Preface

Approximation methods are of vital importance in many challenging applications from computational science and engineering. This book collects papers from world experts in a broad variety of relevant applications of approximation theory, including pattern recognition and machine learning, multiscale modelling of fluid flow, metrology, geometric modelling, the solution of differential equations, and signal and image processing, to mention a few.

The 30 papers in this volume document new trends in approximation through recent theoretical developments, important computational aspects and multidisciplinary applications, which makes it a perfect text for graduate students and researchers from science and engineering who wish to understand and develop numerical algorithms for solving their specific problems. An important feature of the book is to bring together modern methods from statistics, mathematical modelling and numerical simulation for solving relevant problems with a wide range of inherent scales. Industrial mathematicians, including representatives from Microsoft and Schlumberger make contributions, which fosters the transfer of the latest approximation methods to real-world applications.

This book grew out of the fifth in the conference series on *Algorithms for Approximation*, which took place from 17th to 21st July 2005, in the beautiful city of Chester in England. The conference was supported by the National Physical Laboratory and the London Mathematical Society, and had around 90 delegates from over 20 different countries.

The book has been arranged in six parts:

Part I. Imaging and Data Mining;
Part II. Numerical Simulation;
Part III. Statistical Approximation Methods;
Part IV. Data Fitting and Modelling;
Part V. Differential and Integral Equations;
Part VI. Special Functions and Approximation on Manifolds.

Part I grew out of a workshop sponsored by the London Mathematical Society on *Developments in Pattern Recognition and Data Mining* and includes contributions from Donald Wunsch, the President of the *International Neural Networks Society* and Chris Burges from Microsoft. The numerical solution of differential equations lies at the heart of practical application of approximation theory. The next two parts contain contributions in this direction. Part II demonstrates the growing trend in the transfer of approximation theory tools to the simulation of physical systems. In particular, radial basis functions are gaining a foothold in this regard. Part III has papers concerning the solution of differential equations, and especially delay differential equations. The realisation that statistical Kriging methods and radial basis function interpolation are two sides of the same coin has led to an increase in interest in statistical methods in the approximation community. Part IV reflects ongoing work in this direction. Part V contains recent developments in traditional areas of approximation theory, in the modelling of data using splines and radial basis functions. Part VI is concerned with special functions and approximation on manifolds such as spheres.

We are grateful to all the authors who have submitted for this volume, especially for their patience with the editors. The contributions to this volume have all been refereed, and thanks go out to all the referees for their timely and considered comments. Finally, we very much appreciate the cordial relationship we have had with Springer-Verlag, Heidelberg, through Martin Peters.

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Weighted Integrals of Polynomial Splines

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Summary. The construction of weighted splines by knot insertion techniques such as de Boor and Oslo - type algorithms leads immediately to the problem of evaluating integrals of polynomial splines with respect to the positive measure possessing piecewise constant density. It is for such purposes that we consider one possible way for simple and fast evaluation of primitives of products of a polynomial B-spline and a positive piecewise constant function.

1 Introduction and Motivation

Weighted splines appear in many applications, the most well-known being the cubic version where they arise naturally in minimizing functionals like $V(f) := \sum_{i=1}^{n}(w_i \int_{t_i}^{t_{i+1}} [D^2 f(t)]^2 dt$, $w_i > 0$, sometimes also accompanied by the control of first derivatives: $V(f) := \sum_{i=1}^{n}(w_i \int_{t_i}^{t_{i+1}} [D^2 f(t)]^2 dt + \nu_i \int_{t_i}^{t_{i+1}} [Df(t)]^2 dt)$, $\nu_i \geq 0$, $w_i > 0$, see [6, 7, 9] and [11] for a bivariate version.

The parametric version is often used as a polynomial alternative to the exponential tension spline in computer-aided geometric design, and some shape-preserving software systems (MONCON, TRANSPLINE) have been written for that purpose [13, 9, 10]. It is known that the associated B-splines can be calculated by the knot insertion algorithms. For the cubic version of weighted splines, explicit expressions for the knot insertion matrices exist, which are of the very simple form [8, 14]. In the case of the knot insertion algorithms can in principle be obtained by specializing the general theory of Chebyshev blossoming [12].

