Splines As a Useful and Convenient Statistical Tool

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The framework for a unified statistical theory of spline regression assuming fixed knots using the truncated polynomial or "+" function representation is presented. In particular, a partial ordering of some spline models is introduced to clarify their relationship and to indicate the hypotheses that can be tested by using either standard multiple regression procedures or a little-used conditional test developed by Hotelling (1940). The construction of spline models with polynomial pieces of different degrees is illustrated. A numerical example from a chemical experiment is given by using the GLM procedure of the statistical software package SAS (Barr et al. 1976).

KEY WORDS: Hypothesis testing; Multiple regression; Ordinary least squares; Piecewise polynomials; Splines.

1. Introduction

Splines are generally defined to be piecewise polynomials of degree n whose function values and first $n - 1$ derivatives agree at the points where they join. The abscissas of these joint points are called knots. Polynomials may be considered a special case of splines with no knots, and piecewise polynomials with fewer than the maximum number of continuity restrictions may also be considered splines. The number and degrees of the polynomial pieces and the number and position of the knots may vary in different situations.

If the knots are considered variable, that is, parameters to be estimated, they enter into the regression problem in a nonlinear fashion, and all the problems arising in nonlinear regression are present. It is very difficult to find knot locations that give an absolute minimum for the residual sum of squares, so obtaining the least squares estimators of the parameters is difficult and testing hypotheses virtually impossible, although some research in this direction has been done (e.g., see Gallant and Fuller 1973). The use of variable knot splines also carries the practical danger of overfitting the data. Varying the number and positions of the knots can greatly improve the fit with no theoretical justification for model changes at the determined points. Of course, under- or overfitting can be a problem in any kind of model.

Spline regression with fixed knots, however, is straightforward using ordinary least squares, although deciding on the number of knots and the degrees of the polynomial pieces is still a problem from a statistical viewpoint. Wold (1971, 1974) gives several examples of how splines with fixed knots can be used to advantage as a data-fitting tool. He restricts himself to cubic splines that are popular because they are of low degree, fairly smooth assuming continuity restrictions up to the second derivative, and yet have the power to incorporate several different trends in data simply by increasing the number of knots. Wold also uses a special representation or basis for spline models, called B-splines, because of their computational efficiency when a large number of knots are specified. Just as polynomial models may be written by using orthogonal polynomials instead of terms of the form x^n, B-splines represent one of several ways to write spline models. Unfortunately, they do not lend themselves easily to statistical interpretation, although testing can be accomplished through linear transformations (i.e., change of basis). Buse and Lim (1977) show how all hypotheses about continuity restrictions and higher-order terms in the cubic pieces can be tested by using restricted least squares. Buse and Lim's results extend to fitting piecewise polynomials of varying degree with varying continuity restrictions.

A simpler statistical approach than either of these is the use of truncated polynomials, or "+" functions, discussed in Section 2, as basis elements in the spline models. They are not as computationally efficient as B-splines, but their use allows the data to be fit by ordinary least squares while still permitting tests of hypotheses to be easily made. Truncated polynomials have been applied in a wide variety of situations. For example, Fuller (1969) gives a general discussion of linear and quadratic splines in two variables (bilinear and biquadratic splines) and indicates how to test for the significance of spline terms. He illustrates their use in a fertilizer experiment in which corn yield is written as a function of nitrogen and phosphorus in a 5×5 factorial design. Fuller also discusses the joining of quadratic and linear pieces, using a linear piece for extrapolation. Poirier (1975) discusses the application of bilinear splines in economics and tests for the significance of main effects. Studden and Van Arman (1969), Murty (1971), Draper, Guttman, and Lipow (1977), and Park (1978) employ "+" functions in the context of finding optimal designs for spline models.

Unfortunately, "+" functions have not been used to full statistical advantage. Their application has included the testing of only a few selected hypotheses while the wide range of available tests has not been discussed. Although Poirier (1976) and Seber (1977) mention some of these possibilities in a multiple regression context, neither author goes into any detail nor emphasizes their convenience in light of statistical software packages.

