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Smoothing parameters selection in the additive regression models approach for the fault detection

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Abstract

Smoothing is an important statistical tool and is strongly related to nonparametric prediction. Smoothers can be used to visual description of data, smooth plots of relationship, and diagnose residual plots. This paper presents a nonlinear dynamic systems identification method based on additive regression models with smoothing techniques and knowledge discovery data. In particular, two alternative theoretical smoothing choices are proposed in an attempt to estimate additive models structure. The fault detection of dynamic system based on the obtained model is planned aim of the work.. The final part of this work contains an illustrative example regarding the application of proposed approach to a control valve for measurement tracks in the boiler laboratory setup. All research has been carried out in order to demonstrate the sensitivity of faults for three theoretical smoothing parameters in the analyzed structure.

Keywords: fault detection, additive model, smoothing parameter, identification, dynamic system.

Dobór parametrów wygładzających w modelach addytywnych dla potrzeb detekcji uszkodzeń

Streszczenie

Funkcja wygładzająca jest ważnym narzędziem statystycznym związanym z regresją nieparametryczną i służy do określania zależności pomiędzy zmiennymi wejściowymi a wyjściowymi. W pracy przedstawiono nowe podejście do identyfikacji nieliniowych systemów dynamicznych, oparte na addytywnym modelu regresji wraz technikami wygładzającymi oraz eksploracji danych. W szczególności, aby osiągnąć większą elastyczność przy szacowaniu modelu addytywnego, dokonano wyboru dwóch alternatywnych metod wygładzających. Pozyskana wiedza posłużyła do konstrukcji algorytmów detekcji uszkodzeń, a następnie do oceny wrażliwości na występowanie poszczególnych uszkodzeń w zależności od trzech parametrów wygładzających. Badania przeprowadzono dla przykładowego zaworu regulacyjnego na podstawie danych laboratoryjnych próbkowanych na stanowisku regulacji poziomu wody w zbiorniku walczakowym.

Słowa kluczowe: detekcja uszkodzeń, model addytywny, parametr wygładzający, identyfikacja, obiekty dynamiczne.

1. Introduction

The early detection of faults is critical if one wants to avoid the performance degradation and damage to the machinery or the loss of human life. Therefore, accurate diagnosis helps us to make a right decision on emerging actions and repairs. In order to meet reliability requirements of safety-critical processes, the modern control systems should be equipped with mechanisms of fault detection, that are indicators of prohibited deviations from the normal behaviour in the plant or its instrumentation [1, 2]. For this reason, the diagnostics and protection of processes are crucial. Of equal importance are computer systems that aid operator in diagnostics, or even automatically create a diagnosis.

The classical way of fault detection is to check the limits of single variables and alarming of operators. However, this can be improved significantly by taking into account the information hidden in all measurements and automatic actions to keep the systems in operation. Advanced methods of fault detection are based on mathematical signal and process models, and on methods of system theory and process modelling, to generate fault symptoms [2].

In the automatic control systems, the possibility of signals values acquisition exists. It allows us to create models based on measured data and expert's knowledge about the object. With the growth of computer technology, new possibilities have arisen in terms of storing data acquisition and speed of their processing. The science of extracting useful information from large data sets or databases is known as data knowledge discovery data [3]. The key task of this discipline for diagnostic purposes is the analysis of observational data sets, and how to find the relevant information quicker and more accurately, which aids the decision making about the recognition of changes of the state of the process during its operation.

In this paper, an effective method of modelling and predicting the behaviour of fluid flow through the valve has been presented for detecting purposes. This is a new way in the industrial process diagnosis for which the difficulty associated with the problem of dimensionality is substantially reduced. This important class of flexible models arises in form of additive models [4]. There are many ways to approach the formulation and estimation of additive models. Typically they differ in the way the smoothness constraints are imposed on the functions in the model. The most general method for estimating additive models is the backfitting algorithm with an arbitrary smoother. Analysts who use smoothers have to make choices about bandwidth and smoothing parameters, knot numbers and placement, depending on the type of smoother [4, 5]. These choices all have consequences for how the smoothing the trajectory of the process will follow, and then for the possibility of false symptom genering in the fault detection scheme.