Weighted splines can also be evaluated by an integrated version of the derivative formula [15], which can also be used to define most general Chebyshev B-splines [1]:

$$B^n_{i,d\boldsymbol{\sigma}}(x) = \frac{1}{C_{n-1}(i)} \int_{t_i}^{x} B^{n-1}_{i,d\boldsymbol{\sigma}^{(1)}} d\sigma_2 - \frac{1}{C_{n-1}(i+1)} \int_{t_{i+1}}^{x} B^{n-1}_{i+1,d\boldsymbol{\sigma}^{(1)}} d\sigma_2, \qquad (1)$$

where $B^n_{i,d\boldsymbol{\sigma}}(x)$ is the n^{th}–order Chebyshev spline, $d\boldsymbol{\sigma} = (d\sigma_2 \ldots d\sigma_n)^T$ is the measure vector and $d\boldsymbol{\sigma}^{(1)} = (d\sigma_3 \ldots d\sigma_n)^T$ is the measure vector with respect to the first reduced system. We assume that $d\sigma_i$ are some Stieltjes measures, and that all the B-splines in question are normalized so as to make a partition of unity. The constants in the denominators are integrals of B-splines over its support, with respect to the measure that is missing in the definition of $d\boldsymbol{\sigma}^{(1)}$:

$$C_{n-1}(i) := \int_{t_i}^{t_{i+n-1}} B^{n-1}_{i,d\boldsymbol{\sigma}^{(1)}} \, d\sigma_2.$$

The numerical stability of (1) is doubtful (even for polynomial splines), so evaluation by knot insertion is preferred. However, for weighted splines we need only very simple measures, which are all but one Lebesgue measures, and the one that is not has density which is piecewise constant and positive. To be more precise, weighted B-splines are piecewisely spanned by the Chebyshev system of *weighted powers*:

$$\begin{aligned}
u_1(x) &= 1,\\
u_2(x) &= \int_a^x d\tau_2,\\
u_3(x) &= \int_a^x d\tau_2 \int_a^{\tau_2} \frac{d\tau_3}{w(\tau_3)},\\
&\vdots\\
u_k(x) &= \int_a^x d\tau_2 \int_a^{\tau_2} \frac{d\tau_3}{w(\tau_3)} \int_a^{\tau_3} d\tau_4 \cdots \int_a^{\tau_{k-1}} d\tau_k.
\end{aligned}$$

Finally, one can use algorithms for ordinary polynomial splines and avoid explicit mentioning of weighted splines, but even then integration of products of polynomial splines and piecewise constant function must be performed, as shown by de Boor [3], who also gives closed formulæ for some lower order splines.

2 Recurrence for Integrals of Polynomial B-Splines

Whatever approach we choose, in order to evaluate weighted splines we need to calculate the integrals of ordinary polynomial B-splines

$$C_k(j) = \int_{t_j}^{t_{j+k}} B_j^k(\tau) \frac{d\tau}{w(\tau)}.$$

In what follows, we assume that B_j^k are normalized so as to make the partition of unity, and that the knot sequence $\{t_j\}$, possibly containing multiple knots, coincides with the breakpoint sequence for w. For notation purposes, let $w|_{[t_i,t_{i+1})} = w_i$ which makes w right–continuous. We want to find a recurrence for primitives of polynomial B-splines with respect to the piecewise constant positive function w, i.e.,

$$\int_{t_i}^{x} B_i^k(\tau) \frac{d\tau}{w(\tau)}, \qquad x \in [t_i, t_{i+k}],$$

and, specially:

$$\int_{t_j}^{t_{j+1}} B_i^k(\tau) \frac{d\tau}{w(\tau)}, \qquad j = i, \ldots, i+k-1.$$

