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REGULARIZATION OF FIRST KIND INTEGRAL EQUATIONS WITH APPLICATION TO COUETTE VISCOMETRY

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ABSTRACT. The recovery of flow curves for non-Newtonian fluids from Couette rheometry measurements involves the solution of a quite simple first kind Volterra integral equation with a discontinuous kernel. In this paper, a new implementation of regularization is proposed. It involves the direct regularization of the observational equations through the construction of basis functions that exploit the mathematical structure in the integral equation. The proposed implementation is first derived for a general first kind integral equation and then applied to the Couette rheometer equation. For the regularization of this problem, the basis functions take on a form similar to that for B-splines.

1. Introduction. From a rheological as well as an integral equation and numerical analysis perspective, the recovery of flow curves for non-Newtonian fluids from torque measurements on a Couette (coaxial cylindrical) rheometer has a long and interesting history which dates from Couette's (1890) invention, [21]. Rheologically, because it is a simple and fairly inexpensive experiment to perform, it is still a widely utilized procedure to characterize the viscometric properties of Newtonian and non-Newtonian fluids. Furthermore, when compared with capillary and cone-and-plate rheometry, it has a number of important advantages including ease of construction and alignment, experimental accuracy and predictability of secondary flows. Exact solutions are only known for the inversion of capillary and cone-and-plate measurements, and this is one of the reasons behind their historic popularity, especially before the advent of electronic computers.

However, the importance of Couette rheometers relates more to their industrial rather than their scientific use. They allow an assessment of a non-Newtonian fluid to be made relatively quickly and inexpensively. A snapshot of their wide range of industrial application can be

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found in Calderbank and Moo-Young [5], who examine the power consumption in the agitation of non-Newtonian fluids, Rosenblatt et al. [27], who investigate sedimentation and aggregation in a blood rheology study, Grikshtas and Rao [13] who determined the slip velocities of various tomato concentrates and apple sauces, Ayora et al. [2] where the flow properties of different PVC-natural fiber suspensions were assessed, Baudez and Coussot [3] and Baudez, et al. [4] where pasty materials were the focus of deliberations and Picart et al. [22] where the rheological properties of blood are analyzed.

The basic integral equation that relates the torque measurements to the fluidity is a deceptively simple first kind Volterra integral equation with a discontinuous kernel. As discussed in Section 2, it is only mildly improperly posed. Infinite series solutions, derived independently by Krieger and Elrod [16] and Pawlowski [20] have, until quite recently, been the starting point for the numerical inversion of Couette rheometer measurements. A number of methods have been proposed for the summation of the infinite series including various Euler-Maclaurin sum formula approximations starting with the key paper of Krieger and Elrod [16] (Coleman and Noll [7], Krieger [14, 15], Code and Raal [6], Yang and Krieger [28]). More recently, with the increasing availability of new instrumentation and more comprehensive measurements, completely new methods have been proposed based on discretized Tikhonov regularization [18] and wavelet-vaguelette decomposition [1]. A major driver has been the increasing sophistication of materials manufactured from petro-chemicals and botanical/crop products, which has generated a growing demand not only for new instruments but also for improved algorithms for the recovery of information from indirect measurements, such as Couette flow data.

The paper has been organized in the following manner. The Couette rheometer integral equation is derived in Section 2. An infinite series solution is then used to assess the improperly posedness of this integral equation. A brief discussion follows about the historic evaluation on this series solution including the application of the Euler-Maclaurin sum formula. The published applications of Tikhonov regularization to the Couette equation are briefly assessed, and a new regularization approach is formulated in Section 3 for the standard Tikhonov quadratic functional for a general first kind integral equation. The key step establishes that the equations, resulting from setting the first variation of this discretization to zero, can be solved analytically. This result is used to derive a set of basis functions for the solution of the set of discretized functionals. These results are then utilized in Section 4 to derive a set of basis function for the approximate solution of the Couette integral equation. Though there are various ways in which such functions can be constructed, it turns out that there is a basis that is closely related to B-splines.