In this article, through the use of a partial ordering of splines, we examine fully the possible tests that can be made about spline models with fixed knots us-

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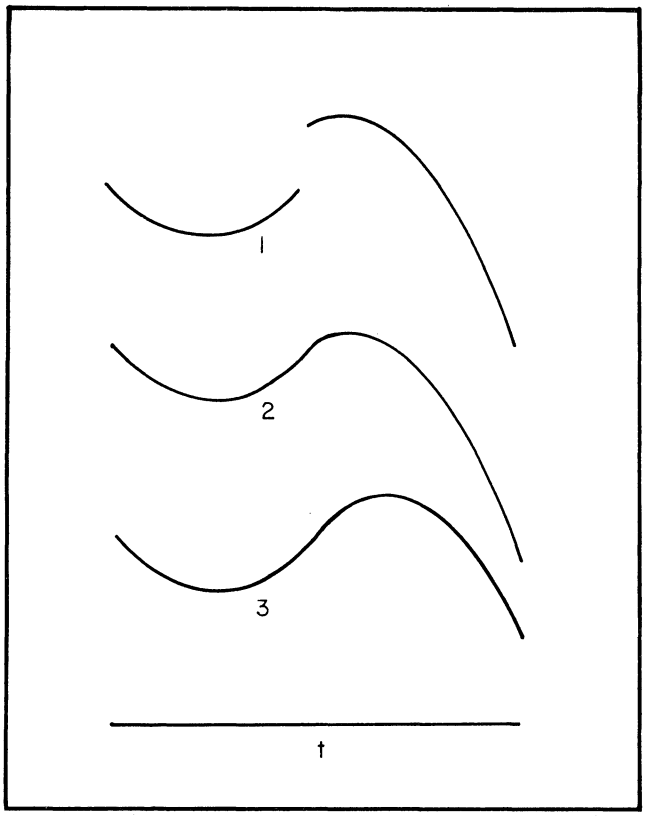


A. Quadratic Splines With One Knot and Varying Continuity Restrictions.

ing "+" functions. Except for tests relating to arbitrary endpoint restrictions, the tests examined include all the tests discussed by Poirier (1973) and Buse and Lim (1977). In addition, a little-used test developed by Hotelling (1940) is discussed to illustrate how, in some cases, additional tests outside the usual multiple regression framework can be made.

We begin by reviewing in Section 2 the use of "+" functions to define spline models with varying degrees of smoothness and the estimation of the parameters by ordinary least squares. Modifications for regression through the origin are also discussed. In Section 3, a partial ordering of some splines is given that shows how splines with different continuity restrictions and degrees of the polynomial pieces relate to each other. This approach is helpful in determining which hypotheses about splines may be tested and what the results mean. In Section 4, these techniques are applied to a set of data using the GLM procedure of SAS (Barr et al. 1976) to illustrate the ease with which data may be fit and hypotheses may be tested in spline models using multiple regression procedures.

2. The "+" Function Representation

In order to use ordinary least squares to fit data assuming a spline model and still allow for easy testing, "+" functions can be used to impose the number and kind of continuity (smoothing) restrictions we desire. The "+" function is defined as

$$\begin{aligned} u_+ &= u \quad \text{if} \quad u > 0 \\ &= 0 \quad \text{if} \quad u \leq 0. \end{aligned}$$

To illustrate the use of "+" functions in spline models, we first consider the particular case of a piecewise quadratic in x with a knot at t and no smoothing conditions:

$$\begin{aligned} S(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{10}(x-t)_+^0 \\ + \beta_{11}(x-t)_+^1 + \beta_{12}(x-t)_+^2 + \epsilon. \quad (2.1) \end{aligned}$$

We assume the ϵ's are independent and normally distributed with mean zero and common variance, and we define $(x-t)_+^0 = 1$ if $x \geq t$ and 0 if $x < t$. The accompanying table gives the form of S and its first derivative $S^{(1)}$. Note that the piecewise polynomials are possibly different quadratics in x and that neither S nor $S^{(1)}$ is necessarily continuous at $x = t$. In Figure A, A1 shows how the graph of (2.1) might look. If the β_{10} term were eliminated from the model, we see from the table that S would be continuous, and if, in addition, the β_{11} term were eliminated, both S and $S^{(1)}$ would be continuous. Thus, we can test whether imposing one or more continuity restrictions results in a significantly worse fit by testing the significance of the least squares estimates of β_{10} and/or β_{11}. A2 and A3 of Figure A show a continuous quadratic spline without and with, respectively, a continuous first derivative. Testing the importance of all the "+" function terms, that is, $\beta_{10} = \beta_{11} = \beta_{12} = 0$, is equivalent to testing whether the spline fits the data significantly better than a quadratic polynomial. These tests are easily performed by using a multiple regression procedure in a statistical computer package that gives sequential sums of squares.