Let $x \in [t_j, t_{j+1})$, then

$$\begin{aligned}
\int_{t_i}^{x} B_i^k(\tau)\frac{d\tau}{w(\tau)} &= \sum_{s=i}^{j-1}\int_{t_s}^{t_{s+1}} B_i^k(\tau)\frac{1}{w_s}d\tau + \frac{1}{w_j}\int_{t_j}^{x} B_i^k(\tau)\,d\tau \\
&= \sum_{s=i}^{j-1}\frac{1}{w_s}\left(\int_{t_i}^{t_{s+1}} B_i^k(\tau)\,d\tau - \int_{t_i}^{t_s} B_i^k(\tau)\,d\tau\right) \\
&\quad + \frac{1}{w_j}\left(\int_{t_i}^{x} B_i^k(\tau)\,d\tau - \int_{t_i}^{t_j} B_i^k(\tau)\,d\tau\right) \\
&= \sum_{s=i}^{j-1}\frac{1}{w_s}\frac{t_{i+k}-t_i}{k}\left(\sum_{r=i}^{s} B_r^{k+1}(t_{s+1}) - \sum_{r=i}^{s-1} B_r^{k+1}(t_s)\right) \\
&\quad + \frac{1}{w_j}\frac{t_{i+k}-t_i}{k}\left(\sum_{r=i}^{j} B_r^{k+1}(x) - \sum_{r=i}^{j-1} B_r^{k+1}(t_j)\right), \qquad (2)
\end{aligned}$$

by the well known formula for integrals of polynomial splines [16, p. 200] and [2, pp. 150-151]. Let

$$\bar\alpha_{i,j+1}^{k+1}(x) := \sum_{r=i}^{j} B_r^{k+1}(x) \quad \text{and} \quad \alpha_{i,j+1}^{k+1} := \bar\alpha_{i,j+1}^{k+1}(t_{j+1}). \qquad (3)$$

Then in terms of $\bar\alpha$'s formula (2) can be written as

$$\int_{t_i}^{x} B_i^k(\tau)\frac{d\tau}{w(\tau)} = \frac{t_{i+k}-t_i}{k}\left(\sum_{s=i}^{j-1}\frac{1}{w_s}\left(\alpha_{i,s+1}^{k+1}-\alpha_{i,s}^{k+1}\right)+\frac{1}{w_j}\left(\bar\alpha_{i,j+1}^{k+1}(x)-\alpha_{i,j}^{k+1}\right)\right). \quad (4)$$

We claim that $\bar\alpha_{i,j+1}^{k+1}(x)$ can be evaluated as convex combination of lower order quantities $\bar\alpha_{i,j}^{k}(x)$. By de Boor–Cox recurrence

$$\begin{aligned}
\sum_{r=i}^{j} B_r^{k+1}(x) &= \sum_{r=i}^{j}\left(\frac{x-t_r}{t_{r+k}-t_r}B_r^k(x) + \frac{t_{r+k+1}-x}{t_{r+k+1}-t_{r+1}}B_{r+1}^k(x)\right) \\
&= \sum_{r=i}^{j}\frac{x-t_r}{t_{r+k}-t_r}B_r^k(x) + \sum_{r=i}^{j}B_{r+1}^k(x) - \sum_{r=i}^{j}\frac{x-t_{r+1}}{t_{r+k+1}-t_{r+1}}B_{r+1}^k(x) \\
&= \sum_{r=i+1}^{j}\left(\frac{x-t_r}{t_{r+k}-t_r} - \frac{x-t_r}{t_{r+k}-t_r}\right)B_r^k(x) + \frac{x-t_i}{t_{i+k}-t_i}B_i^k(x) + \sum_{r=i}^{j-1}B_{r+1}^k(x) \\
&= \frac{x-t_i}{t_{i+k}-t_i}B_i^k(x) + \sum_{r=i+1}^{j}B_r^k(x) = \frac{x-t_i}{t_{i+k}-t_i}B_i^k(x) + \bar\alpha_{i+1,j+1}^k(x),
\end{aligned}$$

because $B_{j+1}^k(x) = 0$ for $x \in [t_j, t_{j+1})$. Thus we have proved the recurrence