2. The Couette rheometer equation and its formal solution. A Couette (concentric cylinder) rheometer consists of an inner cylinder (the bob) of length L and radius r_b and the outer cylinder (the cup) of radius r_c , where the cup is rotated at an angular velocity Ω while a torque M is applied to the bob to hold it stationary.

Mooney [19] was the first to formulate the basic equation from first principles, viewing it as the solution to the problem of "... calculating slip and fluidity from experimental data." As Mooney [19] noted, Reiner's [23] earlier approach floundered because it failed to separate the solution of the inverse problem into the two clearly distinct steps of first formulating a model for the measurements in terms of the unknown flow curve and then solving the resulting mathematical relationship for the flow curve.

The essence of Mooney's [19] derivation is built on the assumption that "... no turbulence or other factor, aside from fluidity and slip, ... affect the measurements; and all surfaces in contact with the moving fluid must be alike" Essentially, this means that the flow of the fluid in the rheometer will be steady-state with only the azimuthal component of the velocity nonzero.

Equilibrium requires that the shear-stress $\tau(r)$ exerted on the fluid between the two cylinders at a radius $r, r_b \leq r \leq r_c$, be

(1)
$$\tau(r) = \frac{M}{2\pi r^2 L}$$

Thus, it follows that

(2)
$$\frac{d\tau}{dr} = -\frac{2\tau}{r}.$$

In the current context, the constitutive relationship can be formulated to take the form

$$\dot{\gamma} = \tau f(\tau),$$

which states that, for an ideal liquid in Couette flow, the rate of shearing, $\dot{\gamma}$, is a function $\tau f(\tau)$ of the local shear stress τ only. Here, $f(\tau)$ denotes the *fluidity* which corresponds to the reciprocal of the viscosity. In the simplest case of a Newtonian liquid, the fluidity is a constant. For many non-Newtonian materials, a power law is a good approximation, though more complex situations arise. For example, in a Bingham fluid, shearing does not commence until the shear stress exceeds the threshold yield stress.

For the azimuthal flow in a Couette rheometer,

$$\dot{\gamma} = -r \, \frac{d\omega}{dr},$$

where $\omega(r)$ denotes the angular velocity of the fluid at a radial distance r from the axis of the rheometer. Substitution of this result in the constitutive relationship yields

$$-r\frac{d\omega}{dr} = -r\frac{d\omega}{d\tau}\frac{d\tau}{dr} = \tau f(\tau),$$

and, on applying equation (2), one obtains

$$2\frac{d\omega}{d\tau} = f(\tau).$$

Integration of this last equation from $\omega = 0$ at the bob, to $\omega = \Omega$ at the cup, and utilizing the fact that the shearing at the bob and the cup, τ_b and τ_c , respectively, are related, through (1), by

$$\alpha = \frac{\tau_c}{\tau_b} = \left(\frac{r_b}{r_c}\right)^2,$$

the required Volterra integral relationship is derived

(3)
$$2\Omega(\tau) = \int_{\alpha\tau}^{\tau} f(\eta) \, d\eta.$$

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One can reinterpret the Couette integral equation (3) as the difference between two integrals of the form

$$F(\tau) = \int_0^\tau f(\eta) \, d\eta,$$

and, thereby, obtain

(4) $2\Omega(\tau) = F(\tau) - F(\alpha \tau)$, or equivalently $F(\tau) = F(\alpha \tau) + 2\Omega(\tau)$.

Iteration of the second equation in (4) to the limit, utilizing the fact that F(0) = 0, yields

$$F(\tau) = 2\sum_{j=0}^{\infty} \Omega(\alpha^{j}\tau),$$

which, when differentiated with respect to τ , gives the following infinite series solution for $f(\tau)$,

(5)
$$f(\tau) = 2\sum_{j=0}^{\infty} \alpha^{j} \Omega'(\alpha^{j} \tau), \quad \Omega' = \frac{d\Omega}{d\tau}$$

This derivation is somewhat simpler than that given in earlier publications.