In general, with k knots, $t_1 < \ldots < t_k$, and the $k+1$ polynomial pieces each of degree n, we may write a spline model with no continuity restrictions as follows:

$$S(x) = \sum_{j=0}^{n} \beta_{0j}x^j + \sum_{i=1}^{k}\sum_{j=0}^{n} \beta_{ij}(x-t_i)_+^j + \epsilon. \quad (2.2)$$

As in the special case just discussed, the presence of a $\beta_{ij}(x-t_i)_+^j$ term allows a discontinuity at t_i in the jth derivative of S, $S^{(j)}(S^{(0)} = S)$, and its absence forces the continuity of $S^{(j)}$ at t_i. Thus, S can be made continuous at knot t_i by omitting from (2.2) the constant term $\beta_{i0}(x-t_i)_+^0$, and $S^{(j)}$ can be made continuous at t_i by omitting the term $\beta_{ij}(x-t_i)_+^j$. If we wanted continuity in the jth derivative of S at a particular knot t_i, we would probably also want continuity in all lower-order derivatives at t_i. This continuity is accomplished by omitting the terms $\beta_{im}(x-t_i)_+^m$, $m = 0, 1, \ldots, j$. Different continuity restrictions can be imposed at different knots simply by deleting the appropriate terms. The more terms we delete, the worse the fit will be. Because the deletion of a "+" term is equivalent to adding a continuity restriction, however, the curve will be smoother. In order to determine which continuity restrictions do not result in a significantly worse fit, we test in (2.2) whether the ap-

Model (2.1)

	$S(x)$	$S^{(1)}(x)$
$x < t$	$\beta_{00} + \beta_{01}x + \beta_{02}x^2$	$\beta_{01} + 2\beta_{02}x$
$x \geq t$	$\beta_{00} + \beta_{01}x + \beta_{02}x^2$	$\beta_{01} + 2\beta_{02}x$
	$+ \beta_{10} + \beta_{11}(x - t) + \beta_{12}(x - t)^2$	$+ \beta_{11} + 2\beta_{12}(x - t)$

propriate coefficients are zero. This test may be done simultaneously or sequentially as in variable elimination, any criticism of the latter also applying to restriction addition.

The smoothest possible spline with polynomial pieces of degree n with k knots is given by

$$S(x) = \sum_{j=0}^{n} \beta_{0j}x^j + \sum_{i=1}^{k} \beta_{in}(x - t_i)_+{}^n + \epsilon,$$

omitting from (2.2) all "+" terms of power lower than n. In this case, S and its first $n - 1$ derivatives will be continuous. Because most regression models are very smooth, polynomials being infinitely differentiable at every point, it is not unreasonable to assume as much smoothness as possible in spline models, as is often the case. Therefore, testing the importance of certain continuity restrictions may be of interest only to obtain a smoother curve, but in some instances there may be theoretical reasons also. Testing the importance of the fixed knots, however, should have a physical interpretation in most cases. Because the knots are fixed in the beginning by the experimenter, he/she should have some reason not only for putting the knots at specific locations but also for assuming that they exist at all.

If all the knots are positive, we can force the regression through the origin simply by deleting β_{00} from (2.2). If one or more of the knots is negative (implying $t_1 < 0$), we can reparameterize model (2.2) by using $S(z)$ with $z = x - t_1 + 1$ and delete β_{00} as before.

If we wish to fit polynomial pieces of different degrees, model (2.2) can be modified and multiple regression techniques applied as usual. In some cases the modification may necessarily be substantial. The simplest type of modification occurs when only polynomial pieces of degrees n and $n - 1$ are used in the model. We must then impose the condition in model (2.2) that some parameters are zero and certain pairs of parameters sum to zero. If polynomial pieces of degrees other than n and $n - 1$ are desired, the modifications to (2.2) are more involved.

To illustrate these concepts, suppose we wish to use three polynomial pieces: the first piece cubic, the second quadratic, and the third linear such that the spline is continuous but not necessarily its first derivative. We begin by using (2.2) to write the model for a three-piece cubic (largest-degree piece) continuous spline:

$$\begin{aligned} S(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{03}x^3 + \beta_{11}(x - t_1)_+ \\ + \beta_{12}(x - t_1)_+{}^2 + \beta_{13}(x - t_1)_+{}^3 + \beta_{21}(x - t_2)_+ \\ + \beta_{22}(x - t_2)_+{}^2 + \beta_{23}(x - t_2)_+{}^3. \end{aligned}$$

The absence of the β_{10} and β_{20} terms guarantees that the function is continuous, and the presence of higher-order terms allows for possible discontinuities in the derivatives. We need to modify this model to get the desired cubic, quadratic, and linear pieces.

