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ANALYSING THE RESULTS OF A DESIGNED EXPERIMENT WHEN THE RESPONSE IS A CURVE

METHODOLOGY AND APPLICATION IN METAL INJECTION MOULDING

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Analysing the results of a designed experiment when the response is a curve: methodology and application in metal injection moulding.

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SUMMARY

In (designed) industrial experiments, the response observed often takes the form of a curve representing, for example, the evolution of a quality characteristic over a period of time. In such context, the polynomial regression approach, usually used in response surface analysis to predict the response as a function of the experimental factors, should be adapted to the functional character of the response.

This paper reviews several possible methods of analysing the results of a designed experiment when the response is a curve and compares them with a case study from the metal injection moulding industry. Four different approaches are presented to fit a model to the (functional) data : two step nonlinear modelling; pointwise functional regression; smoothed functional regression and PLS. All the models derived are able to predict the functional response from any design factor setting chosen in the experimental domain. Two inferential problems are discussed: the significance testing of experimental factor effects, and the calculation of prediction intervals around predicted curves. Asymptotic results and bootstrap procedures are compared in this context.

Keywords: Experimental design, functional regression analysis, nonlinear regression, B-splines, response surfaces.

1. INTRODUCTION

Experimental design techniques and response surface methodology are common tools to maximize the information coming out of experimental campaigns in product development and quality improvement. The following steps usually guide the experimenter's work: an experimental design is first set up according to his or her research objective and constraints; after running the experiment, first or second order polynomial models are fitted to explain the responses from the factor levels; finally, the model are used to interpret the experimental factor effects and/or to

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find optimal production conditions. Books by Box *et al* [1,2] Montgomery[3] or Myers and Montgomery[4] are key references in this context. Classically, each response involved in such experiment is supposed to be a continuous scalar variable. When several responses are involved, they are modelled independently from each other while multi-response optimisation methods may be used in the optimisation phase (Derringer and Suich[5]).

Nowadays, with the availability of modern measurement devices and automatic data storage, recorded experimental responses often take the form of a function (e.g. a process variable over a time or over a temperature interval). In such context, the functional response is often summarised by indices such as the AUC (Area Under the Curve) or the maximum. Each summary index is then analysed individually using classical (polynomial) regression analysis. This procedure is often satisfactory but uses only a part of the information available in the response curve. Moreover, natural and intuitive summary indices do not always exist and, in some contexts, it is interesting to build a model which is able to explain and predict the whole functional response.

The goal of this paper is to present and compare some practical approaches of analysing the results of a designed experiment when the response is a curve. Different problems are discussed: model definition, estimation and validation, tests of significance of factor effects, prediction and optimisation.

The methodology presented in this paper will be illustrated by a case study of metal injection moulding (see details on the context below). The goal of the experiment is to find the optimal composition of a binder involving two constituents X and R. The response is a measure of the evolution of the strength of the binder over a range of temperatures. As shown in Figure 1, a 15 run experiment was performed : 3^2 runs of a factorial design, 4 check points and 2 replications in the centre of the domain. The goal is to build, from these experimental data, a model able to predict the expected curve for any point of the experimental domain.

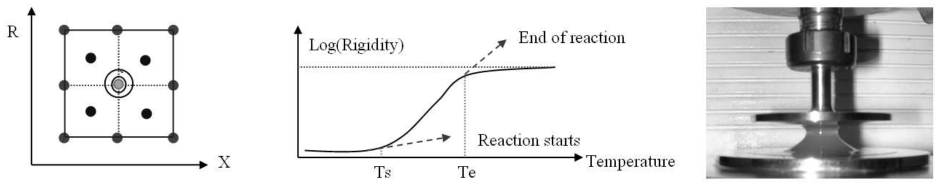

Figure 1: Experimental design, shape of the response curve and measurement device.

The classical methodology for the statistical modelling of the effect of covariates on functional responses is called *longitudinal data analysis* (Diggle *et al* [6]). It was developed in the context of biology to study the behaviour, over time, of individuals submitted to different possible treatments. The data collected in this context are rarely complete curves but consist only of some time points observed for each individual and these are subject to high measurement variation. For this reason, only linear and quadratic models single-variable models are usually used to fit the response curves.

In industrial experiments, response curves are often observed at many time points and measurement errors are usually small with respect to the signal available in the curves. This allows more sophisticated parametric or nonparametric models to be developped, which can, in good cases, fit the observed curves very closely. We will see that a classical nonlinear modelling of the response curves, combined with a polynomial modelling of the nonlinear models coefficients with respect to the experimental factors provide a good solution when all response curves have the shape of a common known parametric function.