2. Nonparametric smoothing techniques

Let us call the physical measurable quantities influencing the process and resulting from the process operation, the input and output signal, respectively. The smoother is a tool for summarizing the trend of an output signal Y as a function of $p > 1$ input signals $X_1, X_2, ..., X_p$. It produces an estimate of the trend that is less variable than Y itself. An important property of a smoother is its nonparametric nature - it doesn't assume a rigid form for the dependence of Y and $X_1, X_2, ..., X_p$. We call the estimate produced by a smoother a *smooth* and a single predictor case a *scatterplot smoothing*. A scatterplot smoother can be used to estimate the dependence of the mean of Y on the input signals, and thus serve as a building block for the estimation of additive models, discussed in the next chapter.

Smoothers fall into three basic classes: kernel smoothers, local polynomial regression, and splines [5]. I restrict my attention, here to local polynomial regression, and natural cubic splines.

Suppose we have a pair $(x_i, y_i)_{i=1}^{n}$ of a random sample, where y_i represent measurement results of the variable Y and x_i are the n observed values of the variable X. The locally polynomial regression specifically denotes a method that is more descriptively known as locally weighted polynomial smoothers - *lowess*. The local polynomials fit to each subset of the data are almost always of first or second degree; that is, either locally linear

$$\phi(x_i) \approx a_0 + a_1(x_i - x) \tag{1}$$

or locally quadratic

$$\phi(x_i) \approx a_0 + a_1(x_i - x) + \frac{a_2}{2}(x_i - x)^2 . \tag{2}$$

Let us focus on the local linear polynomials. The polynomials are fitted using weighted least squares

$$\arg\min_{[a_o, a_1]} \sum_{i=1}^{n} W(\frac{x_i - x}{h})(y_i - (a_0 + a_1(x_i - x)))^2 , \tag{3}$$

giving more weight to points near the point whose output signal is being estimated and less weight to points further away. The value of the regression function for the point is then obtained by evaluating the local polynomial using the input signals values for that data point. The fit is complete after regression function values have been computed for each of the n data points. The weight function $W(\cdot)$ is one-dimensional kernel function and h is by user-specified input smoothing parameter called the *bandwidth* or *span,* which determines how much of the data is used to fit each local polynomial. Large values of h produce the smoothest functions and the smaller h tends to overfit the data.

An alternative smoothing technique is natural cubic splines. For a data set x_i of n points, we can construct a cubic spline with n-1 piecewise cubic polynomials between the data points. Suppose that knots are denoted by $\{t_k\}_{k=1}^{n}$ in n data points x_i of interval $[a,b]$. A simple choice of basis function for picewise-cubic splines, derives from the parametric expression for the smooth

$$\phi(x) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 + \sum_{k=1}^{n} \beta_k (x - t_k)_+^3 , \tag{4}$$

where the notation $(x - t_k)_+$ denotes the positive part of $(x - t_k)$:

$$(x - t_k)_+ = \begin{cases} x - t_k & \text{when} \quad x \ge t_k \\ 0 & \text{when} \quad x < t_k \end{cases} . \tag{5}$$

The $\phi(\cdot)$ in (4) has the required properties: is cubic polynomial in any subinterval $[t_k, t_{k+1}]$, has two continuous derivatives and has a third derivative that is a step function with jumps at knots t_k.

Alternately, we can set $\phi''(a) = \phi''(b) = 0$ resulting in the natural cubic spline. The cubic smoothing splines is the minimizer of the penalized least-squares criterion

$$\sum_{i=1}^{n} (y_i - \phi(x_i))^2 + \lambda \int_a^b \phi''^2(t) dt , \tag{6}$$

where λ is a fixed constants with values typically in (0,1), called *roughness penalty* or *spar*. The first term measures closeness to the data, while second term penalized curvature in the function. The parameter λ plays the same role as the bandwidth in the local polynomial smoother. Large values of λ produce smoother curves while smaller values produce more wiggly curves.

If we focus on the fit at the observed points $x_1,...,x_n$, a smoother can be written as

$$\hat{\phi}(x_i) = \sum_{k=1}^{n} S_{ik} y_k , \tag{7}$$

where S_{ik} is the jk^{th} entry of $n \times n$ smoother matrix S for smoothing against the n unique predictor values $x_1,...,x_n$. Thus, both of mentioned above smoothers are linear smoother and have a single smoothing parameter [4, 5].

