TITLE: Application of Orthogonalisation Procedures for Gaussian Radial Basis Functions and Chebyshev Polynomials

Application of orthogonalisation procedures for Gaussian radial basis functions and Chebyshev polynomials

John C Mason and Andrew Crampton

School of Computing and Mathematics, University of Huddersfield, Huddersfield, UK.
j.c.mason@hud.ac.uk, a.crampton@hud.ac.uk

Abstract

Procedures for orthogonalisation of Gaussians and B-splines are recalled and it is shown that, provided Gaussians are negligible in appropriate regions, the same recurrence formulae may be adopted in both and render the computation relatively efficient. Chebyshev polynomial collocation is well known to be rapidly defined by discrete orthogonalisation, and similar ideas are commonly applicable to partial differentieal equations (PDEs) and integral equations (IEs). However, it is shown that the most elementary mixed methods (both boundary conditions and PDEs being satisfied) for the Dirichlet problem in rectangular types of domain can lead to a singular linear system, which may be rendered non-singular, for example, by a small modification of interpolation nodes.

1 Introduction

Gaussian radial basis functions (RBFs) are negligible outside a certain range, which depends on the accuracy required and the exponent used. For example, if four decimal place accuracy is sufficient, then outside $[-2, 2]$ the function $e^{-\lambda x^2}$ is negligible for $\lambda \geq 2.5$. Indeed the translated RBFs

$$\phi_i(x) = e^{-\lambda(x-i)^2} \quad i = -1, 0, \ldots, n+1, \tag{1.1}$$

resemble, at least superficially, a set of translated cubic B-splines, each having a support of four sub-intervals of length one, contained in $[i-2, i+2]$.

Following work of Mason *et al* [4] and Goodman *et al* [1], we show that these RBFs, rounded to the required accuracy, may be conveniently and efficiently orthogonalised so that

(i) a 4 term recurrence may be adopted identical to the one in [4] for cubic B-splines,

(ii) inner products may be determined very simply in terms of 4 parts of a normal distribution,

(iii) a well conditioned calculation results and best l_2 approximations may be obtained immediately with an orthogonalised basis,

(iv) a continuous or discrete inner product (and best approximation) may be adopted.

In a second application of orthogonalisation, this time to polynomials, it is shown that a two-dimensional $(n+1) \times (n+1)$ polynomial collocation problem, which includes amongst its nodes n Chebyshev polynomial zeros on each of 4 sides of a square, leads to a singular (rank one deficient) system. For all n, one superfluous equation is readily identified and a suitable replacement equation is readily found. Discrete orthogonalisation is used to combine and greatly simplify the equations and prove singularity.

2 Orthogonalised Gaussians

An orthogonal system $\{P_i\}$ is developed from the Gaussians ϕ_i in (1.1) using

$$P_k = \phi_k - a_{k1}P_{k-1} - a_{k2}P_{k-2} - a_{k3}P_{k-3}, \quad k = -1, \ldots, n+1, \tag{2.1}$$

where $a_{13} = a_{03} = a_{02} = a_{-1,3} = a_{-1,2} = a_{-1,1} = 0$.

Now we define coefficients b_{kr}, for $r = 0, \ldots, k+1$ and $k = -1, \ldots, n+1$, as the inner products

$$b_{kr} = \langle \phi_k, \phi_{k-r} \rangle = \int_{I_{k,r}} \phi_k(x)\phi_{k-r}(x)dx, \tag{2.2}$$

where $I_{k,r}$ is the common support of ϕ_k and ϕ_{k-r} and normalising constants n_k are the squared norms

$$n_k = \|P_k\|^2 = \langle P_k, P_k \rangle\,, \tag{2.3}$$

where $\langle \bullet, \bullet \rangle$ is the inner product (2.2) and $\| \bullet \|$ is the corresponding norm.

Then, setting $\langle P_k, P_{k-r} \rangle = 0$ for $r = 1, 2, 3$ gives

$$\langle \phi_k, P_{k-r} \rangle = a_{kr} n_{k-r}. \tag{2.4}$$

Taking the inner product of (2.1) with itself gives

$$n_k = b_{k0} + \sum_{r=1}^{3} \left[-2a_{kr} \langle \phi_k, P_{k-r} \rangle + a_{kr}^2 n_{k-r} \right], \tag{2.5}$$

which, by using (2.4), gives

$$n_k = b_{k0} - \sum_{r=1}^{3} a_{kr}^2 n_{k-r}. \tag{2.6}$$

This is the first basic equation for writing $\{n_k\}$ in terms of $\{a_{kr}\}$ and $\{b_{kr}\}$.