The literature on functional regression and varying-coefficient models gives more general and flexible solutions when no common parametric form for the curves is available. It presents the advantage of treating the curves as functions in an elegant theoretical framework and propose very flexible models to express functional responses as smooth functions of covariate values. Ramsay and Silverman[7] book is a key reference in functional data analysis and the paper of Huang *et al* [8] is an interesting varying-coefficient model reference for the problem discussed in this paper. Faraway[9] discusses directly the problem of regression analysis for functional responses in the context of engineering problems and is the main reference used in this paper.

This paper is organised as follows. The second section defines the available data, related notations and different ways of fitting a predictive model to the data. The next two sections present inferential tools linked to the estimated models; including tests of significance of factor effects and the computation of prediction intervals. The last section illustrates the methodology on the case study and shows how the functional modelling results can be interpreted and represented graphically.

2. MODEL DEFINITION AND ESTIMATION

2.1. Data, general model and notations

Let $\xi_i = (\xi_{i1}, \xi_{i2} ..., \xi_{iq})'$ be the vector of values taken by q experimental factors for the i^{th} run of a design of size n. Let $x_i = (x_{i1}, x_{i2} ..., x_{ip})'$ be defined as a vector of p transformations of the factor settings, such as, for example, the terms of a first or second order polynomial model calculated from standardised ξ_i's. X is the corresponding $n \times p$ model matrix. Let $y_i(t)$ be the curve observed for run i over an interval $[t_{min}, t_{max}]$ where t is a variable such as a time or temperature.

The goal is to build, from these data, a statistical model able to predict the expected curve $\hat{y}_0(t)$ for any point ξ_0 (or, equivalently, x_0) of the experimental domain.

In practice, each curve $y_i(t)$ is usually only available on a grid supposed, in this paper, to be the same for all experimental runs : $(t_1, t_2 ..., t_m)$. Let y_{ik} be defined as $y_i(t_k)$ and Y as the $n \times m$ matrix with the n discretized curves. The common grid hypothesis is only compulsory for Method 2 below.

The three modelling approaches presented below can be written under the following generic linear form:

$$z_i = x_i\beta + \epsilon_i \quad \text{with } z_i = h(y_i(t)) \quad i = 1, 2, ...n \tag{1}$$

where $h(y_i(t))$ is a well chosen transformation of the function $y_i(t)$ to a discrete vector z_i of size $1 \times q$, β is a $p \times q$ matrix of unknown parameters and ϵ_i represents the (transformed) experimental error. It is a $1 \times q$ vector with zero mean and unknown variance covariance matrix Σ where $\epsilon_i(t)$ is independent of $\epsilon_j(t)$ when $i \neq j$. In matrix form, this model becomes:

$$Z = X\beta + \epsilon \tag{2}$$

where Z and ϵ are $n \times q$ matrices.

The three approaches presented below use three different forms for the pre-processing transformation $h(.)$ and an adapted methodology to fit the model to the data. We will suppose that the information lost in this pre-processing step is negligible compared to the uncertainty present in the error term ϵ of the remaining linear model.

2.2. Approach 1 : parametric nonlinear pre-processing

When the observed curves $y_i(t)$ $(i = 1, 2...n)$ have a common shape which can be well approximated by a nonlinear parametric function $f(t; (\theta_1, ..., \theta_q))$ (e.g. logistic or exponential function), the vector of parameters $\theta = (\theta_1, ..., \theta_q)$ is a possible candidate to define $z = h(y)$. More precisely, the first step of the modelling procedure consists of fitting, by nonlinear least-squaress, the function $f(t; \theta)$ to each discretized curve $y_i(t)$, $i = 1, ...n$. This step provides n vectors of estimated parameters $\hat{\theta}_i = (\hat{\theta}_{i1}, \hat{\theta}_{i2}, ...\hat{\theta}_{iq})$, $i = 1, 2, ...n$ which are defined as the response vectors in the second modelling step : $z_i = \hat{\theta}_i = h(y_i(t))$.