Eliminating the β_{13} and β_{23} terms will not remove the cubic contribution from the last two pieces because x^3 contributes to each piece. By eliminating the β_{23} term and imposing the condition $\beta_{03} + \beta_{13} = 0$, however, the last two pieces will not be cubic because the x^3 term in $\beta_{13}(x - t_1)_+{}^3$ will cancel with $\beta_{03}x^3$ for $x > t_1$. We now have

$$\begin{aligned} S(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{03}[x^3 - (x - t_1)_+{}^3] \\ + \beta_{11}(x - t_1)_+ + \beta_{12}(x - t_1)_+{}^2 + \beta_{21}(x - t_2)_+ \\ + \beta_{22}(x - t_2)_+{}^2 \end{aligned}$$

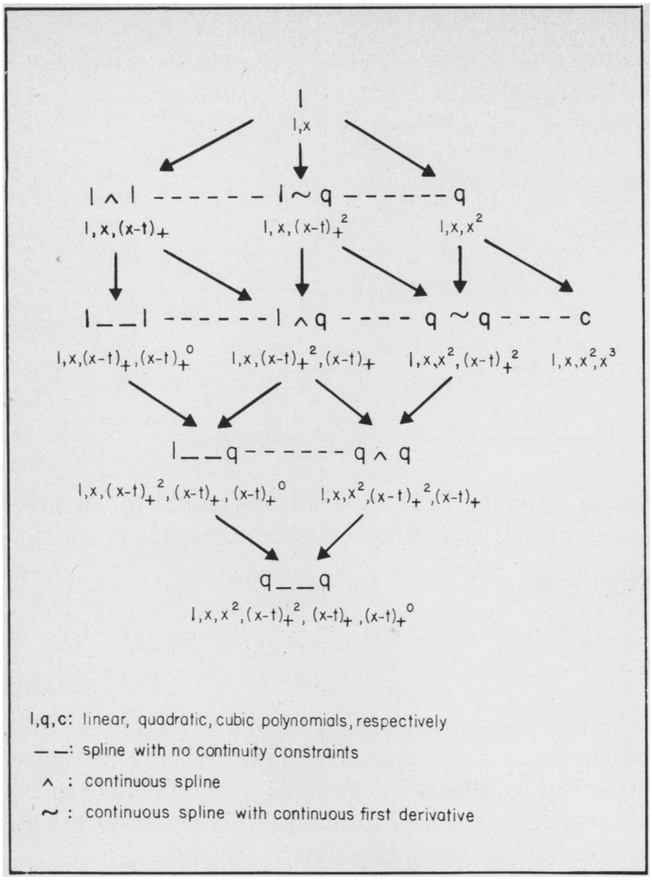
and need only eliminate the quadratic contribution from the third piece to get the desired model. This is accomplished by requiring the sum of the coefficients of the x^2 terms to be zero, that is, $\beta_{02} + 3\beta_{03}t_1 + \beta_{12} + \beta_{22} = 0$. Substituting for β_{22} from this equation yields the final desired spline model:

$$\begin{aligned} S(x) = \beta_{00} + \beta_{01}x + \beta_{02}[(x^2 - (x - t_2)_+{}^2] \\ + \beta_{03}[x^3 - (x - t_1)_+{}^3 - 3t_1(x - t_2)_+{}^2] \\ + \beta_{11}(x - t_1)_+ + \beta_{12}[(x - t_1)_+{}^2 - (x - t_2)_+{}^2] \\ + \beta_{21}(x - t_2)_+. \end{aligned}$$

This same kind of procedure can be followed for more complicated combinations of polynomial pieces.

3. A Partial Ordering of Splines

To illustrate further the kinds of hypotheses that can be tested by using "+" function spline models and how they relate to polynomial models and to each other, a



B. A Partial Ordering of Some Spline Models With a Fixed Knot at t.

NOTE: An F-test may be used to compare models connected by a sequence of arrows. Hotelling's conditional test may be used to compare all adjacent models and some nonadjacent models connected by a dotted line.

partial ordering of some spline models is given in Figure B along with their basis elements. Only splines with at most one knot and of degree 2 are shown (except for the cubic polynomial), but the partial ordering may be extended to splines with more knots and of higher degree. Also, the partial ordering in Figure B assumes that the degree of the polynomial piece on the right is at least as large as the polynomial piece on the left. A similar partial ordering exists with the reverse true and with hypothesis tests available such as those discussed later.