Clearly, for the (physically unrealistic) situation where $\alpha \to 0$, the improper posedness of (3) corresponds to that of a single differentiation. The importance of the series representation of equation (5) is that, more generally, it establishes that the inherent improper posedness associated with the Couette rheometer equation (3) can be viewed as the sum of numerical differentiations of the Ω data. However, the summation appears to play a smoothing role. This can be illustrated in the following manner by reformulating (3) to take the form

$$\frac{2\Omega(\tau)}{(1-\alpha)\tau} = \int_0^T \frac{H(\eta - \alpha\tau) - H(\eta - \tau)}{(1-\alpha)\tau} f(\eta) \, d\eta,$$

where T is the maximum value that τ can take, and $H(\cdot)$ denotes the Heaviside unit step function which takes the value 1 for positive arguments and is zero otherwise. Clearly, from (3), $\Omega(\tau)$ depends on α . Furthermore, in the limit as α tends to one, the kernel becomes the Dirac delta function $\delta(\eta - \tau)$. It therefore follows that

$$\lim_{\alpha \to 1} \left[\frac{2\Omega(\tau)}{(1-\alpha)\tau} \right] = f(\tau).$$

The existence of this limit implies, heuristically, that, at least for $\alpha \sim 1$, the summation in equation (5) tends to play a smoothing role. In fact, the application of the standard integral mean value theorem to equation (3) yields

$$2\Omega(\tau) = (1 - \alpha)\tau f(\hat{\tau}), \quad \alpha \tau < \hat{\tau} < \tau,$$

which yields a clear encapsulation of the nature of that smoothing.

However, there is a dichotomy. From a rheological perspective, the larger the radius of the bob and the narrower the gap between the bob and the cup, for which $\alpha \sim 1$, the more accurately will be the recovery of the non-Newtonian behavior of a fluid to shearing, as a good approximation to shearing between flat parallel plates will be obtained and end effects will decrease. From a numerical analysis perspective, the closer the value of α is to 1, the slower will be the convergence of the infinite series solution (5) and the more problematic will be the evaluation of the Euler-Maclaurin sum formula approximation, since the relative error in the data is often larger for instruments where the bob and the cup are very close. For $\alpha \sim 1$, such approximations will be useful only when the need can be avoided to compute derivatives of Ω higher than the first. Furthermore, as discussed in Section 3, even the published Tikhonov regularization methods proposed for (3) can become problematic.

Krieger and Elrod [16] made the fundamental observation that the Euler-Maclaurin sum formula could be applied to an alternative form of the sum in (5). This has been investigated in a number of independent ways. Formally, if the derivatives of Ω are known exactly, the Euler-Maclaurin sum formula approximation will give a very good approximation for $\alpha \sim 1$. However, since the relative errors in the Ω data are often larger for instruments where the bob and cup are very close to each other, the Euler-Maclaurin sum formula approach can become quite problematic [7]. Aware of this difficulty, Code and Raal [6] developed a reinterpretation of the Euler-Maclaurin sum formula by

modeling the constitutive relationship, of the fluid under investigation, in terms of a power-law departure factor. The goal here was to obtain approximations for the higher order derivatives in terms of lower order derivatives. In a way, this approach can be viewed as a form of ad hoc regularization. It was subsequently pursued in a number of independent ways by Yang and Krieger [28].

The success of the simplicity and applicability of the above approximations was such that they became the standard for decades. Only the advent of improved instrumentation and more comprehensive data stimulated the need for improved algorithms. In addition, the greater amounts of data on finer grids forced the inherent improperly posed nature of equation (3) to be taken explicitly into account.

This has seen the publication of various algorithms based on Tikhonov regularization [18, 29]. Ancey [1] has proposed the use of the wavelet-vaguelette decomposition for performing the regularization.

3. Direct regularization of the observational equations. In this section, a different approach to the regularization of first kind integral equations is proposed.

Equation (3) can be viewed as a special case of a first kind integral equation of the form

(6)
$$\int_0^1 k(t,s)x(s) \, ds = y(t), \quad 0 < t < 1,$$

by using appropriately scaled variables. With respect to given observational data $d_i = y(t_i) + \varepsilon_i$, i = 1, 2, ..., n, where the ε_i denote random measurement errors, equation (6) takes the following discretized form

$$\int_0^1 k(t_i, s) x(s) \, ds = d_i, \quad i = 1, 2, \dots, n.$$

For the recovery of a continuous approximation from the discrete observational data $\{d_i\}$, this set of equations is clearly underdetermined, irrespective of the smoothness of the kernel k(t, s). The underlying improper posedness is further exacerbated as the smoothness of the kernel increases.