Now, using (2.1), with k replaced by $k-1, k-2, k-3$ we obtain

$$\langle \phi_k, P_{k-3} \rangle = b_{k3} = a_{k3} n_{k-3} \tag{2.7}$$

$$\langle \phi_k, P_{k-2} \rangle = b_{k2} - a_{k-2,1} \langle \phi_k, P_{k-3} \rangle .$$

Hence

$$a_{k2} n_{k-2} = b_{k2} - a_{k-2,1} b_{k3}. \tag{2.8}$$

Finally

$$\langle \phi_k, P_{k-1} \rangle = b_{k1} - a_{k-1,1} \langle \phi_k, P_{k-2} \rangle - a_{k-1,2} \langle \phi_k, P_{k-3} \rangle ,$$

so that

$$a_{k1} n_{k-1} = b_{k1} - a_{k-1,1} (a_{k2} n_{k-2}) - a_{k-1,2} b_{k3}. \tag{2.9}$$

Equations (2.6), (2.7), (2.8) and (2.9) may be solved to determine all the required coefficients $\{a_{kr}\}$ and $\{n_k\}$ explicitly by substitution, starting from $n_{-1} = \|\phi_{-1}\|^2$. This involves $\mathcal{O}(n)$ operations for $n+3$ basis functions. The best approximation to a function f (either continuous $f = f(x)$ or discrete $f = (f_1, \ldots, f_m)^T$) by orthogonalised Gaussians may be determined explicitly as

$$f \approx \sum_{j=-1}^{n+1} c_j P_j,$$

where $c_j = \langle P_j, P_j \rangle^{-1} \langle f, P_j \rangle = (n_j)^{-1} \langle f, P_j \rangle .$

2.1 Numerical example

Here we use the procedure for constructing orthogonalised Gaussians to produce an interpolant to data obtained from a fast response oscilloscope[1]. To the left of Figure 1 we see the first three orthogonalised Gaussian functions, with centres specified at the integers -1, 0 and 1, with support growing from left to right. The figure on the right shows the oscilloscope data ** and the fitted o-Gaussian interpolant —.

[1] Oscilloscope data supplied by Centre for Electromagnetic and Time Metrology, National Physical Laboratory, London, UK.

In this example we use 512 centres and choose $\lambda = 2.5$ in (1.1). Since our choice for λ requires only four decimal place accuracy, the normal equations produce the usual identity matrix and the coefficient vector $\{c_{-1}, \ldots, c_{n+1}\}$ can then be determined by the equations $c = A^T f$ where $f = \{f_1, \ldots, f_m\}$ and $A_{i,j} = P_j(x_i)$. The fit is extremely good and vindicates the neglecting of the Gaussians outside the interval considered.

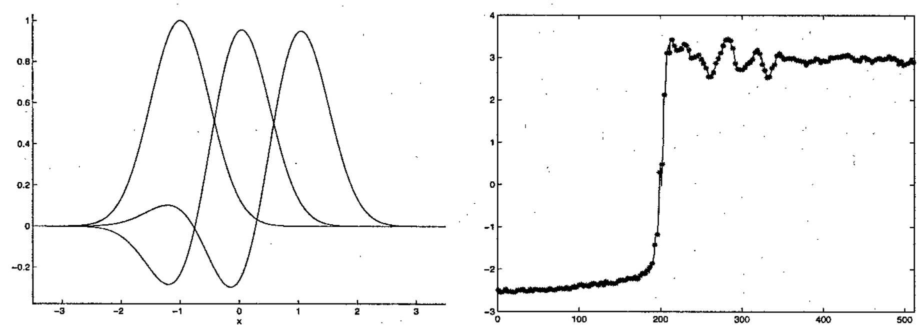

FIG. 1. First three orthogonalised basis functions and o-Gaussian fit to oscilloscope data.