$$\bar\alpha_{i,j+1}^{k+1}(x) = \frac{x-t_i}{t_{i+k}-t_i}B_i^k(x) + \bar\alpha_{i+1,j+1}^k(x), \qquad (5)$$

for $x \in [t_j, t_{j+1})$ and $j = i, \ldots, i+k-1$. We proceed to manipulate (5) to get a more symmetric expression. Obviously,

$$\begin{aligned}
\bar\alpha_{i,j+1}^k(x) &= \sum_{r=i}^{j} B_r^k(x) = B_i^k(x) + \sum_{r=i+1}^{j} B_r^k(x) \\
&= B_i^k(x) + \bar\alpha_{i+1,j+1}^k(x),
\end{aligned}$$

whence $B_i^k(x) = \bar{\alpha}_{i,j+1}^k(x) - \bar{\alpha}_{i+1,j+1}^k(x)$, which, when substituted in (5) gives

$$\begin{aligned}\bar{\alpha}_{i,j+1}^{k+1}(x) &= \frac{x-t_i}{t_{i+k}-t_i}\Big(\bar{\alpha}_{i,j+1}^k(x) - \bar{\alpha}_{i+1,j+1}^k(x)\Big) + \bar{\alpha}_{i+1,j+1}^k(x) \\ &= \frac{x-t_i}{t_{i+k}-t_i}\bar{\alpha}_{i,j+1}^k(x) + \bar{\alpha}_{i+1,j+1}^k(x)\left(1 - \frac{x-t_i}{t_{i+k}-t_i}\right).\end{aligned}$$

Finally, we have the recurrence

$$\bar{\alpha}_{i,j+1}^{k+1}(x) = \frac{x-t_i}{t_{i+k}-t_i}\,\bar{\alpha}_{i,j+1}^k(x) + \frac{t_{i+k}-x}{t_{i+k}-t_i}\,\bar{\alpha}_{i+1,j+1}^k(x), \tag{6}$$

for $x \in [t_j, t_{j+1})$ and $j = i, \ldots, i+k-1$.

We need to evaluate

$$\frac{1}{w_j}\,\frac{t_{i+k}-t_i}{k}\left(\sum_{r=i}^{j} B_r^{k+1}(x) - \sum_{r=i}^{j-1} B_r^{k+1}(t_j)\right) = \frac{t_{i+k}-t_i}{k\,w_j}\Big(\bar{\alpha}_{i,j+1}^{k+1}(x) - \alpha_{i,j}^{k+1}\Big),$$

but have no way of telling whether the subtraction of $\bar{\alpha}$'s will result in dangerous cancellation of significant digits; therefore we must find another way of evaluating differences of $\bar{\alpha}$'s. To this end, let

$$\bar{\delta}_{i,j}^{k+1}(x) := \bar{\alpha}_{i,j+1}^{k+1}(x) - \alpha_{i,j}^{k+1}.$$

From (6) we have

$$\begin{aligned}&\bar{\delta}_{i,j}^{k+1}(x) \\ &= \frac{x-t_i}{t_{i+k}-t_i}\,\bar{\alpha}_{i,j+1}^k(x) + \frac{t_{i+k}-x}{t_{i+k}-t_i}\,\bar{\alpha}_{i+1,j+1}^k(x) - \frac{t_j-t_i}{t_{i+k}-t_i}\,\alpha_{i,j}^k - \frac{t_{i+k}-t_j}{t_{i+k}-t_i}\,\alpha_{i+1,j}^k \\ &= \frac{t_j-t_i}{t_{i+k}-t_i}\,\bar{\delta}_{i,j}^k(x) + \frac{t_{i+k}-x}{t_{i+k}-t_i}\,\bar{\delta}_{i+1,j}^k(x) + \frac{x-t_j}{t_{i+k}-t_i}\Big(\bar{\alpha}_{i,j+1}^k(x) - \alpha_{i+1,j}^k\Big).\end{aligned} \tag{7}$$

