Spline Functions and the Problem of Graduation

I. J. Schoenberg

PNAS 1964;52;947-950
doi:10.1073/pnas.52.4.947

SPLINE FUNCTIONS AND THE PROBLEM OF GRADUATION*

By I. J. Schoenberg

UNIVERSITY OF PENNSYLVANIA AND INSTITUTE FOR ADVANCED STUDY

Communicated by S. Bochner, August 19, 1964

1. *Introduction.*—The aim of this note is to extend some of the recent work on spline interpolation so as to include also a solution of the problem of graduation of data. The well-known method of graduation due to E. T. Whittaker suggests how this should be done. Here we merely describe the idea and the qualitative aspects of the new method, while proofs and the computational side will be discussed elsewhere.

2. *Spline Interpolation.*—Let $I = [a, b]$ be a finite interval and let (x_ν, y_ν), $(\nu = 1, \ldots, n)$, be given data such that $a \leqq x_1 < x_2 < \ldots < x_n \leqq b$. The following facts are known:[1]

Let m be a natural number, $m \leqq n$. The problem of finding a function $f(x)$ $(x \in I)$ having a square integrable mth derivative and satisfying the two conditions

$$f(x_\nu) = y_\nu, \quad (\nu = 1, \ldots, n), \tag{1}$$

$$Jf \equiv \frac{1}{(m!)^2} \int_I (f^m(x))^2 dx = \text{minimum}, \tag{2}$$

has a unique solution which is the restriction to $[a, b]$ of the function $s(x) = S(x;\ y_1, y_2, \ldots, y_n)$ which is uniquely characterized by the three conditions

$$s(x_\nu) = y_\nu,\ (\nu = 1, \ldots, n) \tag{3}$$

$$s(x) \in C^{2m-2}(-\infty,\ \infty) \tag{4}$$

$$\begin{cases} s(x) \in \pi_{2m-1} \text{ in each of the intervals } (x_\nu, x_{\nu+1}),^2 \\ s(x) \in \pi_{m-1} \text{ in } (-\infty, x_1) \text{ and also in } (x_n,\ \infty). \end{cases} \tag{5}$$

The functions defined by the two conditions (4) and (5) are called *spline functions of order* $2m$ (or degree $2m - 1$), having the *knots* x_ν; we denote their class by the symbol $\mathcal{S}_m$.

We have assumed that $1 \leqq m \leqq n$. If $m = 1$, then $s(x)$ is obtained by linear interpolation between successive y_ν, while $s(x) = y_1$ if $x < x_1$ and $s(x) = y_n$ if $x > x_n$. If $m = n$, then $\mathcal{S}_m = \pi_{n-1}$ and $s(x)$ is the polynomial interpolating the y_ν.

3. *Whittaker's Method of Graduation.*—In 1923 E. T. Whittaker[3] proposed the following method of adjusting the ordinates y_ν if these are only imperfectly known and are in need of a certain amount of smoothing: he chooses m, $1 \leqq m < n$, and the (smoothing) parameter, ϵ, $\epsilon > 0$. The graduated sequence $y_\nu^* = y_\nu^*(\epsilon)$ is then obtained as the solution of the problem

$$\epsilon \sum_{\nu=1}^{n-m} (\Delta^m y_\nu^*)^2 + \sum_1^n (y_\nu^* - y_\nu)^2 = \text{minimum}, \tag{6}$$

where

$$\Delta^m y_\nu^* = \sum_{i=\nu}^{\nu+m} y_i^*/\omega'_\nu(x_i), \qquad \omega_\nu(x) = (x - x_\nu) \ldots (x - x_{\nu+m}),$$

are the divided differences.

We use throughout this note the notation

$$Ef = Ef(x) = \sum_{1}^{n} (f(x_\nu) - y_\nu)^2 \tag{7}$$

and define the familiar least squares polynomial $Q(x) \in \pi_{m-1}$ as the solution of the problem

$$Ef = \text{minimum}, \ (f \in \pi_{m-1}). \tag{8}$$

It is easily shown that Whittaker's graduated values $y_\nu^*(\epsilon)$ have the properties

$$\lim_{\epsilon \to 0} y_\nu^*(\epsilon) = y_\nu, \qquad \lim_{\epsilon \to \infty} y_\nu^*(\epsilon) = Q(x_\nu). \tag{9}$$