2.2 Extensions to orthogonalised Gaussians

The following extensions are clearly possible.

(i) Use of generally placed centres (knots) and/or a discrete inner product.

(ii) Use of higher dimensions – as in Anderson *et al* [2].

(iii) Replacement of interval $(-\infty, \infty)$ in a continuous norm by $[0, n]$ and $[0, n]$ by $[0, 1]$ using scaling.

(iv) Consideration of a function with wider (approximate) support, such as $[-3, 3]$ or more generally $[-r, r]$ for $r > 2$.

3 Chebyshev polynomials in two-dimensional collocation

The (first kind) Chebyshev polynomial $T_i(x)$ of degree i is defined by

$$T_i(x) = \cos i\theta \qquad i = 0, \ldots, m, \quad -1 \le x \le 1, \tag{3.1}$$

where $x = \cos\theta$ and $0 \le \theta \le \pi$.

Among its many properties is the discrete orthogonality property

$$\sum_{k=1}^{m} T_i(x_k) T_j(x_k) = \begin{cases} 0 & \text{for} \quad i \ne j; \quad i, j \le m-1 \\ m & \text{for} \quad i = j = 0 \\ \frac{1}{2}m & \text{for} \quad i = j \ne 0, \end{cases} \tag{3.2}$$

where x_k are the m zeros of $T_m(x)$, namely

$$x_k = \cos\left(\frac{(2k-1)\pi}{2m}\right), \quad k = 1, \ldots, m. \tag{3.3}$$

The orthogonality property of (3.2) is not a unique one amongst the Chebyshev polynomials of four kinds. Indeed, Mason and Venturino [5] showed that there are at least fourteen such formulae, depending on alternative weights, choices of Chebyshev-related abscissae and kinds of Chebyshev polynomial.

3.1 The elliptic problem — mixed methods

Let us now exploit this property (3.2) in a pseudo-spectral method for a linear elliptic PDE problem on a square. The PDE

$$Lu = f(x, y), \quad |x|, |y| \leq 1, \tag{3.4}$$

subject to

$$u = g(x, y), \tag{3.5}$$

where $g(x, y)$ is a function known explicitly only on $x = \pm 1$ and $y = \pm 1$, can be solved approximately in the form

$$u = u_{mn} = {\sum_{i=0}^{m}}' {\sum_{j=0}^{n}}' a_{ij} T_i(x) T_j(y), \tag{3.6}$$

where a dashed summation denotes that the first term in a sum is halved.

To obtain equations for a_{ij}, we solve

$$\begin{aligned}
Lu_{mn} &= f, && \text{at the } (m-1) \times (n-1) \text{ zeros of } T_{m-1}(x)T_{n-1}(y), && (3.7)\\
u_{mn} &= g, && \text{on } x = \pm 1 \text{ at zeros of } T_n(y) \quad (2n \text{ equations}), && (3.8)\\
u_{mn} &= g, && \text{on } y = \pm 1 \text{ at zeros of } T_m(x) \quad (2m \text{ equations}). && (3.9)
\end{aligned}$$

Together (3.7)–(3.9) form $(m+1) \times (n+1)$ equations for $\{a_{ij}\}$. However, we claim that the included equations (3.8), (3.9) are singular of joint rank $2m + 2n - 1$. If this is so, then the system is singular without consideration of the PDE collocation equations (3.7). The equations (3.8), (3.9) become

$$g_{k,\pm 1} = {\sum_{i=0}^{m}}' {\sum_{j=0}^{n}}' a_{ij} T_i(x_k) T_j(\pm 1), \quad g_{\pm 1,\ell} = {\sum_{i=0}^{m}}' {\sum_{j=0}^{n}}' a_{ij} T_i(\pm 1) T_j(y_\ell), \tag{3.10}$$

where x_k, y_ℓ are zeros of $T_m(x), T_n(y)$ respectively and where

$$\begin{aligned}
g_{1,\ell} &= g(1, y_\ell), & g_{-1,\ell} &= g(-1, y_\ell),\\
g_{k,1} &= g(x_k, 1), & g_{k,-1} &= g(x_k, -1).
\end{aligned}$$

