RBF collocation methods as pseudospectral methods

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Abstract

We show how the collocation framework that is prevalent in the radial basis function literature can be modified so that the methods can be interpreted in the framework of standard pseudospectral methods. This implies that many of the standard algorithms and strategies used for solving time-dependent as well as time-independent partial differential equations with (polynomial) pseudospectral methods can be readily adapted for the use with radial basis functions. The potential advantage of radial basis functions is that they lend themselves to complex geometries and non-uniform discretizations.
Keywords: radial basis functions, collocation, pseudospectral methods.

1 Pseudospectral methods and radial basis functions

Pseudospectral (PS) methods are known as highly accurate solvers for partial differential equations (PDEs). The basic idea (see, e.g., [4] or [12]) is to use a set of (very smooth and global) basis functions ϕ_j, $j = 1, \ldots, N$, such as polynomials to represent an unknown function (the approximate solution of the PDE) via

$$u^h(x) = \sum_{j=1}^{N} \lambda_j \phi_j(x), \qquad x \in \mathbb{R}. \tag{1}$$

Since most of our discussion will focus on a representation of the spatial part of the solution we ignore the time variable in the formulas for u^h. We will employ standard time-stepping procedures to deal with the temporal part of the solution. Moreover, since standard pseudospectral methods are designed for the univariate

case we initially limit ourselves to single-variable functions. Later we will generalize to multivariate (spatial) problems by using radial basis functions.

An important feature of pseudospectral methods is the fact that one usually is content with obtaining an approximation to the solution on a discrete set of grid points x_i, $i = 1, \ldots, N$. One of several ways to implement the spectral method is via so-called *differentiation matrices*, i.e., one finds a matrix D such that at the grid points x_i we have

$$\boldsymbol{u}' = D\boldsymbol{u}, \tag{2}$$

where $\boldsymbol{u} = [u^h(x_1), \ldots, u^h(x_N)]^T$ is the vector of values of u^h at the grid points. Frequently, orthogonal polynomials such as Chebyshev polynomials are used as basis functions, and the grid points are corresponding Chebyshev points. In this case the entries of the differentiation matrix are explicitly known (see, e.g., [12]).

In this paper we are interested in using (infinitely smooth) radial basis functions (RBFs) in the spectral expansion (1), i.e., $\phi_j(x) = \Phi(\|x - x_j\|)$, where Φ is some positive definite univariate basic function. Possible choices for positive definite functions include, e.g., Gaussians $\Phi(r) = e^{-(\varepsilon r)^2}$, or Matérn functions such as

$$\Phi(r) = e^{-\varepsilon r}\left((\varepsilon r)^3 + 6(\varepsilon r)^2 + 15(\varepsilon r) + 15\right). \tag{3}$$

Here, the univariate variable r is a radial variable, i.e., $r = \|x\|$, and the positive parameter ε is equivalent to the well-known shape parameter used to scale the basic functions. We have chosen the representations above since then $\varepsilon \to 0$ always results in "flat" basic functions for which we have the well-known trade-off principle, i.e., high accuracy at the cost of low stability or vice versa (see, e.g., [11]).

2 Differentiation matrices

We now present a brief discussion of differentiation matrices. Consider expansion (1) and let ϕ_j, $j = 1, \ldots, N$, be an arbitrary linearly independent set of smooth functions that will serve as the basis for our approximation space.

If we evaluate (1) at the grid points x_i, $i = 1, \ldots, N$, then we get

$$u^h(x_i) = \sum_{j=1}^{N} \lambda_j \phi_j(x_i), \qquad i = 1, \ldots, N,$$

or in matrix-vector notation

$$\boldsymbol{u} = A\boldsymbol{\lambda}, \tag{4}$$

where $\boldsymbol{\lambda} = [\lambda_1, \ldots, \lambda_N]^T$ is the coefficient vector, the evaluation matrix A has entries $A_{ij} = \phi_j(x_i)$, and $\boldsymbol{u}$ is as before.

By linearity we can also use the expansion (1) to compute the derivative of u^h by differentiating the basis functions

$$\frac{d}{dx}u^h(x) = \sum_{j=1}^{N} \lambda_j \frac{d}{dx}\phi_j(x).$$

If we again evaluate at the grid points x_i then we get in matrix-vector notation

$$\boldsymbol{u}' = A_x \boldsymbol{\lambda}, \tag{5}$$

where $\boldsymbol{u}$ and $\boldsymbol{\lambda}$ are as above, and the matrix A_x has entries $\frac{d}{dx}\phi_j(x_i)$, or $\frac{d}{dx}\Phi(\|x - x_j\|)|_{x=x_i}$ for radial functions.

In order to obtain the differentiation matrix D we need to ensure invertibility of the evaluation matrix A. This depends both on the basis functions chosen as well as the location of the grid points x_i. For univariate polynomials it is well-known that the evaluation matrix is invertible for any set of distinct grid points. In particular, if the polynomials are written in cardinal (or Lagrange) form, then the evaluation matrix is the identity matrix. For positive definite radial basis functions (an extension of) Bochner's theorem guarantees the invertibility of the matrix A for any set of distinct grid points (also non-uniformly spaced and in $\mathbb{R}^d$, $d > 1$). Cardinal RBFs, on the other hand, are rather difficult to obtain. For the special case of uniform one-dimensional grids such formulas can be found in [9].

