JOURNAL OF COMPUTATIONAL PHYSICS 60, 253–262 (1985)

Extrapolating B Splines for Interpolation

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Received November 29, 1983; revised May 31, 1984

A limit form of Richardson extrapolation is used to obtain interpolation formulae with accuracy of a higher degree than that obtained with the variation diminishing spline approximation.

1. INTRODUCTION

Schoenberg [4] has shown how fundamental interpolation formulae may be written in the form

$$\bar{f}(x, h) = \sum_{j=-\infty}^{\infty} f(x_j)\, L(x - x_j, h), \tag{1}$$

for an equi-spaced grid such that $x_j = jh$ (Schoenberg takes $h = 1$). The interpolation is said to be ordinary when $\bar{f}(x_j, h) = f(x_j)$ and smoothing when $\bar{f}(x_j, h) \neq f(x_j)$ and the characteristic function

$$\phi(u) := \sum_{j=-\infty}^{\infty} L(j, 1)\, e^{iju},$$

satisfies $\phi(0) = 1$ and $|\phi| \leqslant 1$. Schoenberg [4] has also shown that the interpolatory properties of (1) can be described in terms of the Fourier transforms of L. If we use the definition

$$g(t) := \int_{-\infty}^{\infty} L(x, h)\cos(2\pi t x)\, dx, \tag{2}$$

then (1) will reproduce polynomials of degree $k-1$ provided (a) $g(t) - h$ has a zero of order k at $t = 0$ and (b) $g(t)$ has zeros of order k at the points $th = \pm 1, \pm 2, \ldots$.

Schoenberg introduced a fundamental set of interpolating kernels, the central B splines, so that (1), in his notation, becomes

$$\bar{f}(x, h) = \sum_{j=-\infty}^{\infty} f(x_j)\, M_n(x - x_j, h) \tag{3}$$

0021-9991/85 $3.00

where $M_n(u, h)$ is the nth central B spline (of order n, i.e., degree $n-1$). The basis spline $M_2(u, h)$ is the triangular function defined by

$$\begin{aligned} M_2(u, h) &= 1 - |u|/h; \qquad && |u| \leqslant h, \\ &= 0; && \text{otherwise,} \end{aligned} \tag{4}$$

which gives the area weighting interpolation used in particle simulations. The kernel M_2 leads to an ordinary interpolation formula. The higher order M_n give smoothing interpolation formulae. The functions M_n and their first $n-2$ derivatives are continuous. For this reason, in particle simulations (e.g., Hockney and Eastwood [2]) interpolation is usually carried out with M_3. The Fourier transform of $M_n(x, h)$ is (Schoenberg [1] who replaces t by $u/2\pi$)

$$g(t) := \int_{-\infty}^{\infty} M_n(x, h) \cos(2\pi x t)\, dx = h \left[\frac{\sin(\pi t h)}{(\pi t h)} \right]^n \tag{5}$$

and, for $t \sim 0$, $g(t) \sim h - n\pi^2 t^2 h^3/6$. Referring to the conditions above we find that the basis splines only achieve linear interpolation.

The aim of this paper is to show how, starting with interpolants based on M_n, higher order interpolation formulae can be constructed. Schoenberg [1, 4] has also derived higher order interpolation formulae. However, the method we use differs from those used by Schoenberg and the interpolants we find appear to be new.