The model $Z = X\beta + \epsilon$ is a multivariate regression model and it can be shown (Johnson and Whischern[10]) that the generalized least-squaress estimator of β is simply the ordinary least-squaress one:

$$\hat{\beta} = (X'X)^{-1}X'Z$$

For any new observation x_0 in the experimental domain, a predicted curve is derived by inverting the two steps above: $\hat{z}_0 = x_0'\hat{\beta}$ and $\hat{y}_0(t) = f(t; \hat{z}_0)$.

As we will see in Section 4, this approach has the big advantage of providing interpretable outputs but it is only applicable when a (good) nonlinear function is available to approximate the original curves. Low dependence between the nonlinear parameters $\theta_1, ...\theta_q$ is crucial to get interpretable and stable estimates.

2.3. Approach 2 : pointwise functional regression

The second approach is issued from the functional analysis literature (Ramsay and Silverman[7] and Faraway[8]). In this context, model (1) is commonly written in the following linear form :

$$y_i(t) = \sum_{j=1}^{p} x_{ij}\beta_j(t) + \epsilon_i(t)$$

where the $\beta_j(t)$'s are functional parameters.

In discrete form, this model becomes the multivariate regression model (2) : $Z = X\beta + \epsilon$ where z_i is simply the discretized form of $y(t)$: $Z = Y$ and ϵ, the discretized residual matrix. The (generalized) least-squares estimator of β is simply : $\hat{\beta} = (X'X)^{-1}X'Y$ and is equivalent to performing a multiple regression of $(y_{1k}, y_{2k}, ...y_{nk})'$ on X for each time point t_k. The predicted response for a new observation x_0 is given by $\hat{y}_0 = x_0'\hat{\beta}$ where $\hat{y}_0$ is a $1 \times m$ vector.

This method may give a good fit but does not take into account the functional (and autocorrelated) character of the response curves. We will show in Section 4 that, when the original curves are not smooth, the resulting parameter functions $\hat{\beta}_j = (\hat{\beta}_{j1}, \hat{\beta}_{j2}, ...\hat{\beta}_{jm})$ and the predicted curve $\hat{y}_i$ are unnecessarily noisy. Moreover, the predicted curves are discrete and may need further interpolation.

Note also that this approach is equivalent to applying a PLS2 modelling to the X and Y matrix (Martens and Martens[11]). For this reason, PLS will not be further discussed in this paper.

2.4. Approach 3 : B-spline transformation pre-processing

This third approach may be seen as a non-parametric generalisation of the first one and an improvement of the over-parametrized pointwise functional regression one. It consists of replacing the fitting of a parametric nonlinear model in the first method by the expression of each observed curve as a linear combination of basic functions $\phi_k(t)$ able to mimic various types of curves such as cubic B-Splines (de Boor[12]) :

$$y_i(t) \tilde{=} \sum_{k=1}^{q} \theta_{ik}\phi_k(t).$$

If ϕ is the $q \times m$ matrix of discretized base functions over the grid $(t_1, t_2, ...t_m)$, the $(n \times q)$ matrix θ of θ_{ik}'s coefficients is estimated by the OLS formula: $\hat{\theta} = Y\phi(\phi\phi')^{-1}$. If response curves are not observed on the same time grid, this regression should simply be applied to each curve individually.

The Z matrix in the linear modelling step is defined here as the $n \times q$ matrix $\hat{\theta}$. The β matrix is estimated as $\hat{\beta} = (X'X)^{-1}X'Z$ and for a new observation x_0, the predicted discrete response curve is given by: $\hat{y}_0 = x_0'\hat{\beta}\phi$

Section 4 will show that this approach supplies similar results than pointwise functional regression but predicted curves are smoother. Moreover, it can be shown that this two-step approach is equivalent to the two-step estimation method proposed by Fan and Zhang[12] or to one-step least-squares estimation of the linear model:

$$y_{ik} = \sum_{j=1}^{p} x_{ij} \sum_{l=1}^{q} \beta_{jl}\phi_{jk} + \epsilon_{ik} \quad i = 1, 2, ...n, \;\; k = 1, 2, ...m$$

3. FACTOR EFFECT SIGNIFICANCE TESTS

Two common questions arise in the interpretation of models estimated from experimental design results:

1. Which factors or model terms have a significant effect on the response?
2. How do the factors affect the responses?

When responses are functions, these two questions must be answered for the whole curve and not for each t value separately. More precisely, in the modelling framework described in Section 2, a term of the linear model $Z = X\beta + \epsilon$ will be declared significant if a multivariate test applied to the corresponding line of the β matrix is significant.

