Structure selection with ANOVA: local linear models

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Abstract

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Keywords: Identification, Nonlinear models, Analysis of variance

STRUCTURE SELECTION WITH ANOVA: LOCAL LINEAR MODELS

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1. PROBLEM DESCRIPTION

The problem that will be discussed in this paper is the one of easing the process of building good, parsimonious models of nonlinear systems. The tool used for obtaining this goal is the statistical method analysis of variance (ANOVA). (Miller, 1997) is a comprehensive reference.

In earlier work, it has been shown that ANOVA can be used to extract structure information from input/output data, see (Lind, 2000; Lind, 2001; Lind, 2002). This can be done without estimating any complex model, which is a great benefit due to the complexity of the estimation task. In this contribution it will be shown how the structure information from ANOVA can be applied to the local linear model structure.

2. THE KEY TO STRUCTURE INFORMATION

The key to extracting structure information from the data lies in utilising a point model with a special parameterisation, called a linear statistical model (here for a two-dimensional function):

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}, \quad (1)$$

The overall mean effect is denoted by μ . τ_i is the mean effect of the i th level of the factor A , where

$i = 1, \dots, a$, while β_j is the mean effect of the j th level of the factor B , where $j = 1, \dots, b$. The means are taken over all the levels of the other factor. The interactions between the factors are denoted by $(\tau\beta)_{ij}$, which is indexed by the levels of both factors. The random error component ε_{ijk} is assumed to come from a Gaussian distribution with constant variance σ^2 and the index k denotes the sample number from the ij :th level combination. The number of free parameters in the model is restricted by the following equations, that define all the effects as deviations from lower order interactions (with the overall mean as interaction of order zero): $\sum_{i=1}^a \tau_i = 0$, $\sum_{j=1}^b \beta_j = 0$, $\sum_{i=1}^a (\tau\beta)_{ij} = 0, \forall j$ and $\sum_{j=1}^b (\tau\beta)_{ij} = 0, \forall i$.

It is possible to divide the residual quadratic sum from this point model into orthogonal parts related to the τ_i 's, β_j 's, $(\tau\beta)_{ij}$'s and the random error component respectively. These then form F -distributed test variables that can be used to determine whether factor A and/or B affect the output at all, additively or with interaction.

For a higher-dimensional point model, the used parameterisation has many more than a sufficient number of parameters. The reason to use this parameterisation is that the high-order interactions are very seldom present in the data, so many of the interaction

effect parameters can be discarded with the F -tests, thereby simplifying the model while giving the wanted structural information.

The linear statistical model structure also benefit the transparency of the model. People tend to think about functional relationships in two- and three-dimensional views and have a hard time understanding complex interactions between many variables. If the model should be useful for physical interpretations the order of the interactions should be kept low. This type of model thinking has been incorporated by (Harris *et al.*, 2002) in their SUPANOVA algorithm which is a support vector machine built on the ideas to separate low-order interaction effects from high-order interaction effects by a special function expansion.

3. LOCAL MODELS

A local model, as described in (Nelles, 2001; Töpfer *et al.*, 2002), is a nonlinear model of the following form:

$$\hat{y} = \sum_{i=1}^M \Phi_i(\varphi) g_i(\varphi), \quad (2)$$

where a set of local models, the $g_i(\varphi)$:s, are weighted by the weighting, activation or membership functions $\Phi_i(\varphi)$. The regressor vector φ can consist of, e. g., different input time lags, old output lags and/or transformations of these. This model is an alternative function expansion to the one used in neural networks. The idea is that the input space is divided into parts in which a simple model g_i , most often a linear one, describes the output satisfactory. The Φ_i :s take care of to which part of the input space the input belongs and the possible smoothing of the transitions between the parts. The partitioning of the input space can be done in the following ways; a grid structure, recursive partitioning or a partitioning of arbitrary form. The choice of partitioning is called structure identification. The model can also be seen as a linear model with operating-point dependent parameters;