Clearly, some form of regularization is required in order to identify and stabilize the recovery of a unique approximation f to the solution x. There are various ways in which regularization can be applied to this set of discretized equations. However, if it is known that the solution is smooth and the measurement errors are independently and identically distributed, then Tikhonov regularization, which takes the following form, is appropriate

(7)
$$\mathcal{F}(f; \mathbf{d}) = \sum_{i=1}^{n} \left[\int_{0}^{1} k(t_i, s) f(s) \, ds - d_i \right]^2 + \lambda \int_{0}^{1} (f^{(m)}(s))^2 \, ds$$
$$\lambda > 0,$$

where **d** denotes the *n*-dimensional vector with components d_i and

$$f^m(s) = \frac{d^m f(s)}{ds^m}, \quad m \ll n.$$

Heuristically, in this form of regularization, uniqueness and stability are achieved as a balancing, controlled by the value of the regularization parameter λ , between the need for a smooth approximation f and an appropriate fit to the data. The results derived below can be generalized to a much wider class of regularization procedures than is encapsulated in (7) which, among other possibilities, could involve introducing known weightings into the two integral components in (7). Such an extension would arise naturally if the measurement errors $\{\varepsilon_i\}$ were not independently and identically distributed.

As explained for the Couette rheometer equation (3) in Yeow et al. [29] and Leong and Yeow [18], the popular strategy for deriving an approximation f on the basis of the quadratic functional (7) is to first construct a discretization of this functional and to then minimize the resulting algebraic quadratic form with respect to the components in the discretization of f. Historically, the essence of this idea dates back to Whittaker's [27] work on graduation. As explained in various places such as Shaw and Tigg [26] for the implementation proposed by Yeow et al., and more generally by Engl et al. [11, Chapter 9], this normally is a quite natural and sensible strategy that results in the solution of a relatively small number of equations. However, for the Couette equation (3) in order to obtain an accurate approximation to $f(\tau)$ using the method proposed by Yeow et al. [29] it will be necessary to construct and solve quite large matrix equations. In particular, when $\alpha \sim 1$, because of the small range $[\alpha \tau, \tau]$ over which the kernel k(t, s), as a function of s, is defined, the number of discretization points on each of the intervals $[\alpha \tau, \tau]$ must be reasonably large. Thus, when $\alpha \sim 1$, there will be many small intervals, and, consequently, it will be necessary to work with quite large matrices. This fact has been acknowledged in [18].

It turns out however that the optimal solution of equation (7) can be determined without resorting to approximation, in an analogous way in which Schoenberg [25] generalized the work of Whittaker [27]. In fact, for the case of the Couette equation (3), an analogue of the Curry and Schoenberg [9] B-splines can be derived as shown in Section 4.

On setting the first variation of the functional in (7) to zero, one obtains the following ordinary differential equation

(8)
$$f^{(2m)}(s) = \sum_{i=1}^{n} \beta_i k(t_i, s), \quad \beta_i = \frac{(-1)^m r_i}{\lambda},$$

along with the natural boundary conditions

(9)
$$f^{(m+j-1)}(0) = f^{(m+j-1)}(1) = 0, \quad j = 1, 2, \dots, m,$$

where the r_i are the residuals

$$r_i = \left[\int_0^1 k(t_i, \eta) f(\eta) \, d\eta - d_i\right].$$

From Taylor's theorem, utilizing the fact that

$$f^{(m+j-1)}(0) = 0, \quad j = 1, 2, \dots, m,$$

it follows that

$$f^{(m+j-1)}(s) = \frac{1}{(m-j)!} \int_0^s (s-\eta)^{m-j} f^{(2m)}(\eta) \, d\eta, \quad j = 1, 2, \dots, m.$$