Let X_0 and X_1 be two $(n \times p_0)$ and $(n \times p_1)$ full rank model matrices corresponding to two nested models M_0 and M_1 $(M_0 \subset M_1)$. If the significance of a single term of model M_1 is under consideration, X_0 is simply matrix X_1 where the corresponding column term is suppressed. For the three estimation approaches described above, the significance test can be seen as a multivariate multiple regression test on the following hypotheses :

$$H_0 : Z = X_0\beta^{(0)} + \epsilon^{(0)} \quad H_1 : Z = X_1\beta^{(1)} + \epsilon^{(1)}.$$

Let $\hat{z}_i^{(0)}$ and $\hat{z}_i^{(1)}$ represent the predicted vectors in ξ_i under these two models and $e_i^{(0)}$ and $e_i^{(1)}$ the corresponding residuals: $e_i^{(j)} = z_i - \hat{z}_i^{(j)}$, $j = 0, 1$.

Assuming that the residuals normaly distributed, the maximum likelihood estimator of the $q \times q$ variance covariance matrix Σ for each model M_j is given by :

$$\hat{\Sigma}^{(j)} = \frac{1}{n}\sum_{i=1}^{n} e_i^{(j)} e_i^{(j)\prime}$$

For small q (that is in approach (1) and (3)), the likelihood ratio test (LR) based on the ratio $-log(|\hat{\Sigma}^{(1)}|/|\hat{\Sigma}^{(0)}|)$ is a possible way to test M_0 against M_1. For large n, the corresponding test statistic is proportional to a chi-square distribution (see Johnson and Wichern[10]).

Shen and Faraway[14] show that the LR test is not suitable to large q or real functional data because it loses power and becomes unstable when q increases. They propose an alternative test applicable to all q values which does not depend on q, the finest of the grid for functional data. It is based on the test statistic :

$$\mathcal{F} = \frac{(rss_0 - rss_1)/(p_1 - p_0)}{rss_1/(n - p_1)}$$

where rss_j is the sum of squares of residuals under H_j : $ssr_j = \sum_{i=1}^{n} \sum_{k=1}^{q} (z_{ij} - \hat{z}_{ij}^{(j)})^2$. They show that, when n is sufficiently large, $\mathcal{F}$ may be approximated by an F distribution with $(p_1 - p_0)\delta_0$ and $(n - p_1)\delta_1$ degrees of freedom. δ_j is defined as trace$(\hat{\Sigma}^{(j)})^2$/trace$(\hat{\Sigma}^{(j)2})$.

Bootstrap is an alternative test procedure. Faraway[9] suggests a test procedure based it on the following test statistic:

$$T = \frac{1}{n} \sum_{i=1}^{n} \sum_{q=1}^{m} (\hat{z}_{ij}^{(0)} - \hat{z}_{ij}^{(1)})^2$$

This works as follows :

1. Compute T from the original Z data and calculate $\hat{z}_i^{(0)}$ and $e_i^{(0)}, i = 1, ...n$ the predicted response and residual vectors under H_0.
2. Resample with replacement from the $e_i^{(0)}$'s and create resampled response vectors as : $\tilde{z}_i = \hat{z}_i^{(0)} + \tilde{e}_i^{(0)}$.
3. Refit the two models M_0 and M_1 with these new response vectors and calculate the resampled test statistic T^*.
4. Repeat step 2 and 3 B times and calculate the bootstrap p-value as $\sharp\{T_b^* > T, b = 1, 2...B\}/B$

Section 4 illustrates these three tests on the case study in metal injection moulding.

The interpretation of factor effects on the response curves depends on the modelling and estimation procedure. For Approach 1, since the number of nonlinear model parameters θ_k, $k = 1...q$ is usually small, the analysis of the response surface estimated for each model parameter can give very good results when each parameter has a proper interpretation (as in the logistic case below). For Approach 2, the only way to interpret the effects of the model terms on the response is to look to the sign, size and shape of the $\hat{\beta}_i(t)$ parameter functions. Finally, if basis function like B-splines are used in the Approach 3, it can be shown that the parameter vectors $\hat{\beta}_i = (\hat{\beta}_{i1}, ...\hat{\beta}_{iq})$ have a similar shape and interpretation tho the $\hat{\beta}_i(t)$'s of the functional regression approach.