2. Integral Form

There is a considerable analytical convenience in working with an integral rather than the sum in (1). The error involved in switching from one to the other can be estimated using the Poisson summation formula. We find

$$\sum_{j=-\infty}^{\infty} f_j M_n(x - x_j, h) = \int_{-\infty}^{\infty} f(uh)\, M_n(x - uh, h)\, du + \varepsilon_n(h), \tag{6}$$

where

$$\varepsilon_n(h) = 2 \sum_{r=1}^{\infty} \int_{-\infty}^{\infty} f(uh)\, M_n(x - uh, h) \cos(2\pi r u)\, du. \tag{7}$$

If we expand $f(uh)$ about the point $uh = x$ we find

$$\varepsilon_n(h) \sim \frac{2}{h} \sum_{r=1}^{\infty} \sum_{a=0}^{\infty} \frac{f^{(a)}(x)}{a!} I_{ra}(x, h), \tag{8}$$

where

$$I_{ra}(x, h) := \int_{-\infty}^{\infty} \omega^a M_n(\omega, h) \cos[2\pi r(x-\omega)/h]\, d\omega$$
$$= \cos(2\pi rx/h)\, C_{ra} + \sin(2\pi rx/h)\, S_{ra} \tag{9}$$

with

$$C_{ra} := \int_{-\infty}^{\infty} \omega^a M_n(\omega, h) \cos(2\pi\omega r/h)\, d\omega \qquad (=0 \text{ for } a \text{ odd})$$

$$S_{ra} := \int_{-a}^{\infty} \omega^a M_n(\omega, h) \sin(2\pi\omega r/h)\, d\omega \qquad (=0 \text{ for } a \text{ even}).$$

Upon differentiating the integral in (5) with respect to t we see that, except possibly for a sign, the nonzero values of C_{ra} and S_{ra} are given by $g^{(a)}(t)/(2\pi)^a$ at $t=r/h$. And this, upon differentiating the right hand side of (5), is seen to be $h(h/2)^a\, \psi^{(a)}(\pi r)$, where

$$\psi(\sigma) := (\sin \sigma/\sigma)^n$$

is entire and has zeroes of order n at $\pm\pi$, $\pm 2\pi$,.... Hence the inner sum in (8) begins at $a=n$, so

$$\varepsilon_n(h) \propto h^n. \tag{10}$$

In general, if the kernel has a Fourier transform $g(t)$ which has a zero of order n at $th = \pm 1, \pm 2, \ldots$, then $\varepsilon_n(h) \propto h^n$. For our problem we see that we can use the integral in (6) in place of the summation in (1) provided $n \geqslant 3$ since then the error $\varepsilon_n(h)$ is of higher degree in h than the interpolation error. Our interpolant is essentially

$$\tilde{f}(x, h) = \frac{1}{h} \int_{-\infty}^{\infty} f(x')\, M_n(x-x', h)\, dx'; \qquad n \geqslant 3. \tag{11}$$

By expanding $f(x')$ about the point x we find

$$\tilde{f}(x, h) = f(x) + \frac{f''(x)}{2h} \int_{-\infty}^{\infty} M_n(u, h)\, u^2\, du + \cdots. \tag{12}$$

Since $M_n(u, h)$ is an even function of u all terms involving odd derivatives of $f(x)$ vanish. From (5) we find

$$\int_{-\infty}^{\infty} M_n(u, h)\, u^{2a}\, du = \frac{(-1)^a}{(2\pi)^{2a}} \left(\frac{d^{2a} g(t)}{dt^{2a}}\right)_{t=0} = O(h^{2a+1}), \tag{13}$$

and (12) can be written

$$\bar{f}(x, h) = f(x) + a(x)\, h^2 + \cdots. \tag{14}$$

Note that the error in the interpolant (11) is always of even degree in h and is $O(h^m)$ if the Fourier transform of the kernel has the expansion

$$g(t) - h \propto t^m. \tag{15}$$

Interpolants of the form (11) therefore reproduce polynomials of degree $k-1$ provided $g(t)-h$ has a zero of order k at $t=0$. They are equivalent to a summation interpolation formula which reproduces polynomials of degree $k-1$ provided $g(t)$ also has a zero of order k at the points $th = \pm 1, \pm 2, \ldots$.