The simplest model is the simple linear model, denoted l. Models have an increasing number of terms as we move down from l and thus will give a better fit to the data. For example, if the data are believed to behave in a different linear fashion on either side of a fixed point t, the knot, we may wish to use a spline model and fit the data with two possibly different lines on each side. The model may or may not be continuous at the knot ($1 \wedge 1$ and $1 -- 1$, respectively). The model $1 -- 1$ will be at least as good as $1 \wedge 1$ because it has one more term, and we can test for a significant difference between the two fits by testing the significance of the estimate of the coefficient of $(x - t)_+{}^0$. The improvement of each of these over model l can also be tested. In general, models connected by a sequence of arrows in Figure B may be tested for a significant difference in fit by testing that the coefficients of the extra terms in the more complicated model are zero.

An important question to be answered is whether a spline should be used at all. If we make an assumption about the form of the model, for example, that there is one knot, we are assuming that the underlying mechanism is not of the same kind throughout the range of the independent variable observed. If the difference is only slight, then even though a change may in fact occur at the knot, it may be so minor that a model without a knot is adequate to describe the process. Testing the hypothesis that the coefficients of all the "+" terms are zero will provide us with the answer. If this hypothesis is rejected and there is more than one knot, we may wish to test further (and conditionally on the results of the previous test) the importance of particular knots or continuity restrictions. This kind of sequential testing (mentioned earlier in Section 2) is akin to techniques in variable selection in which a variable is dropped from the regression (or in spline models, a continuity restriction is added) if, for instance, it is not significant and has the smallest adjusted sum of squares. Therefore, any drawbacks to this technique would also apply to spline models. Sequential tests need not be performed, however, if certain hypotheses of interest are specified before the data are fit.

Some hypotheses may be more easily tested than others because of the basis terms used. For example, in the model $q \wedge q$,

$$S(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{11}(x - t)_+ + \beta_{12}(x - t)_+{}^2 + \epsilon, \quad (3.1)$$

we easily see from Figure B that by testing that $\beta_{02} = 0$ we are testing whether model $q \wedge q$ is significantly better than model $1 \wedge q$. Testing that $\beta_{12} = 0$, however, is not equivalent to testing whether $q \wedge q$ is significantly better than $q \wedge 1$ (not shown in Figure B) because the x^2 term will still appear on both sides of the knot even when $\beta_{12} = 0$. In fact, such a test would not be of statistical or practical importance because we would still have a continuous quadratic spline ($q \wedge q$) but with a worse fit. We can test that the model should be $q \wedge 1$ by testing that $\beta_{02} + \beta_{12} = 0$, for then the x^2 term to the right of t disappears. This can be done by examining the usual F ratio after finding the error sum of squares from the model

$$S(x) = \beta_{00} + \beta_{01}x + \beta_{02}(x^2 - (x - t)_+{}^2) + \beta_{11}(x - t)_+ + \epsilon.$$

An easier approach, however, is to write the model as

$$S(x) = \beta_{00} + \beta_{01}x + \beta_{02}x^2 + \beta_{11}(t - x)_+ + \beta_{12}(t - x)_+{}^2 + \epsilon$$

and test that $\beta_{02} = 0$. This alternate representation is only advantageous, however, if we are interested in testing if $q \wedge 1$ but not $1 \wedge q$ is as good as $q \wedge q$. Thus, we may possibly test hypotheses by specifying only one model using a convenient basis and examining selected coefficients. In other instances, regardless of the basis, we may have to find the residual sum of squares from more than one model if our hypotheses make statements about certain linear combinations of the parameters.

For data in which the independent variables are considered fixed, we may possibly test for a significantly different fit between two spline models that are not connected by an arrow in Figure B. The usual test between two models is based on the difference in error sum of squares between the constrained and unconstrained models, the terms in one model being a subset (or linear combination) of the terms in the other model. If, however, constraining one of the models does not result in the other, this method does not apply. For example, we see from Figure B that the model $q \sim q$ gives at least as good a fit as either of the models q or $1 \sim q$, both of which give at least as good a fit as model 1. Of these four models, only $1 \sim q$ and q cannot be compared in the usual way, but a test can be made if the independent variable is considered fixed.