Selecting an appropriate smoothing parameter is a key part of nonparametric regression fitting. In order to obtain a proper or "good" fit, the modeler must find a balance between the variance and bias. For choosing the smoothing parameter, we can use an automatic selection by the generalized cross-validation *GCV* [4] or a graphical method helping us to choose the appropriate value. In generalized cross-validation, the data are divided into subsets. The model is successively fit omitting each subset in turn and then the fitted model is used to predict the output signal for the left-out subset. Although cross-validation and the other automatic methods for selecting a smoothing parameter seem well founded, their performance in practice is sometimes questionable. Alternatively, it is reasonable to select the value of smoothing parameter simply by specifying the degrees of freedom *df* of a smoother in order to make different smoothers comparable with respect to the amount of fitting they do [4,5]. The degrees of freedom is a trace of the smoother matrix S and values for *df* should be greater than 1, with *df*=1 implying a linear fit. This measure gives a useful a priori choice in situations where automatic choice is not feasible.

3. Additive model

The additive model is defined by

$$Y = \alpha + \sum_{j=1}^{p} \varphi_j (X_j) + \varepsilon, \tag{8}$$

where error ε is a sequence of independent and identically distributed random variables (*iid*) with the mean $E(\varepsilon) = 0$ and the finite variance $Var(\varepsilon) = \sigma^2$. The φ_j s are unknown, arbitrary univariate functions one for each predictor X_j. Functions φ_j s can be, for example, roots, logarithms or trigonometric functions. Let us point that we do not assume that the signals X_j are independent [7]. The additive model can be nonlinear with respect to signals X_j but it's still linear with respect to signals $\varphi_j(X_j)$. Let's notice that without making an additional assumption about the constant in the model (8), there will be free constants in each of the functions. In order to avoid the above nonuniqueness, we need to impose the condition $E[\varphi_j(X_j)] = 0$, or equivalently $E(Y) = \alpha$ for all functions.

For a pair $\{(x_{ij}, y_i)_{i=1}^{n}\}_{j=1}^{p}$ of a random sample, where y_i represent measurements of the variable Y, and x_{ij} are the n observed values of the variable X_j, the additive model can be estimated by minimization of the residual sum of squares

$$\arg\min_{\{\alpha, \varphi_j\}} \sum_{i=1}^{n} (y_i - \alpha - \sum_{j=1}^{p} \varphi_j (x_{ij}))^2 , \tag{9}$$

which finds the value of parameter α and the set of one dimensional functions φ_j. Thus, we avoid the necessity of estimation in the multidimensional space. For more flexibility, relations between output signal and input signals are fitted by the use of iterative smoothing process called *backfitting algorithm*, with an arbitrary smoother like locally polynomial or natural cubic spline.

The backfitting algorithm is an iterative procedure for fitting additive models in which, at each step, one component is estimated keeping the other components fixed, the algorithm proceeding component by component and iterating until convergence. Convergence of the algorithm has been studied in [4, 5, 7].

4. Fault detection algorithm

Model-based methods of fault detection use the analytical relations in the form of process model equations [2]. The relations between the measured input signals and output signal are represented by the additive model of the process. Fault detection methods then generate quantities called residuals r_i, which are the comparisons of the actual behavior of the monitored output to the behavior predicted on the basis of the additive model. The residuals are normally equal to zero. They become nonzero as a result of faults.

The detection performance of the diagnostic technique is characterized by important and quantifiable benchmarks, like the fault sensitivity and the reaction speed, that is, the ability of the technique to detect faults of a reasonably small size, and with a reasonably small delay after their arrival. Also its robustness, i.e., the ability of the technique to operate in the presence of noise, disturbances and modelling errors, is affected by the design of detection algorithm [1].

The simplest possible detection algorithm is to compare each observation of the scalar residual individually with the threshold values. Symptom of fault is detected if diagnostic signal $s(r_i)$ is equal to 1, i.e. when the threshold value K_1 or K_2 was exceeded by the *i*-th residual:

$$s(r_i) = \begin{cases} 0 & \text{when} \quad K_1 \le r_i \le K_2 \\ 1 & \text{when} \quad r_i < K_1 \ \vee \ r_i > K_2 \end{cases}. \tag{10}$$

The threshold values are obtained based on the training sample, i.e., on residuals from the normal behaviour of process, as following:

$$\begin{aligned} K_1 &= \min\{r_i\} - \hat{\sigma}\{r_i\} \\ K_2 &= \max\{r_i\} + \hat{\sigma}\{r_i\} \end{aligned}, \tag{11}$$

where $\hat{\sigma}\{r_i\}$ is sample standard deviation of residuals r_i.

5. Exploratory data analysis

All research has been carried out based on the example of a control valve for measurement tracks in a boiler laboratory setup, controlled by industrial IT control systems, with the use of the R-project [7] designed to advanced statistical calculations. This work can be seen as a continuation of the work in [8].