$$\begin{aligned} \hat{y} &= \sum_{i=1}^M (w_{i0} + w_{i1}\varphi_1 + \dots + w_{ip}\varphi_p) \Phi_i(\varphi) = \\ &= w_0(\varphi) + w_1(\varphi)\varphi_1 + \dots + w_p(\varphi)\varphi_p, \end{aligned}$$

with

$$w_q = \sum_{i=1}^M w_{qi} \Phi_i(\varphi).$$

It is not necessarily the case that all regressors in φ are included in both $g_i(\varphi)$ and $\Phi_i(\varphi)$. In the following, the part of φ that occurs in g_i will be called $\mathbf{x}$ and the part that occurs in Φ_i will be called $\mathbf{z}$. $\mathbf{x}$ and $\mathbf{z}$ can be partly constituted by the same regressors. As already mentioned the $g_i(\mathbf{x})$ are often linear(or affine) functions. Also the notion of cells will be used. Each part of the input space defined in an axis-orthogonal grid is called a cell, see Figure 1.

Fig. 1. These are examples of an axis-orthogonal grid to the left and an axis-orthogonal recursive partitioning to the right.

Sometimes the $\Phi_i(\mathbf{z})$ are decomposed into functions of the form $f_{i1}(z_1)f_{i2}(z_2)\dots f_{ik}(z_k)$, where each $f_{ij}(z_j)$ is a bell shaped function. The spread of the bell depends on whether a smooth transition between different parts of the input space is wanted or not. This decomposition gives an axis-orthogonal partitioning of the input space, see Figure 1.

Here the questions are how many and which $f_{ij}(z_j)$ are needed for successful modelling and which parts of φ that should be included in $\mathbf{x}$ and $\mathbf{z}$ respectively. This is exactly the kind of information ANOVA can contribute with. Also process knowledge will be helpful.

4. REDUCING STRUCTURAL COMPLEXITY

In this section, data from the system

$$y = \text{sgn}(u_1) \cdot u_2 + u_3 + e$$

will be used as example. If u_1 is the derivative of the position, this system is a very simple example in which different dynamics apply when braking or accelerating. Here, e comes from a zero mean normal distribution with variance 1. The data are collected such that u_1 , u_2 and u_3 each assume the levels -1 , 1 , 3 and 5 and all level combinations of these factors are present four times. This gives 256 input/output data. If the factors are different lags of the same signal, the level combinations can be obtained by using a pseudo-random multi-level signal (Godfrey, 1993).

The reduction of the structural complexity can be seen as a three-step procedure:

- (1) Apply ANOVA to your data (Lind, 2001). The result is an ANOVA table, see Table 1. From this table, the significant regressors and their interaction pattern can be concluded. In this case, the three-factor interaction is not significant, i. e., all the factors contribute non-additively to the output, and the two-factor interactions between u_1 and u_3 and between u_2 and u_3 are not significant. The main effect from u_3 is significant, but it is not interesting to consider the main effects from u_1 or u_2 since the interaction between these factors is significant.
- (2) The significant effects can be investigated further by looking at plots of the cell means, i. e., the

Effect	Degrees of Freedom	Mean Square	F	p-level
u_1	3	248	224	0.0000
u_2	3	111	100	0.0000
u_3	3	427	386	0.0000
$u_1 * u_2$	9	111	100	0.0000
$u_1 * u_3$	9	0.9	0.8	0.64
$u_2 * u_3$	9	1.4	1.2	0.28
$u_1 * u_2 * u_3$	27	1.0	1.0	0.53
Error	192	1.1		

Table 1. Analysis of Variance Table. The columns are from the left; the degrees of freedom associated with each sum of squares, the sum of squares divided by its degrees of freedom, the value of the F-distributed test variable associated with the corresponding interaction effect and, finally, the probability level that the interaction is not present.

mean over all the data in each cell, together with their confidence intervals. If a straight line can be drawn through the confidence intervals, in a way that will be explained further, the effect of the factor on the x-axis can be considered to be linear, given the other factor(s) involved in the plot.

- (3) Use the information when deciding what possible partitionings to use for estimating the local linear model. See section 4.2.