Hotelling (1940) developed a conditional test between p models, each with k terms, $k - 1$ of which are the same in all models; that is, the models are identical except for one term. Specifically, suppose $k - 1$ predictors have already been chosen for a regression model, and we wish to know which one of p additional predictors $x_1, \ldots, x_p$ should be included also. If ρ_i is the partial correlation between the dependent variable y and x_i adjusted for the original $k - 1$ predictors, Hotelling's procedure uses an F ratio to test H_0: $\rho_1 = \rho_2 = \cdots = \rho_p$. In the simple case of choosing between two variables, x_1 and x_2, when no other predictors are involved, for a sample of size n the test statistic has a t distribution with $n - 3$ degrees of freedom and equals

$$(r_1 - r_2)[((n - 3)/2D)(1 + r_0)]^{1/2}$$

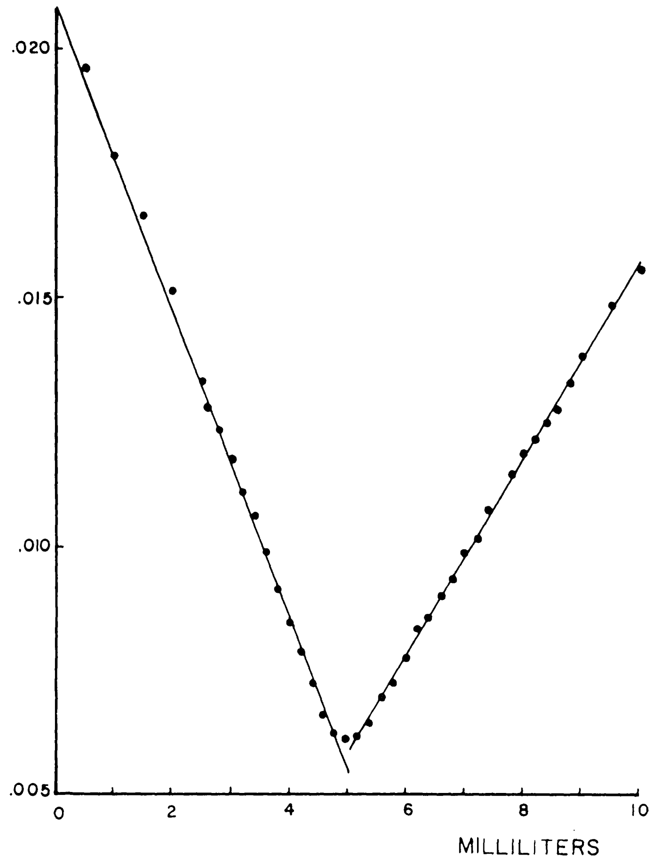
where r_i is the sample correlation between y and x_i, r_0 is the sample correlation between x_1 and x_2, and D is the determinant of the matrix

$$\begin{bmatrix} 1 & r_1 & r_2 \\ r_1 & 1 & r_0 \\ r_2 & r_0 & 1 \end{bmatrix}.$$

The test applies to all linear models where the independent variables are considered fixed, not random. Spline models that may be compared by using Hotelling's test are connected by a dotted line in Figure B.