Further,

$$\begin{aligned}\bar{\alpha}_{i,j+1}^k(x) - \alpha_{i+1,j}^k &= \bar{\alpha}_{i,j+1}^k(x) - \bar{\alpha}_{i+1,j+1}^k(x) + \bar{\alpha}_{i+1,j+1}^k(x) - \alpha_{i+1,j}^k \\ &= \bar{\alpha}_{i,j+1}^k(x) - \bar{\alpha}_{i+1,j+1}^k(x) + \bar{\delta}_{i+1,j}^k(x) \\ &= \sum_{r=i}^{j} B_r^k(x) - \sum_{r=i+1}^{j} B_r^k(x) + \bar{\delta}_{i+1,j}^k(x) \\ &= B_i^k(x) + \bar{\delta}_{i+1,j}^k(x),\end{aligned} \tag{8}$$

where the last line follows from the defining equation (3) for $\bar{\delta}_{i+1,j}^k(x)$. On substituting (8) in (7) we get

$$\bar{\delta}_{i,j}^{k+1}(x) = \frac{t_j-t_i}{t_{i+k}-t_i}\,\bar{\delta}_{i,j}^k(x) + \frac{t_{i+k}-t_j}{t_{i+k}-t_i}\,\bar{\delta}_{i+1,j}^k(x) + \frac{x-t_j}{t_{i+k}-t_i}\,B_i^k(x),$$

for $x \in [t_j, t_{j+1})$ and $j = i, \ldots, i+k-1$. Finally, from (4) we have

$$\frac{k}{t_{i+k}-t_i}\int_{t_i}^{x} B_i^k(\tau)\frac{d\tau}{w(\tau)} = \sum_{s=i}^{j-1}\frac{\delta_{i,s}^{k+1}}{w_s} + \frac{1}{w_j}\,\bar{\delta}_{i,j}^{k+1}(x), \tag{9}$$

with

$$\delta_{i,s}^{k+1} := \bar{\delta}_{i,s}^{k+1}(t_{s+1}),$$

$x \in [t_j, t_{j+1})$ and $j = i, \ldots, i+k-1$. Specially,

$$\frac{k}{t_{i+k} - t_i} \int_{t_i}^{t_{i+k}} B_i^k(\tau) \frac{d\tau}{w(\tau)} = \sum_{s=i}^{i+k-1} \frac{\delta_{i,s}^{k+1}}{w_s},$$

and by (9)

$$\frac{k}{t_{i+k} - t_i} \int_{t_j}^{t_{j+1}} B_i^k(\tau) d\tau = w_j \left(\int_{t_i}^{t_{j+1}} B_i^k(\tau) \frac{d\tau}{w(\tau)} - \int_{t_i}^{t_j} B_i^k(\tau) \frac{d\tau}{w(\tau)} \right) = \delta_{i,j}^{k+1},$$

where $\delta_{i,j}^{k+1}$ is calculated recursively:

$$\delta_{i,j}^{2} = \begin{cases} 1 \text{ for } j = i, \\ 0 \text{ for } j \neq i, \end{cases}$$

$$\delta_{i,j}^{k+1} = \frac{t_j - t_i}{t_{i+k} - t_i} \delta_{i,j}^{k} + \frac{t_{i+k} - t_j}{t_{i+k} - t_i} \delta_{i+1,j}^{k} + \frac{t_{j+1} - t_j}{t_{i+k} - t_i} B_i^k(t_{j+1}), \tag{10}$$

for $j = i, \ldots, i+k-1$.

3 Conclusion

There are other ways of calculating weighted integrals of polynomial splines, like Gaussian integration or conversion to Bezier form, and also some approximative ones [17]. In fact, (10) is a special case of recurrence used to evaluate inner products of B-splines ([4]) in which one of the B-splines is of order one. The proof given here is more in the spirit of 'B-splines without divided differences' [5], contains some new recurrences (5), and can be extended to obtain a recurrence for inner products. For inner products though, the greater complexity ($\mathrm{O}(k^4)$) compared to Gaussian integration ($\mathrm{O}(k^3)$) makes the recurrence seldom used, while for weighted splines it is preferable, being of the same complexity and machine independent.

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