4.1 Investigating interaction effects

To see if an interaction effect is linear in one of the factors given the others, e. g., $y = \text{sgn}(u_1) \cdot u_2$ which is linear in u_2 given u_1 , it is possible to check the plots of the cell means, see Figure 2. These plots are computationally “free” and they also give an indication of how reliable the linear assumption is. No extra computations are needed for the plots of cell means, since all the cell means are computed in order to make the ANOVA table. A good estimate of the error variance is also obtained, so confidence intervals for the cell means are easily computed. The linearity tests done by looking at these plots can be done formally by defining linear contrasts, which is a linear combination of the cell means nominally adding to zero. A confidence interval for the linear contrast will tell if the difference from zero is significant (no linearity) or not.

It is enough to look at the cell mean plots for the highest order interaction of significance (for each factor combination). Assume that the cell means (in a two-dimensional grid) are linear functions of factor B for each fixed level i of factor A, that is,

$$\mu_{ij} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} = v_i + \rho_i \delta_j,$$

where μ_{ij} is the cell mean in cell (i, j) , v_i is a constant offset, ρ_i is the slope and δ_j is the distance between level 1 and level j of factor B. The row means μ_j are computed as

$$\begin{aligned} \mu_j &= \frac{1}{a} \sum_{i=1}^a \mu_{ij} = \mu + \beta_j = \\ &= \frac{1}{a} \sum_{i=1}^a v_i + \left(\frac{1}{a} \sum_{i=1}^a \rho_i \right) \delta_j = v + \rho \delta_j, \end{aligned}$$

where the second equality is due to the parameter restrictions and $v = \frac{1}{a} \sum_{i=1}^a v_i$ and $\rho = \frac{1}{a} \sum_{i=1}^a \rho_i$. Hence, it is obvious that if the two-dimensional cell means show a linear relation for factor B, also the one-dimensional cell means (the row means) will show a linear relation.

If high-order interaction effects are present, as shown by the ANOVA table, there will be more plots to look at. The axes of the high-dimensional cell means plot have to be permuted such that each regressor in the significant interaction effect gets to be at the x-axis once. Then the regressors that only need to be included in $\mathbf{x}$, the regressor vector for the local linear models, will be detected. The number of plots for each permutation will vary depending on how many levels each factor has and the order of the significant interaction.

4.2 Corresponding local linear model structure

Listed below are the possible outcomes of steps 1 and 2 and the corresponding choices of $\mathbf{x}$, $\mathbf{z}$ and $\Phi_i(\mathbf{z})$, for an analysis with three factors. How many $\Phi_i(\mathbf{z})$:s that are needed cannot be concluded from these tests. The idea is quite simple, but there are many slightly different cases, hence the length of the list.

- 1a; Three-factor interaction between u_1 , u_2 and u_3 . No linearities detected in the cell means plots. Let $\mathbf{x} = [u_1, u_2, u_3]$ and $\mathbf{z} = [u_1, u_2, u_3]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i1}(u_1) \cdot f_{i2}(u_2) \cdot f_{i3}(u_3)$.
- 1b; Three-factor interaction between u_1 , u_2 and u_3 . Linear in u_1 given the levels of u_2 and u_3 . Let $\mathbf{x} = [u_1, u_2, u_3]$ and $\mathbf{z} = [u_2, u_3]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i2}(u_2) \cdot f_{i3}(u_3)$.
- 1c; Analogue to case 1b, but with u_2 linear given the others.
- 1d; Analogue to case 1b, but with u_3 linear given the others.
- 1e; Three-factor interaction between u_1 , u_2 and u_3 . Linear in u_1 given the levels of u_2 and u_3 , and in u_2 given the levels of u_1 and u_3 . Choose between using the setup in case 1b (u_2 as regime variable) or the setup in case 1c (u_1 as regime variable).
- 1f; Analogue to case 1e, but with u_1 or u_3 linear given the others.
- 1g; Analogue to case 1e, but with u_2 or u_3 linear given the others.
- 1h; Three-factor interaction between u_1 , u_2 and u_3 . Linear in u_1 given the levels of u_2 and u_3 , in u_2 given the levels of u_1 and u_3 , and in u_3 given the levels of u_1 and u_2 . Choose between using the setup in case 1b (u_2 and u_3 as regime variables), the setup in case 1c (u_1 and u_2 as