4. PREDICTION AND PREDICTION INTERVAL

In the framework of section 2, the prediction of the response curve $\hat{y}_0(t)$ for a new point x_0 of the experimental domain may be written in discrete form as :

$$\hat{y}_0 = h^{-1}(x_0'\hat{\beta}) = (\hat{y}_{01}, \hat{y}_{02}..., \hat{y}_{0m})$$

where $h^{-1}(.)$ is $f((t_1, ...t_m); x_0'\hat{\beta})$ for approach 1, $x_0'\hat{\beta}$ for approach 2 and $x_0'\hat{\beta}\phi$ for approach 3.

If we suppose that negligible information is lost in the h(.) pre-processing transformation, the prediction $(m \times m)$ variance-covariance matrix of $\hat{y}_0$ is given by:

$$\Omega \tilde{=} V(\hat{y}_0) = F\Sigma F'(1 + x_0'(X'X)^{-1}x_0)$$

where F is an $m \times q$ matrix of the partial derivatives of the transformation $h^{-1}(.)$. For Approach 1, $F_{ik} = \frac{\delta f(t_i;z_0)}{\delta z_{0j}}$; for Approach 2, $F = I_m$ and, for Approach 3, $F = \phi'$; This variance formula is exact for linear Approaches 2 and 3 and asymptotic for Approach 1.

As before, the estimator of the $q \times q$ residual variance covariance matrix Σ is given by :

$$\hat{\Sigma} = \frac{1}{n}\sum_{i=1}^{n}(z_i - \hat{z}_i)(z_i - \hat{z}_i)'$$

and an asymptotic $(1-\alpha)$ prediction interval for a single observation y_{i0} follows :

$$[\hat{y}_{0i} - z_{1-\alpha/2}\hat{\Omega}_{ii}, \hat{y}_{0i} + z_{1-\alpha/2}\hat{\Omega}_{ii}]$$

Faraway[9] introduces a bootstrap prediction interval defined as : $\hat{y}_{0i} \pm c\hat{\Omega}_{ii}$ where c is derived by the following procedure :

1. Estimate the model with the original data and calculate the fitted vectors $\hat{z}_i$, the predicted discrete curve $\hat{y}_0$ and the residual vectors $e_i, i = 1, ...n$.
2. Resample with replacement from the e_i's and create resampled response vectors $\tilde{z}_i = \hat{z}_i + \tilde{e}_i$.
3. Refit the model $Z^* = X\beta^* + \epsilon^*$ with this resampled data and predict the response curve $\hat{y}_0^*$.
4. Calculate c^b as $sup_{1\leq k\leq m}|\hat{y}_{0k}^* - \hat{y}_{0k}\|/\hat{\Omega}_{kk}$.
5. Repeat steps 2 to 4 B times and calculate c as the $(1-\alpha)^{\text{th}}$ quantile of $(c^1, c^2, ...c^B)$.

5. CASE STUDY

5.1. Context and goal of the study

Metal Injection Moulding (MIM) is an established route for mass production of small and complex metal parts. This process combines a small quantity of binder with metal powder to form a feedstock that can be moulded. After shaping, the binder is extracted and the powder is sintered. The substitution of polymer carried by water is an emerging goal due to health and environmental benefits. So a new aqueous binder formulation, namely xanthan gum and chromium nitrate, is proposed. This study aims to identify the optimal composition which gives the highest gel strength at a low gelling temperature (avoid excessive evaporation) and the lowest chromium concentration (to limit contamination). The gelling properties of the binder were studied as a function of temperature with a rheometer (Bohlin CS) operating in control stress mode using a cone (4°) and plate (40 mm) system. With this tool, it is possible to continuously record the variation of the elastic modulus (representative of gel strength) on heating using small amplitude oscillatory rheometry.

5.2. Design and response curves

A 15-run experimental design (see Figure 1) has been performed to study the effect of xanthan concentration (X) and the chromium/xanthan concentration ratio (R) on the elastic modulus ($y(t)$) at temperature between 10 and 80 °C. Th results where obtained with a Bohlin rheometer. X varied from 1 to 5% and R from 1:1 to 4:1. Figure 2(a) presents the response curves in real and logarithmic values. They show a well defined shape with local measurement noise (which is uninformative with respect to the theoretical gelling properties of each solution). Before analysis, these data were transformed into logarithm and interpolated to get all curves on a commun grid of 701 points between 10 and 80°C.