To be useful for data mining purposes, the databases need to undergo a preprocessing, in the form of data cleaning, data transformation and identifying outliers [3, 6, 8]. Moreover, the monitored plant is usually subjected to random noise. Therefore, the signals must be filtered. In order to do it, the finite impulse response of 2nd order FIR filter was applied.

In this paper the actuator was determined by the following additive model:

$$\begin{aligned} F_t = \alpha &+ \varphi_1(CV_{t-1}) + \varphi_2(CV_{t-2}) + \varphi_3(P1_{t-1}) + \varphi_4(P1_{t-2}) + \\ &\varphi_5(P2_{t-1}) + \varphi_6(P2_{t-2}) + \varepsilon_t, \end{aligned} \tag{12}$$

where ε_t, for $t = 3,...,n$ are *iid* random errors.

Table 1 shows variables used in model.

Tab. 1. Variables used in the modeling
Tab. 1. Zmienne użyte w modelowaniu

Variable symbol	Variable description	Range	Unit
F	Water flow beyond the valve	0-5	m³/h
CV	Control value (controller output)	0-100	%
*P*1	Water pressure (valve inlet)	0-400	kPa
*P*2	Water pressure (valve outlet)	0-200	kPa

5.1. Selecting the smoothing parameter

To compare how well different smoothers perform using simulated data, the additive model (12) was fitted by the backfitting algorithm with the different nonparametric smoothing techniques. In the comparative analysis, natural cubic spline (s) and locally weighted linear smoother (lo) were used. For natural cubic spline I selected the smoothing parameter by degrees of freedom $df \in \{2,4,6\}$, the same for each term, and by roughness penalty λ (*spar*) via *GCV*. Table 2 shows the values of roughness penalty for each term.

Tab. 2. Values of roughness penalty
Tab. 2. Wartości współczynnika wygładzającego

Variable symbol	CV_{t-1}	CV_{t-2}	$P1_{t-1}$
spar	1.01×10^{-11}	9.19×10^{-12}	9.06×10^{-8}
Variable symbol	$P1_{t-2}$	$P2_{t-1}$	$P2_{t-2}$
spar	2.84×10^{-8}	1.33×10^{-13}	1.98×10^{-13}

For the lowess smoother, I applied various spans via the visual method. In my analysis the span is a member of interval [0.25,0.75].

5.2. The modelling results

Based on the training sample, for each smoothing technique, I obtained estimated flow values (predicted F), and real flow values from the process (F). For model checking the mean squared error (MSE), mean absolute deviation error (MADE), mean absolute percentage error in relation to range of measured output signal (MAPE) and variance of errors (VAR) for each smoothed fit were obtained. The results were showed in Table 3.

Tab. 3. Criteria of the additive model fitting for training sample
Tab. 3. Wskaźniki jakości dopasowania modelu addytywnego dla próby uczącej

Model with smoothing parameter	Measures			
	MSE	MADE	MAPE	VAR
s(*df* = 2)	7e-04	0.019	0.6%	7e-04
s(*df* = 4)	3e-04	0.01	0.26%	3e-04
s(*df* = 6)	2e-04	0.01	0.28%	2e-04
s(*spar*)	1e-06	4e-04	0.13%	1e-06
lo(*span* = 0.25)	5e-04	0.016	0.57%	5e-04
lo(*span* = 0.35)	3e-04	0.009	0.3%	3e-04
lo(*span* = 0.55)	1e-04	0.007	0.24%	1e-04
lo(*span* = 0.65)	8e-04	0.02	0.71%	8e-04
lo(*span* = 0.75)	0.001	0.025	0.88%	0.001

Using the mean squared error criterion the difference between smoothing splines and lowess is negligible. Lowess fits that are smoother have MADE values that are slightly higher than that for the natural cubic spline. So while one can get a very good fits with lowess, the fit with smoothing splines is better. Moreover, the results, here, demonstrate that natural cubic spline fits with automatic parameter selection (*spar*) produce the best fits that closely match the true relationship between real and predicted flow values.

5.3. The quality detection results

In order to examine detection algorithms based on the additive model, a test sample consisting of data from the normal process behaviour f_0 and data with simulated faults were applied.

Model (12) can be designed for detection of the actuator faults. Therefore, we can expect that residuals will be affected by the faults f_1 - second control valve is opened in 10%, f_2 - opened bypass flow-meter, f_3 - valve clogging, f_4 - applying antipressure on the servo-motor chamber.