3. Richardson Extrapolation

Returning now to (14) we wish to devise a means of eliminating the term $a(x)\, h^2$. If we could do this the interpolation error in (11) would be $O(h^4)$. Richardson extrapolation is a well-known way of improving the accuracy of a formula and we can apply it here since, for a uniform grid with separation H,

$$\bar{f}(x, H) = f(x) + a(x)\, H^2 + \cdots. \tag{16}$$

We can then combine (14) and (16) so as to remove the error term. In this way we find the new interpolant

$$\int_{-\infty}^{\infty} f(x')\, \Phi_n(x - x', h, H)\, dx', \tag{17}$$

where

$$\Phi_n(u, h, H) = \left\{ \frac{H^2}{h} M_n(u, h) - \frac{h^2}{H} M_n(u, H) \right\} / (H^2 - h^2). \tag{18}$$

The interpolant has errors of $O(h^4)$ but, as it stands, it is useless because the integration cannot be expressed accurately by a summation on either grid. To escape this difficulty we take the limit of (18) as $H \to h$. We find

$$\operatorname*{Lim}_{H \to h} \Phi_n(u, h, H) = \frac{1}{2h} \left(3M_n - h \frac{\partial M_n}{\partial h} \right), \tag{19}$$

and the new interpolation kernel

$$W_n(u, h) := \frac{1}{2} \left[3M_n - h \frac{\partial M_n}{\partial h} \right], \tag{20}$$

where we require $n \geqslant 3$ because otherwise the derivative of M_n is not defined everywhere. The new integral interpolation formula now satisfies

$$\bar{f}(x, h) = \frac{1}{h} \int_{-\infty}^{\infty} f(x') \, W_n(x - x', h) \, dx' = f(x) + A(x) \, h^4 + \cdots, \tag{21}$$

but it will be clear from the earlier discussion that the practical interpolation formula

$$\bar{f}(x) = \sum_{j=-\infty}^{\infty} f_j W_n(x - x_j, h), \tag{22}$$

may not achieve the same accuracy. In fact, because W_n involves a derivative of M_n, it will not be as smooth as M_n and its Fourier transform will not vanish as quickly as that for M_n as $t \to \infty$. Since we require $n \geqslant 4$ for $\varepsilon_n(h)$ (see (10)) to be at least as small as $O(h^4)$, and W_n is less smooth than M_n we can expect that (22) will only achieve the same accuracy as (21) if $n > 4$. These are only very rough arguments. They can be made more precise by using Schoenberg's criteria. From (5) and (20) we find (setting $\sigma = \pi t h$)

$$\begin{aligned} G_n(t) &= \int_{-\infty}^{\infty} W_n(v, h) \cos(2\pi u t) \, du \\ &= \frac{1}{2} \left[3h \left(\frac{\sin \sigma}{\sigma} \right)^n - h \frac{\partial}{\partial h} \left\{ h \left(\frac{\sin \sigma}{\sigma} \right)^n \right] \\ &= h \left(\frac{\sin \sigma}{\sigma} \right)^{n-1} \left[\left(1 + \frac{n}{2} \right) \frac{\sin \sigma}{\sigma} - \frac{n}{2} \cos \sigma \right]. \end{aligned} \tag{23}$$

Referring back to the rules given in the introduction, and noting also that

$$G_n(t) - h = -\frac{h(n-1)(11n-6)(\pi t h)^4}{360} \tag{24}$$

as $t \to 0$, we conclude that (22) will only achieve $O(h^4)$ interpolation if $n \geqslant 5$. In this case the interpolation formula (22) will reproduce polynomials of degree 3.