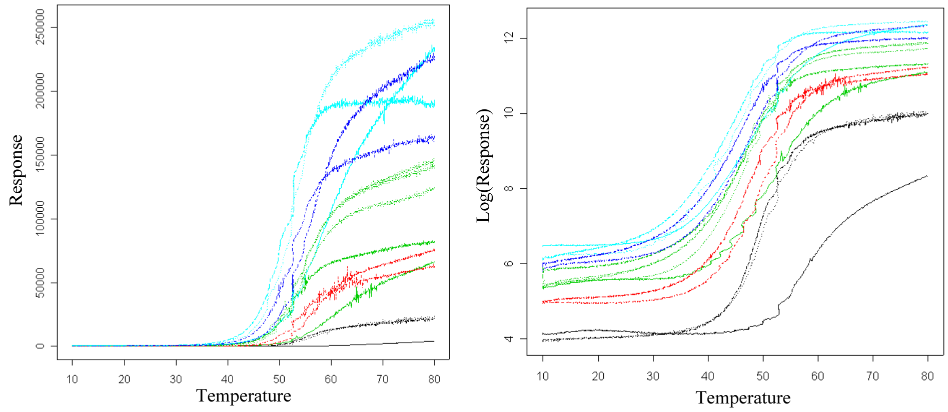

Figure 2: Response curves in original (left) and logarithmic (right) values

5.3. Design and response curves

The three estimation methods (NL : nonlinear pre-processing, FR : functional regression and BS : B-spline pre-processing) were used to fit a model to these curves and explain them from the factor settings. A partial third order polynomial model was used to build the X model matrix from the standardised design matrix :

$$z = \beta_0 + \beta_1 X + \beta_2 R + \beta_3 X^2 + \beta_4 R^2 + \beta_5 XR + \beta_6 X^2 R + \beta_7 XR^2 + \epsilon$$

The nonlinear model used to fit the original curves was a four parameters logistic model:

$$y(t) \simeq \theta_1 + \frac{\theta_2 - \theta_1}{1 + exp(-\theta_4(t - \theta_3))} = f(t;\theta)$$

The three methods give very good results as shown in Figure 3 where the original curves are compared with the predicted curves in the nonlinear approach. The two other methods gave very similar results. The global R^2's are $R^2_{NL} = 0.9968$, $R^2_{FR} = 0.9975$ and $R^2_{BS} = 0.9974$.

Figure 4 shows the fitted curves in $X = 3$ and $R = 2$. The left pane shows the original curve, the fitted logistic curve and the logistic curve predicted from the factor settings. The rigth pane shows the results given by the other two methods. It shows that the (10 knots) cubic B-splines fit the original curves much better than the logistic model. Moreover, it illustrates the fact that the predicted curve obtained from the B-spline approach is a smooth version of that obtained with pointwise functional regression. An analysis of the residual curves showed an outlier at $X = 2$ and $R = 1.75$ but replicated runs at this point and at $X = 1$, $R = 1$ confirmed the results.

5.4. Factor effect significance test and interpretation

The three multivariate regression test methods (LR: likelihood ratio, SF: Shen and Faraway F test and B: Bootstrap test) where applied to these models to test the (global) significance of polynomial model terms. Corresponding p-values are given in Table 1. The p-values obtained from the functional regression and B-spline approaches are nearly equal for SF and B tests. For the three models, the SF and B