The other natural boundary condition

$$f^{(m+j-1)}(1) = 0, \quad j = 1, 2, \dots, m,$$

when applied to this result, yields

$$f^{(m+j-1)}(1) = \frac{1}{(m-j)!} \int_0^1 (1-\eta)^{m-j} f^{(2m)}(\eta) \, d\eta = 0,$$

$$j = 1, 2, \dots, m.$$

Substitution of equation (8) into this result gives

(10)
$$f^{(m+j-1)}(1) = \sum_{j=1}^{n} \beta_{i} c_{ij} = 0,$$
$$c_{ij} = \frac{1}{(m-j)!} \int_{0}^{1} (1-\eta)^{m-j} k(t_{i},\eta) \, d\eta,$$
$$j = 1, 2, \dots, m.$$

The next step is the identification of the conditions that guarantee that the minimization of $\mathcal{F}(f; \mathbf{d})$ is unique. If it is assumed that the functional $\mathcal{F}(\cdot; \mathbf{d})$ has two minimizers f and f + p, then it follows that, because the first variation of $\mathcal{F}(f; \mathbf{d})$ is zero,

$$\mathcal{F}(f+p;\mathbf{d}) = \mathcal{F}(f;\mathbf{d}) + \sum_{i=1}^{n} \left(\int_{0}^{1} k(t_{i},s)p(s) \, ds \right)^{2} + \int_{0}^{1} (p^{(m)}(s))^{2} \, ds.$$

As minimizers of $\mathcal{F}(\cdot; \mathbf{d})$, the solutions f and f + p guarantee that the values of $\mathcal{F}(f + p; \mathbf{d})$ and $\mathcal{F}(f; \mathbf{d})$ must be the same, which can only occur if

$$\int_0^1 (p^{(m)}(s))^2 \, ds = 0,$$

and

$$\sum_{i=1}^{n} \left(\int_{0}^{1} k(t_{i}, s) p(s) \, ds \right)^{2} = 0.$$

The former condition implies that p must be a polynomial of the form

$$p_{m-1}(\eta) = \sum_{j=1}^{m} \gamma_j (1-\eta)^{m-j} \equiv 0.$$

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The latter condition implies that

$$\int_0^1 k(t_i, \eta) p_{m-1}(\eta) \, d\eta = 0, \quad i = 1, 2, \dots, n,$$

and, hence,

$$\sum_{j=1}^{m} \gamma_j \int_0^1 k(t_i, \eta) (1-\eta)^{m-j} \, d\eta = \sum_{j=1}^{m} c_{ij} \gamma_j = 0.$$

Uniqueness of the minimizer of $\mathcal{F}(\cdot; \mathbf{d})$ implies that $C\gamma = 0$ if and only if γ equals zero, which implies that the rank of the matrix $C \in \mathbf{R}^{n \times m}$ is m.

Let $G \in \mathbf{R}^{(n-m) \times n}$ denote a matrix of rank n-m, the rows of which are orthogonal to the columns of C; namely,

(11)
$$GC = 0, \quad \sum_{i=1}^{n} g_{qi} c_{ij} = \sum_{i=1}^{n} g_{qi} \int_{0}^{1} k(t_i, \eta) \eta^{m-j} d\eta,$$
$$q = 1, 2, \dots, m-n, \quad j = 1, 2, \dots, m.$$

Together, equations (10) and (11) imply that the vector $[\beta_1, \beta_2, \ldots, \beta_n]$ is orthogonal to the columns of the matrix C and, therefore, must lie in the span of the matrix G^T . This implies that the $\{\beta_i\}$ can be rewritten as a linear combination of the $\{g_{qi}\}, q = 1, 2, \ldots, n - m$; namely,

(12)
$$\beta_i = \sum_{q=1}^{n-m} \zeta_{m+q} g_{qi}.$$

The application of the Taylor series expansion with integral remainder to f(s) yields

$$f(s) = \sum_{j=1}^{2m} \frac{s^{j-1}}{(j-1)!} f^{j-1}(0) + \frac{1}{(2m-1)!} \int_0^s (s-\eta)^{2m-1} f^{(2m)}(\eta) \, d\eta.$$