If $n = 4$ the new interpolation formula has errors of order h^3 which, incidentally, is also the estimate of the error incurred, apart from trionometric functions, in switching from the integration (21) to the summation (22) (using (23) instead of (5) in the analogs of (6) through (10) its zeroes are third order). For this case

$$\begin{aligned} W_4(u, h) &= 1 - \frac{5v^2}{2} + \frac{3v^3}{2}, && 0 \leqslant v \leqslant 1, \\ &= \tfrac{1}{2}(2 - v)^2 (1 - v), && 1 \leqslant v \leqslant 2, \end{aligned} \tag{25}$$

where $v = |u|/h$. This kernel gives an ordinary interpolation formula which reproduces polynomials of degree 2. The kernel W_4 and its first derivative are continuous (the latter matches centred first derivatives at the break points) so that, in its smoothness, W_4 is similar to M_3. It is also similar to the kernel $B(u, h)$ which gives Bessel's interpolation formula if third and higher differences are neglected. This kernel is defined by

$$\begin{aligned} B(u, h) &= (1-v)(1+\tfrac{1}{4}v), \qquad & 0 \leqslant v \leqslant 1, \\ &= \tfrac{1}{4}(1-v)(2-v), & 1 \leqslant v \leqslant 2. \end{aligned} \tag{26}$$

$B(u, h)$ has the same support, degree of polynomial reproduced (two) and order of accuracy (h^3). It also leads to an ordinary interpolation formula. W_4 is smoother than B but its degree is higher. The kernel $E(u, h)$ which gives Everett's interpolation formula (see also Schoenberg, [1] p. 57) if fourth and higher differences (they are all even order) are neglected, has the form

$$\begin{aligned} E(u, h) &= \tfrac{1}{2}(2-v)(1-v^2), \qquad & 0 \leqslant v \leqslant 1, \\ &= \tfrac{1}{6}(2-v)(3-v)(1-v), & 1 \leqslant v \leqslant 2. \end{aligned} \tag{27}$$

This kernel also leads to ordinary interpolation, is of the same degree as W_4, and is less smooth than W_4, but its order of accuracy (h^4) is higher. Because of its smoothness and accuracy W_4 would appear to be a good alternative to M_3 in particle simulations.

Finally we give the detailed form of $W_5(u, h)$, the first of the sequence of kernels to interpolate with errors $O(h^4)$:

$$\begin{aligned} W_5(u, h) &= \tfrac{1}{48}\,(v-\tfrac{5}{2})^3\Big(7v-\frac{15}{2}\Big), \qquad & \tfrac{3}{2} \leqslant v \leqslant \tfrac{5}{2}, \\ &= \tfrac{1}{48}\,(165/4 + 20v - 150v^2 + 120v^3 - 28v^4), & \tfrac{1}{2} \leqslant v \leqslant \tfrac{3}{2}, \\ &= \tfrac{1}{48}\,(345/8 - 75v^2 + 42v^4), & 0 \leqslant v \leqslant \tfrac{1}{2}, \\ &= \quad 0, & \text{otherwise.} \end{aligned} \tag{28}$$

W_5 and its first two derivatives are continuous. The resulting formula is a smoothing interpolation formula. Because of its complicated form it is probably of less practical value than (25) which, though less accurate, is simpler to use.

4. Extensions to Other Kernels

The procedure we have used to generate new interpolating kernels from the basis splines can be applied to other kernels. In most cases there are no complications, but there are certain kernels useful in particle simulations which do not fit Schoenberg's analysis. As an example, consider the interpolation formula

$$\bar{f}(x) = h \sum_{j=-\infty}^{\infty} f_j \frac{e^{-(x-jh)^2/a^2}}{a\sqrt{\pi}} \tag{29}$$

where, typically, $a \gtrsim h$. This formula does not even reproduce a nonzero constant exactly. However it would be premature to dismiss it. As before we can convert the summation into an integration with an error which can be estimated from the Poisson summation formula. (Here we retain only the term with $r = 1$ since the contributions for $r > 1$, though of the same form are much smaller.) This error is

$$2h \int_{-\infty}^{\infty} f(uh) \frac{e^{-(x-uh)^2/a^2}}{a\sqrt{\pi}} \cos(2\pi u)\, du, \tag{30}$$