Figure 1 shows graphs of signals measured and modelled for test sample including the individual faults. The first and second panel of Figure 1 contains a natural cubic spline plot where the amount of smoothing was estimated by degrees of freedom - s(*df*=4), and via GCV - s*(spar)*. On the third panel I plot lowess with the lowest MADE, i.e. for lo(*span*=0.55).

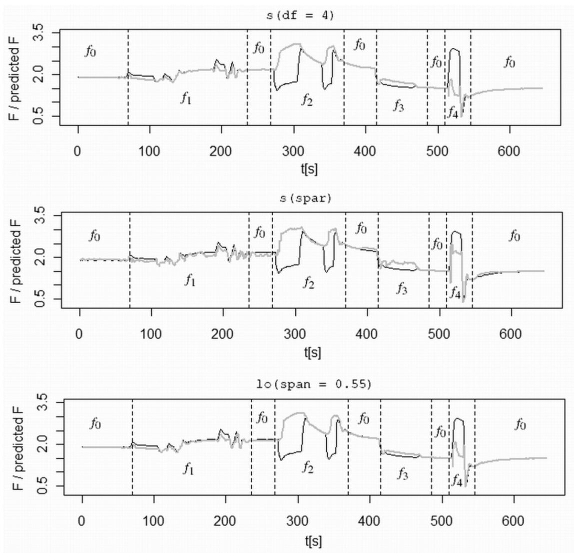

Fig. 1. The process of signals measured and modeled for test sample including the individual faults
Rys. 1. Przebiegi sygnałów, pomierzonego i modelowanego dla próby testowej zawierającej poszczególne uszkodzenia

First, this is no sign of undersmoothing or a jagged fit for all smoothing techniques. Second, the fit is also highly nonlinear. While there are some minor differences, we observe the same pattern. The smoothing parameter *df*=4 for natural cubic spline produces the smoothest curve. The natural cubic spline curve with *spar* parameter is a fairly rough fit. The third curve for lowess with *span*=0.55 goes through all the data points, but is not quite as smooth.

Then the diagnostic test (10) with $K_1 = -0.0467$ and $K_2 = 0.0437$ was applied to evaluate model sensitivity to individual faults. The results of faults detection for the smoothing with different parameters values were presented in Table 4. For natural cubic spline with smoothing parameter *df*=2 and *df*=4, the results are satisfactory, because on the basis of the mean percentage number of deviation from the normal behaviour process (with 5% threshold), test (10) detected all symptoms of simulated faults, and at the same time any incorrectness in the learning sample were noticed. The use of splines with automatic parameter *spar* selection tends to provide fits that are too local and as such produce fits that are overly nonlinear. This change of smoothing parameter for natural cubic splines has caused detection of 37.8% incorrectness in sample from normal behaviour process f_0. The results for lowess smoother with *span*=0.25 and *span*=0.35 are quite good, but the rest of span values implies that the model (12) is not sensitive to the occurrence of fault f_3. Therefore, the fault detection by the additive model depends on choice of the smoothing techniques and parameters.

Tab. 4. The results of detection test for different smoothing techniques and parameters
Tab. 4. Wyniki detekcji w zależności od metody i parametru wygładzania

Model with smoothing parameter	Test samples				
	f_0	f_1	f_2	f_3	f_4
s(*df* = 2)	0%	13.9%	53.4%	46.9%	45.7%
s(*df* = 4)	0%	36.7%	54.4%	58%	50%
s(*df* = 6)	0.5%	34.9%	55.3%	58.3%	50%
s(*spar*)	37.8%	79.5%	78.6%	67.9%	58.7%
lo(*span* = 0.25)	4.8%	44.6%	57.3%	60.5%	52.2%
lo(*span* = 0.35)	0%	33.7%	54%	57.8%	50%
lo(*span* = 0.55)	0.4%	20.5%	54.4%	1.2%	45.7%

6. Conclusions

The additive nonparametric regression allows researchers to combine flexible nonparametric modelling of multidimensional inputs with smoothing techniques. Smoothers invariably require the analyst to make choices about the amount of smoothing to apply and the criteria for this choice amount to visual examination. Received results show that the picking best smoothing parameter from data is an important task for the fault detection scheme. If the smoothing parameter is too small, the estimate is too noisy, exhibiting high various and extraneous wiggles. If the smoothing parameter is too large, then the estimate may miss key features due to oversmoothing, washing out small details and the fault detection is unusable. In general, good selection of smoothing parameters indicates the effectiveness of the fault detection by the additive models in the analyzed structures.

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