Fig. 2. Cell mean plots with confidence intervals. The upper two plots show the two-dimensional cell means, corresponding to the interaction between u_1 and u_2 . The plot to the left have u_1 on the x-axis and one line for each value of u_2 , while the plot to the right have u_2 on the x-axis. From the plots, the following conclusions can be drawn: u_1 and u_2 affect y with interaction, since the curves within each plot do not have the same shape. u_2 affects y linearly if the value of u_1 is fixed, since it is possible to draw a straight line through the confidence intervals for μ_{ij} for each value of i . (The lines in the plot only connects the cell means, they are not straight lines). The lower plots show the one-dimensional cell means with u_2 and u_3 on the x-axis respectively. The left plot confirms that the important information is present in the two-dimensional cell means plots. The right plot shows that the effect from u_3 could be linear.

regime variables), or the setup in case 1d (u_1 and u_3 as regime variables).

- 2; Two-factor interactions between u_1 and u_2 , between u_1 and u_3 and between u_2 and u_3 but no three-factor interaction. The model can be decomposed into three additive sub-models. See further cases 5.1, 5.2 and 5.3. When there are possible choices of which variables should act as regime variables it could be wise to consider the possible choices in the other sub-models too.
- 3.1; Two-factor interactions between u_1 and u_2 , and between u_1 and u_3 . The model can be decomposed into two additive sub-models. See further cases 5.1 and 5.3.
- 3.2; Two-factor interactions between u_1 and u_3 , and between u_2 and u_3 . The model can be decomposed into two additive sub-models. See further cases 5.1 and 5.2.
- 3.3; Two-factor interactions between u_1 and u_2 , and between u_2 and u_3 . The model can be decomposed into two additive sub-models. See further cases 5.2 and 5.3.
- 4.1; Two-factor interaction between u_1 and u_2 and main effect from u_3 . The model can be decom-

posed into two additive sub-models. See further cases 5.1 and 7.3.

- 4.2; Two-factor interaction between u_1 and u_3 and main effect from u_2 . The model can be decomposed into two additive sub-models. See further cases 5.2 and 7.2.
- 4.3; Two-factor interaction between u_2 and u_3 and main effect from u_1 . The model can be decomposed into two additive sub-models. See further cases 5.3 and 7.1.
- 5.1a; Two-factor interaction between u_1 and u_2 . No linearities. Let $\mathbf{x} = [u_1, u_2]$ and $\mathbf{z} = [u_1, u_2]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i1}(u_1) \cdot f_{i2}(u_2)$.
- 5.1b; Two-factor interaction between u_1 and u_2 . Linear in u_1 given the levels of u_2 . Let $\mathbf{x} = [u_1, u_2]$ and $\mathbf{z} = [u_2]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i2}(u_2)$.
- 5.1c; Two-factor interaction between u_1 and u_2 . Linear in u_2 given the levels of u_1 . Let $\mathbf{x} = [u_1, u_2]$ and $\mathbf{z} = [u_1]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i1}(u_1)$.
- 5.1d; Two-factor interaction between u_1 and u_2 . Linear in u_1 given the levels of u_2 and linear in u_2 given the levels of u_1 . Choose between the setup in case 5.1b (u_2 as regime variable), and the setup in case 5.1c (u_1 as regime variable).