which is the real part of

$$\frac{2h}{a\sqrt{\pi}} e^{-\pi^2 a^2/h^2 + 2\pi x i/h} \int_{-\infty}^{\infty} f(uh)\, e^{-(h^2/a^2)[u - qa^2/2h^2]^2}\, du, \tag{31}$$

where

$$q = \frac{2xh}{a^2} + 2\pi i. \tag{32}$$

By shifting the integration contour from the real axis to a straight line parallel to the real axis passing through the point $qa^2/2h^2$, we can write (31) as

$$\frac{2h}{a\sqrt{\pi}} \exp\left[-\frac{\pi^2 a^2}{h^2} + \frac{2\pi i x}{h}\right] \int_{-\infty}^{\infty} f\left(x + \frac{\pi a 2i}{h} + yh\right) e^{-y^2 h^2/a^2}\, dy, \tag{33}$$

which can be approximated in most cases by

$$2 \exp\left[-\frac{\pi^2 a^2}{h^2} + \frac{2\pi i x}{h}\right] f\left(x + \frac{\pi a^2 i}{h}\right). \tag{34}$$

This result, apart from some slight notational changes, agrees with that found by Goodwin [5] for the case where x is zero (note that Goodwin's error term is defined to be $\sqrt{\pi}$ times our error term). If f is a constant A and $a = 1$, the error is $\sim 10^{-4} \times A$ when $h = 1$ and $10^{-17} \times A$ when $h = 0.5$. Therefore the error involved in replacing the summation in (29) by an integration can be made negligible. If $f(x)$ is not a constant (33) may need to be evaluated more carefully but the error can be made negligible by choosing $a \gtrsim h$. We can therefore work with the interpolant

$$\bar{f}(x, a) = \int_{-\infty}^{\infty} f(x') \frac{e^{-(x-x')^2/a^2}}{a\sqrt{\pi}}\, dx', \tag{35}$$

taking $a \gtrsim h$. By Taylor series expansion we find

$$\bar{f}(x, a) = f(x) + \frac{f''(x)}{4} a^2 + \cdots. \tag{36}$$

The previous arguments concerning Richardson extrapolation can be applied, and we can construct a new kernel W by replacing M_n in (19) by the gaussian kernel in (29). We find

$$W(u, a) = \frac{h}{a\sqrt{\pi}} e^{-u^2/a^2} \left[\frac{3}{2} - \frac{u^2}{a^2}\right] \tag{37}$$

With this kernel the interpolant

$$\bar{f}(x, a) = \int_{-\infty}^{\infty} f(x')\, W(x - x', a)\, dx', \tag{38}$$

has errors of $O(a^4)$. The summation form of the interpolation formula interpolates with errors which are approximately of $O(a^4)$ but include errors in replacing the integration by a summation. This error is larger than that involved in using the gaussian kernel but by making $a \gtrsim h$ this error can be made negligible.

The Fourier transform of $W(u, a)$ is

$$\int_{-\infty}^{\infty} W(u, a) \cos(2\pi u t)\, du = h e^{-\pi^2 t^2 a^2}(1 + \pi^2 a^2 t^2), \tag{39}$$

the rapid decrease with increasing t is due to the smoothness of $W(u, a)$. When t is sufficiently small the Fourier transform (39) has the expansion

$$h(1 - \tfrac{1}{2}\pi^4 a^4 t^4), \tag{40}$$

which shows, again, that the integral interpolant (38) has errors of $O(a^4)$.

In ordinary numerical practice the gaussian interpolation formulae are not very useful because their desirable smoothness is outweighed by the disadvantage that at least eight grid points may need to be used (we take the gaussian as negligible beyond $\sim 3a$). Nevertheless the kernel (37) has been used effectively in particle simulations of shock tube phenomena (Monaghan and Gingold [3]).