4. *Graduation by Spline Functions.*—In an attempt to combine the spline interpolation described in section 2 with Whittaker's idea, we propose the following

PROBLEM 1. *Let $m < n$ and $\epsilon > 0$. Among all $f(x)$, defined in I, having a square integrable mth derivative we propose to find the solution of the problem*

$$\epsilon Jf + Ef = \text{minimum}. \tag{10}$$

If the solution $Q(x)$ of the problem (8) is such that $EQ = 0$, then it is clear that $f = Q$ also solves the problem (10) for all $\epsilon > 0$. In order to exclude this trivial case we shall assume throughout that

$$EQ > 0, \text{ or equivalently } Js > 0. \tag{11}$$

THEOREM 1. *The minimum problem* (10) *has a unique solution $f(x) = S(x, \epsilon)$ which is a spline function of the family $\mathcal{S}_m$.*

We state the analogues of the relations (9) as

THEOREM 2. *The functions $s(x)$ and $Q(x)$ being as defined before, the following relations hold*

$$\lim_{\epsilon \to 0} S(x, \epsilon) = s(x), \qquad \lim_{\epsilon \to \infty} S(x, \epsilon) = Q(x). \tag{12}$$

5. *An Equivalent Approach.*—The quantity Jf evidently measures the departure of $f(x)$ from being an element of π_{m-1}; likewise Ef measures how well $f(x)$ describes the data (x_i, y_i). A sensible approach to the problem of graduation is as follows:

Assuming (11), *we choose u in the range $0 \leqq u \leqq Js$ and propose to find the solution of the problem*

$$Ef = \text{minimum}, \textit{ among functions } f(x) \textit{ subject to } Jf \leqq u. \tag{13}$$

That this approach again leads to the solution of Problem 1, as described by Theorem 1, is stated as

THEOREM 3. *The solution $f(x) = S_u(x)$ of the problem* (13) *is unique and such that*

$$S_u(x) \in \mathcal{S}_m, \ JS_u = u.$$

The two families of spline functions

$$S_u(x), \ (0 \leqq u \leqq Js) \text{ and } S(x,\epsilon) \ (0 \leqq \epsilon \leqq \infty)$$

are identical. If we regard $v = ES_u$ as a function of $u = JS_u$ and express the dependence as

$$v = \Phi(u), \ (0 \leqq u \leqq Js), \tag{14}$$

then the graph of (14) *is a smooth and strictly convex arc with*

$$\Phi(0) = EQ, \ \Phi'(0) = -\infty, \ \Phi(Js) = 0, \ \Phi'(Js) = 0. \tag{15}$$

It follows that the function $\Phi(u)$ *is strictly decreasing in its domain of definition. Finally, the relation between* u *and the smoothing parameter* ϵ *of section* 4 *is described by the relation*

$$\epsilon = -\Phi'(u). \tag{16}$$

The convexity of the graph of (14) and (15) allows us to see readily on the graph why $S_u(x)$ is the solution of the problem

$$\epsilon JS + ES = \text{minimum, for } S \in \mathcal{S}_m,$$

and why therefore $S_u(x) = S(x, \epsilon)$. I add that (14) may be represented in parametric form and that u and v are rational functions of the parameter ϵ.

6. *A Formal Comparison with Whittaker's Method.*—We return to section 2 and wish to express $JS(x; y_1, \ldots, y_n)$ in terms of the y_ν. This can be done as follows: We denote by $M_i(x)$ the kernel in the integral representation of the divided difference

$$\Delta^m g(x_i) = \frac{1}{m!}\int_{x_i}^{x_{i+m}} M_i(x) g^{(m)}(x)dx \qquad (i = 1, \ldots, n - m)$$

and extending the definition of $M_i(x)$ to all x by setting $M_i(x) - 0$ if x is outside (x_i, x_{i+m}), we write

$$L_{ij} = \int_{-\infty}^{\infty} M_i(x)M_j(x)dx, \qquad (i,j = 1, \ldots, n - m).$$

The matrix $||L_{ij}||$ is positive definite, and if we introduce its inverse

$$||\Lambda_{ij}|| = ||L_{ij}||^{-1},$$

then[4]

$$JS(x; y_1, \ldots, y_n) = \sum_1^{n-m} \Lambda_{ij}\Delta^m y_i \Delta^m y_j. \tag{17}$$

