with a similar model). Its values are given in table 1. It is obvious that according to our rule of thumb (1) linearization cannot said to be satisfactory.

<u>table 1</u>		
M^*		
lubricant	1	2
	.43	.44

The values of ϵ , shown in table 2, also show that linearization is inappropriate.

<u>table 2</u>		
ϵ		
	<u>maximum</u>	<u>mean</u>
lubricant 1	1.8	.3
2	2.0	.4

The large values in tables 1 and 2 were caused by large deviations from linearity on the one or two largest principal axes of the confidence ellipsoid, whereas on the other axes the deviations from linearity were negligible.

3. A measure of intrinsic non-linearity

3.1. Definition

It is possible to reduce non-linearity by parameter transformation. Let φ be a transformation. Then τ can be represented as:

$$\tau(\varphi) = f(\hat{\beta}) + \frac{\partial f}{\partial \varphi(\hat{\beta})} (\varphi - \varphi(\hat{\beta})) .$$

M is invariant under translations and orthogonal linear transformations (β fixed) so φ can be chosen such that

$$\varphi(\hat{\beta}) = 0 \quad \text{and} \quad \frac{\partial \varphi}{\partial \hat{\beta}} = I .$$

So:

$$\tau(\varphi) = f(\hat{\beta}) + \frac{\partial f}{\partial \hat{\beta}} \varphi .$$

Let γ be the minimal transformation, i.e. minimizing the distance between θ and τ . γ has to satisfy:

$$\|f(\beta) - \tau(\gamma)\| \text{ minimum}$$

or

$$(2) \quad \|f(\beta) - f(\hat{\beta}) - \frac{\partial f}{\partial \hat{\beta}} \gamma\| \text{ minimum} .$$

This is a linear least squares problem. The value of M corresponding to γ is a measure of intrinsic (irreducible) non-linearity and will be denoted by m. M can be called a measure of extrinsic non-linearity.

3.2. Interpretation

Again we assume $\underline{e} \sim N(0, \sigma^2 I)$. An unbiased confidence region with approximate ^{*}) confidence $1-\alpha$ is given by:

$$(3) \quad \{\beta \mid S(\beta) - S(\hat{\beta}) \leq ps^2_{n-p} F^p_{n-p}(\alpha)\} .$$

^{*}) Unbiased because equal likelihood contours are also equal residual sum of squares contours and approximate because the confidence is asymptotically and in the linear case equal to $1-\alpha$.

A theoretical measure of intrinsic non-linearity (say m_t) was introduced by Beale. He showed, provided m_t is not too large, that the confidence region (3) is *conservative* (confidence $\geq 1-\alpha$) if the right-hand side of (3) is multiplied by

$$1 + n/(n-1)m_t \quad (p = 1)$$

and

$$1 + n/(n-p)(p+2)/pm_t \quad (p > 1) .$$

m is an approximation to m_t so we may hope this statement also to be valid with m instead of m_t .

3.3. Example

m^* was computed for the two lubricants. The relation between m and m^* is the same as that between M and M^* . The m^* values are shown in table 3. In table 4 the values of ϵ are displayed.

<u>table 3</u>		
	m^*	
lubricant	<u>1</u>	<u>2</u>
	.0008	.0036

<u>table 4</u>		
	ϵ	
	<u>maximum</u>	<u>mean</u>
lubricant 1	.11	.02
2	.18	.03

A substantial reduction of non-linearity seems possible.

4. Conclusions

At first sight the values of M give no reason to expect satisfactory results from linearization of the viscosity model. On the contours of the linearized confidence ellipsoid the linearized sum of squares is almost equal or substantially smaller than the actual sum of

squares. So the linearized confidence ellipsoid ^{seems to} include the unbiased confidence region. This and the value of m^* give reason to believe the linearized confidence statements to be conservative.

Because m^* is small the parameter transformation $\gamma = \gamma(\beta)$, given by the normal equations corresponding to (2), reduces non-linearity to negligible proportions, but in general it will be extremely difficult to find $\beta = \gamma^{-1}(\gamma)$.

5. References

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