- 5.2; Two-factor interaction between u_1 and u_3 . Analogue to case 5.1.
- 5.3; Two-factor interaction between u_2 and u_3 . Analogue to case 5.1.
- 6.1; Main effects from u_1 and u_2 . No interactions. The model can be decomposed into two additive sub-models. See further cases 7.1 and 7.2.
- 6.2; Main effects from u_1 and u_3 . The model can be decomposed into two additive sub-models. See further cases 7.1 and 7.3.
- 6.3; Main effects from u_2 and u_3 . The model can be decomposed into two additive sub-models. See further cases 7.1 and 7.2.
- 7.1a; Main effect from u_1 . u_1 is linear. Let $\mathbf{x} = [u_1]$ and $\mathbf{z}$ empty. No partitioning is needed.
- 7.1b; Main effect from u_1 . u_1 is nonlinear. Let $\mathbf{x} = [u_1]$ and $\mathbf{z} = [u_1]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i1}(u_1)$.
- 7.2; Main effect from u_2 . Analogue to case 7.1.
- 7.3; Main effect from u_3 . Analogue to case 7.1.
- 8; No significant effects. None of the tested factors show systematic effects in the data.

From the example data set, we have gained the information that all the factors u_1 , u_2 and u_3 are present in the model. The model structure according to the ANOVA table is

$$y = h_1(u_1, u_2) + h_2(u_3) + e,$$

which is case 4.1 above. The interaction between u_1 and u_2 was then investigated further (Figure 2), giving the result that $h_1(u_1, u_2) = f(u_1) \cdot u_2$, that is, u_1 belongs to the regime variables $\mathbf{z}$ while u_2 belongs to $\mathbf{x}$. If $h_2(u_3)$ is a nonlinear function, u_3 need to be in both $\mathbf{z}$ and $\mathbf{x}$. Since u_1 and u_3 do not interact the weighting functions Φ_i will be either $f_{i1}(u_1)$ or $f_{i3}(u_3)$, but not $f_{i1}(u_1) \cdot f_{i3}(u_3)$. The linearity can be tested by plotting the cell means against the levels of factor C (u_3), see Figure 2, which shows that $h_2(u_3)$ could be linear and u_3 does not need to be included in $\mathbf{z}$. The total model consist of two additive sub-models, one corresponding to case 5.1c and the other to case 7.3a.

4.3 Another example

The second example is a bit more complicated than the first one;

$$y = \text{sgn}(u_1) \cdot u_2 \cdot u_3 + u_3^2 + e.$$

The inputs and the noise are chosen exactly as in the first example and the amount of data is the same. The ANOVA table is given in Table 2 and shows that we have case 1 in the list in Section 4.2. The linearity is investigated in the cell mean plots, see Figures 3, 4 and 5. These show that we have case 1c. That means that we should choose $\mathbf{x}$ as $[u_1, u_2, u_3]$ and $\mathbf{z}$ as $[u_2, u_3]$. Possible $\Phi_i(\mathbf{z})$:s are $f_{i2}(u_2) \cdot f_{i3}(u_3)$, but exactly where the partitionings should go is an identification issue.

Effect	Degrees of Freedom	Mean Square	F	p-level
u_1	3	1008	910	0.0000
u_2	3	435	392	0.0000
u_3	3	12122	10941	0.0000
$u_1 * u_2$	9	435	392	0.0000
$u_1 * u_3$	9	423	382	0.0000
$u_2 * u_3$	9	183	165	0.0000
$u_1 * u_2 * u_3$	127	170	154	0.0000
Error	192	1.1		

Table 2. Analysis of Variance Table for the second example.

Fig. 3. Cell mean plots with confidence intervals. u_1 on the x-axis.

Fig. 4. Cell mean plots with confidence intervals. u_2 on the x-axis. The effects seem linear.

Fig. 5. Cell mean plots with confidence intervals. u_3 on the x-axis.

5. CONCLUSIONS

It is possible to gain enough structure information from the input/output data to assist the structure identification task in local linear modelling by using ANOVA. The information that can be extracted from the ANOVA table and the cell means plots are what regressors that should be used for the linear models in each part of the input space, what regressors that should determine the partitioning of the input space and how complex the partitioning should be (that is, how many regressors interact in each weighting function). The cell means plots with confidence intervals appeal also to intuition. They are very similar to scatter plots, but with the benefit that the statistical properties of the input/output data are made visible. Left to consider in the structure identification task is how many partitionings to use and where the limits of each part should be.

6. ACKNOWLEDGEMENTS

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