4. A Numerical Example

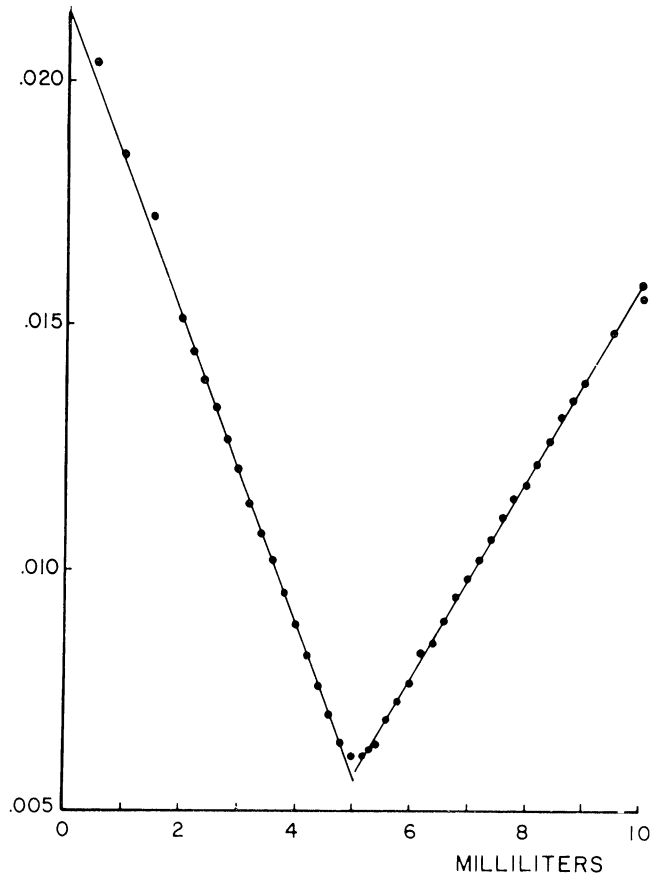
The graph of equivalents of base added versus conductance obtained from a chemical conductivity experiment in which a strong monoprotic acid is titrated with a known concentration of base yields a spline with one knot. The location of the knot is at the point at which one equivalent of the titrant base has been added. The polynomial piece to the left of the knot is generally linear or quadratic depending on the strength of the base, and the other piece is linear. If the analyst wishes to determine the quantity of acid present in a sample, the knot is variable; that is, its location is unknown. On the other hand, the knot is fixed if the concentration of acid is known (and thus the equivalence point and the location of the knot) and the analyst wishes to determine the cell constant with respect to his/her particular experimental conditions.



C. Milliliter of Titrant vs. Conductance: Trial 1.

The standard procedure for fitting the data in the latter case is to fit two straight lines on either side of the known equivalence point but not restrict them to cross there. The spline representation of such a fit is $y = \beta_0 + \beta_1 x + \beta_2(x - t)_+ + \beta_3(x - t)_+^0 + \epsilon$, allowing a discontinuity at the knot t by the presence of the last term. The analyst usually looks only at the size of the residuals to determine whether there are problems with the experimental conditions. Because the lines theoretically should cross at the known equivalence point, however, a discontinuity that is too large as determined by a test of the hypothesis $\beta_3 = 0$ should also indicate deviations from the model system (or expected results), which must be interpreted by the experimenter. We see from Figure B that this is a test between the competing models 1--1 and $1 \wedge 1$.

In the example considered here, .1 M NaOH solution was titrated at a temperature of 23°C into 5.0395 ml of .1 M HCl diluted with 75 ml of deionized



D. Milliliter of Titrant vs. Conductance: Trial 2.

H_2O. A standard cell of cell constant .1 was used. If we know this cell constant is .1, the approximate value of a second cell constant of a cell of identical geometry can be determined from the shift in conductivity at the known equivalence point. The conductance was regressed on the amount of the titrant by using the spline model 1−−1 given above with $t = 5.0395$ ml, the known equivalence point. Two trials were run, and the hypothesis H_0: $\beta_3 = 0$ was tested. A graph of the data and fitted spline in each of the trials is shown in Figures C and D. In the first trial, H_0 was rejected (P-value = .0001), and in the second trial it was accepted (P-value = .3950), which indicates that the results obtained in the second trial are more reliable. Thus, in using the same solution for another trial with a different cell of unknown cell constant, computations based on data from the second trial should be used.

5. Conclusions

We have provided the framework for a unified statistical theory of spline regression assuming fixed knots and using the "+" function representation. Through the use of a partial ordering, we have detailed the relationship of spline models with regard to the degrees of the polynomial pieces and the continuity constraints imposed. Because the "+" function representation permits parameters to be estimated by ordinary least squares and tests of hypotheses to be carried out by using standard multiple regression procedures, the partial ordering provides a convenient way to determine which hypotheses can be tested and how to interpret the role of the various coefficients. The "+" function representation is especially advantageous because it allows the use of multiple regression procedures in statistical packages such as SAS. A numerical example illustrated some of these concepts.

The basis elements used in this article, the "+" functions, are not the most computationally efficient, and the design matrices are ill conditioned for a large number of knots, but the advantage of the "+" functions is that they may be used easily by statisticians to test hypotheses in spline models by using standard techniques. It would be useful to investigate which linear transformations on B-splines would be necessary to test relevant statistical hypotheses. Then the computational efficiency of B-splines could be combined with the statistically advantageous "+" functions into one technique, which, we hope, would become a standard procedure in statistical software packages.

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