Setting $S(x_i, \epsilon) = \eta_i$, hence $S(x, \epsilon) = S(x; \eta_1, \ldots, \eta_n)$ it follows from (17) that the solution of the problem (10) reduces to the solution of the algebraic problem

$$\epsilon \sum_1^{n-m} \Lambda_{ij}\Delta^m \eta_i \Delta^m \eta_j + \sum_1^n (\eta_\nu - y_\nu)^2 = \text{minimum}. \tag{18}$$

A comparison of the first sums in (6) and (18) shows that the new method arises if we replace in (6) the form $\sum_1^{n-m} \xi_i^2$ by the positive definite quadratic form $\sum \Lambda_{ij}\, \xi_i\xi_j$. This increase in complexity might be compensated by the new method furnishing also the approximating spline function $S(x, \epsilon)$, if such an approximation is desirable [e.g., compare the first relations (9) and (12)]. A further actual comparison of the two methods will require numerical experimentation.

7. *The Case of Periodic Data.*—In a recent paper[5] I introduced the method of trigonometric spline interpolation. The discussion of sections 4 and 5 carries over to the periodic case and need not be elaborated. The analogue of Problem 1 is as follows: assuming $2m + 2 \leqq n$, $\epsilon > 0$, we are seeking the function $f(x)$, of period 2π, having a square integrable $(2m + 1)$st derivative and which solves the problem

$$\epsilon \int (\Delta_m f)^2 dx + \sum_1^n (f(x_\nu) - y_\nu)^2 = \text{minimum}, \; [\Delta_m = D(D^2 + 1^2) \dots (D^2 + m^2)],$$

the integration being over an entire period while the x_ν are increasing with $x_n - x_1 < 2\pi$. The unique solution is a trigonometric spline function $S(x, \epsilon)$ having properties analogous to those stated in Theorems 1, 2, and 3. Naturally, the role of $Q(x)$ is now played by the trigonometric polynomial $T(x)$, of order m, which solves the problem

$$\sum_1^n (T(x_\nu) - y_\nu)^2 = \text{minimum}.$$

* Work done with partial support by a grant from the National Science Foundation contract GP-2442.

[1] For references, see *Proc. Roy. Netherl. Acad.*, **A67**, 155–163 (1964). A recent paper is by T. N.E. Greville (Math. Res. Center Tech. Report No. 450, Madison, Wis., January 1964).

[2] We denote by π_k the class of real polynomials of degree not exceeding k.

[3] Whittaker, E. T., *Proc. Edinburgh Math. Soc.*, **41**, 63–75 (1923).

[4] See these PROCEEDINGS, **51**, 28 (1964), formula (15), for a simplification occurring in the case when the x_ν are in arithmetic progression.

[5] To appear in the November 1964 issue of *J. Math. Mech.*

---

*OCCURRENCE OF SOLUBLE ANTIGEN IN THE PLASMA OF MICE WITH VIRUS-INDUCED LEUKEMIA**

BY BURGHARD STÜCK,† LLOYD J. OLD, AND EDWARD A. BOYSE

DIVISION OF EXPERIMENTAL CHEMOTHERAPY, SLOAN-KETTERING INSTITUTE FOR CANCER RESEARCH, SLOAN-KETTERING DIVISION, CORNELL MEDICAL COLLEGE, AND DEPARTMENT OF PATHOLOGY, NEW YORK UNIVERSITY SCHOOL OF MEDICINE

Communicated by Richard E. Shope, August 24, 1964

The cells of leukemias induced in mice by several different viruses possess specific antigens that can be demonstrated by serological methods.[1–8] Leukemias induced by Friend, Moloney, and Rauscher viruses share antigenic determinants that are not present in leukemias induced by Gross virus.[6, 8] It has recently been shown that the antigen characteristic of leukemias induced by Rauscher virus may be acquired by the cells of unrelated transplanted leukemias during passage in mice infected with Rauscher virus, a phenomenon which has been named "antigenic conversion."[9] These converted cells are susceptible to the cytotoxic activity of specific Rauscher antiserum, and this sensitivity persists indefinitely on serial transplantation of converted lines. Permanent antigenic conversion by Rauscher virus has now been shown to occur *in vitro* in an established tissue culture line of the leukemia EL4.[10] Thus it is clear that leukemia cells can support the continued multiplication of an