If we add/subtract the first pair and also the second pair of equations in (3.10), noting that

$$T_j(1) = 1, \quad T_j(-1) = (-1)^j,$$

we deduce that

$$d_k^{(0)} = \sum_{i=0}^{m}{}' \sum_{\substack{j=0 \\ (j \text{ even})}}^{n}{}' a_{ij} T_i(x_k), \quad d_k^{(1)} = \sum_{i=0}^{m}{}' \sum_{\substack{j=0 \\ (j \text{ odd})}}^{n}{}' a_{ij} T_i(x_k), \quad k = 1, \ldots, m, \tag{3.11}$$

$$e_k^{(0)} = \sum_{\substack{i=0 \\ (i \text{ even})}}^{m}{}' \sum_{j=0}^{n}{}' a_{ij} T_j(y_\ell), \quad e_k^{(1)} = \sum_{\substack{i=0 \\ (i \text{ odd})}}^{m}{}' \sum_{j=0}^{n}{}' a_{ij} T_j(y_\ell), \quad \ell = 1, \ldots, n, \tag{3.12}$$

where,

$$\begin{aligned} d_k^{(0)} &= \tfrac{1}{2}(g_{k,1} + g_{k,-1}), & d_k^{(1)} &= \tfrac{1}{2}(g_{k,1} - g_{k,-1}), \\ e_k^{(0)} &= \tfrac{1}{2}(g_{1,\ell} + g_{-1,\ell}), & e_k^{(1)} &= \tfrac{1}{2}(g_{1,\ell} - g_{-1,\ell}). \end{aligned}$$

Multiplying (3.11) by $2T_r(x_k)/(m+1)$ and summing over k, and multiplying (3.12) by $2T_s(y_\ell)/(n+1)$ and summing over ℓ, discrete orthogonality (3.2) gives

$$R_{r+1}^{(0)} \equiv \sum_{\substack{j=0 \\ (j \text{ even})}}^{n}{}' a_{rj} = b_{r+1}^{(0)}, \quad R_{r+1}^{(1)} \equiv \sum_{\substack{j=r \\ (j \text{ odd})}}^{n} a_{rj} = b_{r+1}^{(1)}, \quad r = 0, \ldots, m-1, \tag{3.13}$$

$$C_{s+1}^{(0)} \equiv \sum_{\substack{i=0 \\ (i \text{ even})}}^{m}{}' a_{is} = c_{s+1}^{(0)}, \quad C_{s+1}^{(1)} \equiv \sum_{\substack{i=0 \\ (i \text{ odd})}}^{m} a_{is} = c_{s+1}^{(1)}, \quad s = 0, \ldots, m-1, \tag{3.14}$$

where

$$\begin{aligned} b_{r+1}^{(0)} &= \frac{2}{m+1} \sum_{k=1}^{m} d_k^{(0)} T_r(x_k) & b_{r+1}^{(1)} &= \frac{2}{m+1} \sum_{k=1}^{m} d_k^{(1)} T_r(x_k), \\ c_{s+1}^{(0)} &= \frac{2}{n+1} \sum_{\ell=1}^{n} e_k^{(0)} T_s(y_\ell) & c_{s+1}^{(1)} &= \frac{2}{n+1} \sum_{\ell=1}^{n} e_k^{(1)} T_s(y_\ell). \end{aligned}$$

This constitutes a greatly simplified system to replace (3.10). Indeed we may verify that, for $m = n$,

$$\sum_{\substack{i=0 \\ (m-i \text{ odd})}}^{m-1}{}' R_{i+1}^{(t)} = \sum_{\substack{i=0 \\ (m-i \text{ odd})}}^{m-1}{}' C_{i+1}^{(t)}, \tag{3.15}$$

where $t = 0, 1$ for $m =$ odd, even, respectively, and hence that the equations (3.13) and (3.14) are singular. For example, for $m\ (= n) = 2$, we seek equations in $a_{00}, \ldots, a_{22}$, and (3.13) gives

$$\begin{aligned} R_1^{(0)} &\equiv \tfrac{1}{2}a_{00} + a_{02}, \qquad & R_1^{(1)} &\equiv a_{01}, \\ R_2^{(0)} &\equiv \tfrac{1}{2}a_{10} + a_{12}, \qquad & R_2^{(1)} &\equiv a_{11}, \end{aligned} \tag{3.16}$$

meanwhile (3.14) gives

$$\begin{aligned} C_1^{(0)} &\equiv \tfrac{1}{2}a_{00} + a_{20}, \qquad & C_1^{(1)} &\equiv a_{10}, \\ C_2^{(0)} &\equiv \tfrac{1}{2}a_{01} + a_{21}, \qquad & C_2^{(1)} &\equiv a_{11}. \end{aligned} \tag{3.17}$$