5. Extensions to Higher Dimensions

To fix ideas we will consider the case of three dimensions. The simplest extension of our previous results is to use the interpolant

$$\begin{aligned}\bar{f}(x, y, z, h) = \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} & f(jh, kh, lh)\, M_n(x - x_j, h) \\ & \times M_n(y - y_j, h)\, M_n(z - z_j, h),\end{aligned} \tag{41}$$

where we have assumed, for simplicity, that the grid has the same separation in each dimension and the basis splines have the same order for each dimension. The integral interpolant

$$\bar{f}(x, y, z, h) = \frac{1}{h^3} \int\int\int f(x', y', z')\, M_n(x - x', h)\, M_n(y - y', h)\, M_n(z - z', h)\, dx'\, dy'\, dz' \tag{42}$$

can be examined as before. The final result is that each M_n can be replaced by a corresponding W_n to achieve (when $n \geqslant 5$) interpolation of $O(h^4)$.

A more interesting case occurs if we consider interpolation with guassians in the form

$$\bar{f}(\mathbf{r}) = h^3 \sum_r \sum_k \sum_l f(\mathbf{r}_{jkl}) \frac{e^{-|\mathbf{r} - \mathbf{r}_{jkl}|^2/a^2}}{a^3 \pi^{3/2}}. \tag{43}$$

The 3-dimensional version of the Poisson summation formula shows that (43) can be replaced by

$$\bar{f}(\mathbf{r}, a) = \int\int\int f(\mathbf{r}') \frac{e^{-|\mathbf{r} - \mathbf{r}'|^2/a^2}}{a^3 \pi^{3/2}}\, \mathbf{dr}', \tag{44}$$

with an error which consists of three terms each of which is similar in form to (34). As before this error is usually negligible if $a \gtrsim h$. If $f(\mathbf{r}')$ is expanded about the point $\mathbf{r}$, it is easy to show that (44) interpolates with error of $O(a^2)$. We could improve the order of accuracy by writing the gaussian as a product of three gaussians, one for each dimension, but it is more interesting to deal directly with the 3-dimensional gaussian. From (44)

$$\bar{f}(\mathbf{r}, a) = f(\mathbf{r}) + F(\mathbf{r})\, a^2 + \cdots,$$

so that, by changing the parameter a to A

$$\bar{f}(\mathbf{r}, A) = f(\mathbf{r}) + F(\mathbf{r})\, A^2 + \cdots.$$

We can combine these two expressions to remove the first error terms which is equivalent to using the kernel

$$\Psi(\mathbf{u}, a, A) = \left\{ \frac{A^2}{a^3}\, Q(\mathbf{u}, a) - \frac{a^2}{A^3}\, Q(\mathbf{u}, A) \right\} / (A^2 - a^2) \tag{45}$$

where $Q(\mathbf{u}, a)$ is the gaussian kernel in (44). Taking the limit as $A \to a$ we find

$$\operatorname*{Lim}_{A \to a} \Psi = \frac{1}{2A^3} \left[5Q(\mathbf{u}, a) - a \frac{\partial Q}{\partial a} \right], \tag{46}$$

and the new kernel

$$W(\boldsymbol{u}, a) = \frac{1}{2}\left[5Q(\mathbf{u}, a) - a\frac{\partial Q}{\partial a}\right]. \tag{47}$$

For the general case of n dimensions we find

$$W(\mathbf{u}, a) = \frac{1}{2}\left[(n+2)\, Q(\mathbf{u}, a) - a\frac{\partial Q(\mathbf{u}, a)}{\partial a}\right].$$

Replacing Q by the gaussian we find the new kernel

$$\frac{1}{\pi^{3/2}}\, e^{-u^2/a^2}\left[\frac{5}{2} - \frac{u^2}{a^2}\right]. \tag{48}$$

Other interpolation formula, with a kernel depending on $(\mathbf{r} - \mathbf{r}_{jkl})$, as in (43), can be treated in a similar way. Care must always be taken however to ensure the switch from summation to integration is valid.

ACKNOWLEDGMENT

I thank Blair Swartz for his painstaking effort to correct Sections 1–3 of earlier versions of this paper.

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