Combining this result with equation (8) and the natural boundary conditions (9), at the origin, yields

$$f(s) = \sum_{j=1}^{m} \frac{s^{j-1}}{(j-1)!} f^{j-1}(0) + \sum_{i=1}^{n} \beta_i K_{2m}(t_i, s),$$

where

$$K_j(t_i, s) = \frac{1}{(j-1)!} \int_0^s (s-\eta)^{j-1} k(t_i, \eta) \, d\eta, \quad j = 1, 2, \dots, 2m.$$

In conjunction with equation (12), this last equation becomes

$$f(s) = \sum_{j=1}^{m} \frac{s^{j-1}}{(j-1)!} f^{j-1}(0) + \sum_{i=1}^{n} \sum_{q=1}^{n-m} \zeta_{m+q} g_{qi} K_{2m}(t_i, s),$$

which, on changing the order of summation, yields

$$f(s) = \sum_{j=1}^{m} \frac{s^{j-1}}{(j-1)!} f^{j-1}(0) + \sum_{q=1}^{n-m} \zeta_{m+q} \sum_{i=1}^{n} g_{qi} K_{2m}(t_i, s).$$

Thus, on introducing the basis functions

(13)
$$\phi_q(s) = \frac{s^{q-1}}{(q-1)!}, \quad \zeta_q = f^{(q-1)}(0), \quad q = 1, 2, \dots, m,$$

and

(14)
$$\phi_{m+q}(s) = \sum_{i=1}^{n} g_{qi} K_{2m}(t_i, s), \quad q = 1, 2, \dots, n-m,$$

it follows that the solution of equations (8) and (9) can be written as

(15)
$$f(s) = \sum_{q=1}^{n} \zeta_q \phi_q(s).$$

This establishes the fact that the minimizer of the functional (7) can be written as a linear combination of the basis functions $\phi_q(s)$, $q = 1, 2, \ldots, n$.

Substitution of this approximation for f(s) into equations (7) and differentiation of the resulting set of equations with respect to the unknowns ζ_l yields the following matrix counterpart of the fact that the first variation of the underlying matrix quadratic form is zero

 $A\zeta=\mathbf{z},$

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where

$$a_{lj} = \sum_{i=1}^{n} \int_{0}^{1} k(t_i, s) \phi_j(s) \, ds \int_{0}^{1} k(t_i, \bar{s}) \phi_l(\bar{s}) \, d\bar{s} + \lambda \int_{0}^{1} \phi_j^{(m)}(s) \, ds \int_{0}^{1} \phi_l^{(m)}(\bar{s}) \, d\bar{s}, \zeta = (\zeta_1, \zeta_2, \dots, \zeta_n)^T, \quad \mathbf{z} = (z_1, z_2, \dots, z_n)^T,$$

and

$$z_{l} = \sum_{i=1}^{n} d_{i} \int_{0}^{1} k(t_{i}, s) \phi_{l}(s) \, ds.$$

It is clear from the above construction that the structure of the $\{k(t_i, s)\}$ now plays an explicit role in determining the form of the regularized approximation (15) to the solution of the integral equation (6). Furthermore, the choice of the design points $\{t_i\}$, at which the measurements $\{d_i\}$ are made, controls the choice of the $\{k(t_i, s)\}$ and, thereby, the resulting form of the $\{\phi_j(s)\}$.

4. Construction of the basis functions $\phi_l(s)$ for the Couette flow problem. It follows from a comparison of equations (3) and (6) that

$$k(t,s) = H(\alpha t - s) - H(t - s),$$

and, hence, that

$$K_j(t,s) = \frac{1}{j!} \left[(s - \alpha t)_+^j - (s - t)_+^j \right].$$

For this problem, it is convenient to rescale $K_j(t,s)$ as follows

$$\widetilde{K}_{j}(t,s) = \frac{1}{j!} \frac{\left[(s - \alpha t)_{+}^{j} - (s - t)_{+}^{j}\right]}{(1 - \alpha)t},$$

which is zero for $s < \alpha t$ and a polynomial of degree j - 1 in t for s > t.