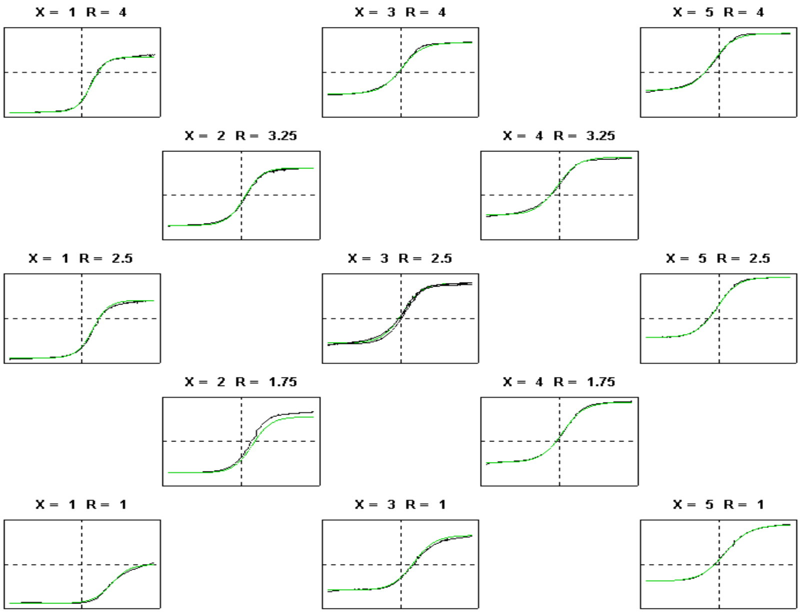

Figure 3: Observed and predicted curves for the nonlinear (logistic) approach

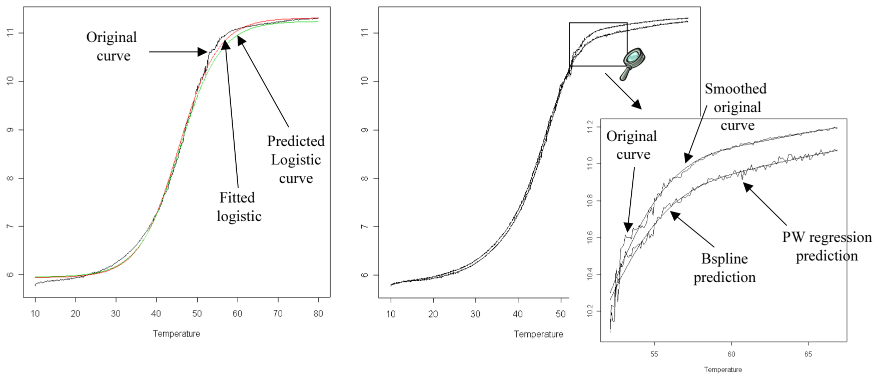

Figure 4: Curve fitted by all methods at point $X = 3$ and $R = 2$

p-values give similar conclusions. The results provided by the LR test are somewhat different from the others. These results allow to conclude that X, X^2 and R^2 have a very strong effec, R and XS have a moderate effect and X^2R and XR^2 a less clear effect.

Figure 5 provides the best way to interpret these polynomial models. It shows, through classical response surfaces, the effect of X and R on the four parameters of the logistic regression models. They can be interpreted in the usual way and confirm the strong effect of X, X^2 and R^2.

Figure 6 presents the estimated parameter curves $\hat{\beta}_i(t)$ obtained with the functional regression approach. These are less easy to interpret but show, in the constant term, the average shape of the curves and confirm a big positive effect for X, a lower effect for R and a negative effect for R^2. Note that the corresponding graphics ob-

	Nonlinear pre-processing			Functional regression		B-spline pre-processing	
	ML	SF	B	SF	B	SF	B
X	0.0000	0.0000	0.0007	0.0000	0.0006	0.0000	0.0007
R	0.0002	0.0000	0.0010	0.0022	0.0016	0.0009	0.001
X^2	0.0010	0.0013	0.0004	0.0002	0.0002	0.0000	0.0002
R^2	0.0023	0.0000	0.0000	0.0003	0.0001	0.0000	0.0002
XS	0.0717	0.0021	0.0005	0.0023	0.0004	0.0004	0.0002
X^2R	0.0075	0.0310	0.0047	0.0186	0.0038	0.0142	0.0031
XR^2	0.1321	0.0040	0.0004	0.0369	0.0070	0.0200	0.0064

Table 1: P-values for test of significance of polynomial model terms

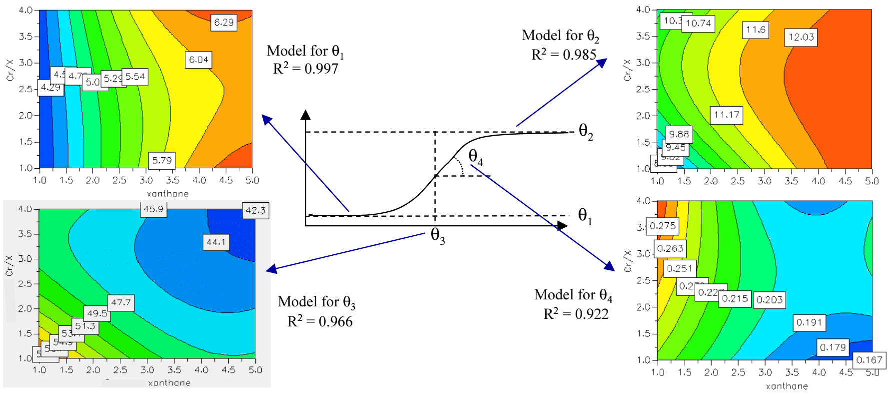

Figure 5: Response surfaces for the four polynomial models fitted in the nonlinear (logistic) pre-processing approach.

tained from the β matrix of the BS approach have very similar shapes and drive to the same conclusions.