Clearly $R_2^{(1)} = C_2^{(1)}$, consistent with (3.15) for $m = 2$. Which equation do we eliminate? For simplicity, in the case of m even, we delete the equation for $C_2^{(1)}$ and replace it by the equation for $R_{m+1}^{(0)}$. It is easy to verify that, within the system (3.13) and (3.14), this leads to full rank, and $R_{m+1}^{(0)}$ is equivalent to boundary specifications of either of

$$\begin{gathered} u(0,1) + u(0,-1), \\ u(1,1) + u(-1,1) + u(1,-1) + u(-1,-1). \end{gathered} \tag{3.18}$$

For $m = n = 2$, this is equivalent to

$$R_3^{(0)} \equiv \frac{1}{2}a_{20} + a_{22}. \tag{3.19}$$

In the case when m is odd, we delete the equation for $C_1^{(0)}$ and replace it by the equation for $C_{m+1}^{(1)}$, the latter being equivalent to adding four boundary point conditions anti-symmetrically, i.e.,

$$u(1,1) - u(-1,1) + u(-1,-1) - u(1,-1). \tag{3.20}$$

If $g(x, y)$ is known everywhere in the square, then we could of course consider replacing a mixed collocation problem by an interior collocation problem by including the boundary conditions automatically in the form of approximations. For example, we could replace the form (3.6) by

$$u_{mn} = (x^2 - 1)(y^2 - 1) \sum_{i=0}^{m-2}{}' \sum_{j=0}^{n-2}{}' a_{ij} T_i(x) T_j(y) + g(x, y), \tag{3.21}$$

or by an alternative form such as

$$u_{mn} = \sum_{i=0}^{m}{}' \sum_{j=0}^{n}{}' a_{ij} \left(T_i(x) - T_{\underline{i}}(x)\right) \Big(T_j(y) - T_{\underline{j}}(y)\Big) + g(x, y), \tag{3.22}$$

where $T_i = T_0(x)$ or $T_1(x)$ according as i is even or odd. These forms have the disadvantage of being difficult to generalise to other kinds of (non-rectangular) boundaries, although (3.21) is adaptable to the case where an equation of the boundary is known (see Mason [3]).

The best Chebyshev method available for the Poisson problem on a rectangle is probably a "differentiation matrix" method, such as is described in Trefethen [6], which represents the solution by nodal values rather than Chebyshev coefficients.

Acknowledgement: We thank the referees for their perceptive remarks.

Bibliography

1. T. N. T. Goodman, C. A. Micchelli, G. Rodriguez and S. Seatzu, On the Cholesky factorization of the Gram matrix of locally supported functions, BIT **35**(2), 1995, 233–257.
2. I. J. Anderson, J. C. Mason, G. Rodriguez and S. Seatzu, Training radial basis function networks using separable and orthogonalised Gaussians, in *Mathematics of Neural Networks*, S. W. Ellacot, J. C. Mason and I. J. Anderson (eds), Kluwer, 1997, 265–269.
3. J. C. Mason, Chebyshev polynomial approximations for the L-membrane eigenvalue problem, in *SIAM J. of Appl. Math* **15** (1967), 172–186.
4. J. C. Mason, G. Rodriguez and S. Seatzu, Orthogonal splines based on B-splines with applications to least squares, smoothing and regularisation problems, in *Numerical Algorithms* **5** (1993), 25–40.
5. J. C. Mason and E. Venturino, Integration methods of Clenshaw- Curtis type based on four kinds of Chebyshev polynomials, in *Multivariate Approximation and Splines*, G. Nuernberger, J. W. Schmidt and G. Walz (eds), Birkhauser, Basel, 1997, 158–165.
6. L. N. Trefethen, *Spectral Methods in MATLAB*, SIAM, 2000.