It is well known that, in general, the truncated polynomials $(t - t_i)_+^q$, defined on some nondecreasing set $t = \{t_i\}$, do not define computationally a suitable set of basis functions for the application of spline functions. The resulting linear systems of equations tend to be poorly



FIGURE 1. A plot of a representative set of the basis functions.

conditioned Greville [12, p. 21]. On the other hand, B-splines, generated by taking appropriate divided differences of truncated polynomials, are known to yield much better conditioned linear systems. In part, this is due to their relatively small support [10].

The concept of a B-spline dates back to Curry and Schoenberg [9]. Following de Boor [10], the *i*th normalized B-spline of order k for a given knot sequence t is denoted by $B_{i,k,t}(s)$ and defined by

$$B_{i,k,t}(s) := (t_{i+k} - t_i)[t_i, \dots, t_{i+k}](\cdot - s)_+^{k-1},$$

for all $s \in R$, where $[t_i, \ldots, t_{i+k}]h(\cdot)$ denotes the *k*th divided difference of the values of the function h(t) at the knot points $\{t_i\}$. The *k*th divided difference eliminates polynomials in *t* of degree less than *k*. Hence, their support is limited to the interval $[t_i, t_{i+k}]$.

Consequently, it is natural to define the basis function $\{\phi_i\}$ to take the form

$$\phi_l(s) = [t_{l-m}, \dots, t_{l+m}] \widetilde{K}_{2m}(\cdot, s), \quad l = m+1, \dots, n-m.$$

This choice yields essentially the same structure as the more general functions $\{\phi_i\}$ of equations (13) and (14), in that they correspond to

a linear combination of the $K_{2m}(t_i, s)$. Furthermore, since $K_{2m}(t, s)$ is zero for $s < \alpha t$ and is a polynomial of degree 2m-1 on s > t, it follows that the support of the basis functions ϕ_l , $l = m + 1, \ldots, n - m$, is restricted to the interval $[\alpha t_{l-m}, t_{l+m}]$. Since $0 < \alpha t_{l-m} < t_{l+m} < 1$, it follows that the boundary conditions (9) are satisfied.

The remaining 2m basis functions correspond to the m functions

(16)
$$\phi_{n-m+l}(s) = [t_{n-2m+l}, \dots, t_n] \widetilde{K}_{2m}(\cdot, s), \quad l = 1, \dots, m,$$

which have support on $[t_{n-2m+l}, 1]$, and the *m* functions

(17)
$$\phi_l(s) = [t_1, \dots, t_{m+l}] \hat{K}_{2m}(\cdot, s), \quad l = 1, \dots, m,$$

with support on $[0, \alpha t_{m+l}]$, where

$$\widehat{K}_{j}(t,s) = \frac{1}{j!} \frac{\left[(s - \alpha t)_{-}^{j} - (s - t)_{-}^{j} \right]}{(1 - \alpha)t}.$$

That the boundary conditions are satisfied by these basis functions can be verified in the following manner. First consider the basis functions of equation (16). It follows that

(18)
$$\phi_{n-m+l}^{(m+j-1)}(s) = [t_{n-2m+l}, \dots, t_n] \widetilde{K}_{m-j+1}(\cdot, s), \quad l = 1, \dots, m.$$

Now $\widetilde{K}_{m-j+1}(t,s)$ is zero for $s < \alpha t$ and is a polynomial of degree m-j in t on $[t_n, 1]$ which is eliminated by the divided differences in equation (18). Thus, the supports for each $\phi_{n-m+l}^{(m+j-1)}(s)$ is the interval $[\alpha t_{n-2m+l}, t_n]$ and hence the boundary conditions (9) are satisfied. A similar argument applies for the basis functions of equation (17).

Because of the limited local support of these basis functions as well as the kernel of the integral equation (5), the resulting matrix equations will be quite sparse. An illustration of the resulting set of basis functions for m = 1 is given in Figure 1.

Note added to proofs. It has come to our attention that the derivation of the basis functions of equations (13) and (14) is similar to that used by D. Nychka, G. Wahba, S. Goldfarb and T. Pugh (*Cross*validation spline methods for the estimation of three-dimensional tumor size distributions from observational on two-dimensional cross sections, JASA **79** (1984), 832–846) where reproducing kernel Hilbert space results are employed.

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