5.5. Prediction and optimisation

The response surfaces of Figure 5 allowed $X = 5$ and $R = 2$ to be chosen as optimal factor settings. Figure 7 (left pane) gives the predicted curves obtained with the three models under these conditions, and the six prediction intervals computed from the asymptotic and bootstrap approaches. They all show very similar results. The rigth pane of Figure 7 shows the predicted curve and the prediction interval obtained using the B-spline pre-processing approach with a validation run which shows a curve inside the prediction interval.

6. CONCLUSIONS

This paper has presented different approaches to analysing the results of a designed experiment when the response is a curve. The three modelling approaches are based on a pre-processing step followed by a multivariate polynomial regression on the transformed curves. From the interpretability point of view, the nonlinear

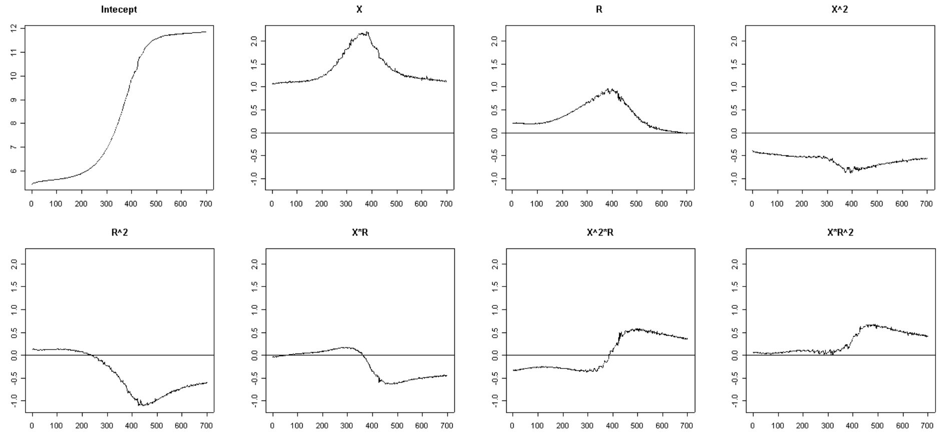

Figure 6: Functional parameters for the 8 terms of the polynomial model estimated with the functional regression approach.

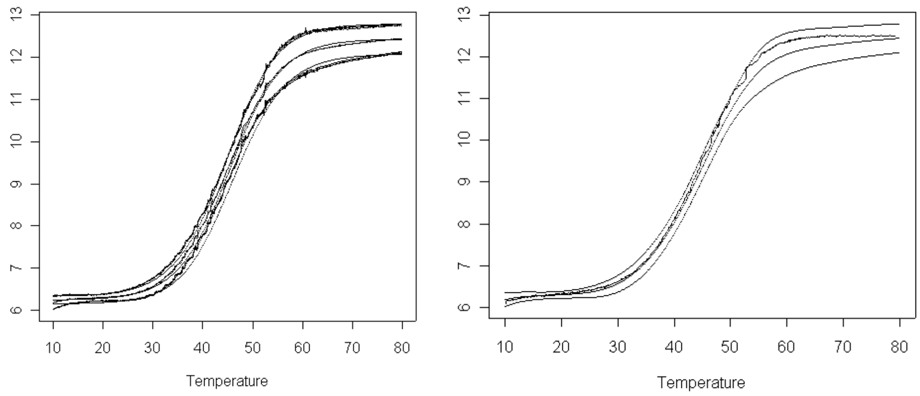

Figure 7: Predicted curve, prediction interval and validation run in point $X = 5$ and $R = 2$.

pre-processing approach is certainly the most attractive for the practitioner, but it is restricted to curves that follow a common and known parametric model. The pointwise function regression is the easiest method to apply, but has the drawback of providing non-smooth predictions and necessitating data observed on a common grid. The B-spline pre-processing approach solves these two problems and is certainly the best choice when a (potentially) general method is required. We are currently testing this last procedure on more complex curves to delimit its real range of applications.

This paper also discusses procedures to test the significance of the model terms and calculate prediction intervals. The case study illustrates their applicability nicely but further work is necessary to investigate small sample properties of the testing procedures (in the line of the work started by Shen and Faraway[14]).

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