Thus we can use (4) to solve for the coefficient vector $\boldsymbol{\lambda} = A^{-1}\boldsymbol{u}$, and then (5) yields

$$\boldsymbol{u}' = A_x A^{-1} \boldsymbol{u},$$

so that the differentiation matrix D corresponding to (2) is given by

$$D = A_x A^{-1}.$$

For more complex linear differential operators $\mathcal{L}$ with constant coefficients we can use the same argument as above to obtain a discretized differential operator (differentiation matrix)

$$L = A_{\mathcal{L}} A^{-1}, \tag{6}$$

where the matrix $A_{\mathcal{L}}$ has entries $A_{\mathcal{L},ij} = \mathcal{L}\phi_j(x_i)$. In the case of radial basis functions these entries are of the form $A_{\mathcal{L},ij} = \mathcal{L}\Phi(\|x - x_j\|)|_{x=x_i}$.

In the context of spectral methods the differentiation matrix L can now be used to solve all kinds of PDEs (time-dependent as well as time-independent). Sometimes only multiplication by L is required (e.g., for many time-stepping algorithms), and for other problems one needs to be able to invert L. In the standard PS case it is known that the Chebyshev differentiation matrix has an N-fold zero eigenvalue (see [1], p.70), and thus is not invertible by itself. However, once boundary conditions are taken into consideration the situation changes (see, e.g., [12], p.67).

A linear elliptic PDE problem

$$\mathcal{L}u = f \quad \text{in } \Omega$$

with Dirichlet boundary condition

$$u = g \quad \text{on } \Gamma = \partial\Omega$$

can be solved using spectral methods. If the basis functions do not already satisfy the boundary conditions (see, e.g., [12], Program 36) one starts with the differentiation matrix L based on all grid points x_i, and then replaces the diagonal entries corresponding to boundary points with ones and the remainder of those rows with zeros. This corresponds to enforcing the boundary condition $u = g$ explicitly.

By reordering the rows and columns of the resulting matrix we obtain a block matrix of the form

$$L_\Gamma = \begin{bmatrix} M & P \\ 0 & I \end{bmatrix}, \tag{7}$$

where the non-zero blocks M and I are of size $(N - N_B) \times (N - N_B)$ and $N_B \times N_B$, respectively, and N_B denotes the number of grid points on the boundary Γ.

The solution of the PDE with boundary conditions on the grid is then given by the solution of the block linear system

$$L_\Gamma \boldsymbol{u} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}, \tag{8}$$

where the vectors $\boldsymbol{f}$ and $\boldsymbol{g}$ collect the values of f and g at the respective grid points.

We can decompose the vector of grid values of the solution into $\boldsymbol{u} = [\boldsymbol{u}_\Omega, \boldsymbol{u}_\Gamma]^T$, where $\boldsymbol{u}_\Omega$ collects the values in the interior of the domain Ω and $\boldsymbol{u}_\Gamma$ collects the values on the boundary. Solving (8) for $\boldsymbol{u}_\Gamma = \boldsymbol{g}$ and substituting this back in we obtain

$$\boldsymbol{u}_\Omega = M^{-1}(\boldsymbol{f} - P\boldsymbol{g}),$$

or, for homogeneous boundary conditions,

$$\boldsymbol{u}_\Omega = M^{-1}\boldsymbol{f}.$$

We now see that we need to be able to decide whether the matrix M is invertible. In the case of Chebyshev polynomial basis functions and the second-derivative operator $\frac{d^2}{dx^2}$ coupled with different types of boundary conditions this question has been answered affirmatively by Gottlieb and Lustman ([5], or, e.g., Section 11.4 of [1]). Program 15 of [12] also provides a discussion and an illustration of one such problem.

For the non-symmetric RBF collocation approach (Kansa's method, see [8]) we also use the spectral expansion (1). If the approximate solution is evaluated on

the grid of collocation points, then this corresponds to the discretized differential operator

$$L_\Gamma = \begin{bmatrix} \tilde{A}_{\mathcal{L}} \\ \tilde{A} \end{bmatrix} A^{-1} \tag{9}$$

with the (rectangular) matrices $\tilde{A}_{\mathcal{L}}$ and $\tilde{A}$ being of the form

$$\tilde{A}_{\mathcal{L},ij} = \mathcal{L}\phi_j(x_i) = \mathcal{L}\Phi(\|x - x_j\|)|_{x=x_i}, \quad i = 1, \ldots, N - N_B,\ j = 1, \ldots, N,$$
$$\tilde{A}_{ij} = \phi_j(x_i) = \Phi(\|x_i - x_j\|), \quad i = N - N_B + 1, \ldots, N,\ j = 1, \ldots, N.$$

A much more detailed discussion of the connection between RBF collocation and PS methods is given in [3].

A drawback of Kansa's method is the fact that it is known that certain grids do not allow invertibility of the system matrix in (9) (see, e.g., the counterexamples in [7]). This implies that we can safely use the non-symmetric RBF pseudospectral approach whenever inversion of the discretized differential operator is not required (e.g., in the context of explicit time-stepping for parabolic PDEs), but have to be careful when using a non-symmetric RBF PS approach for elliptic problems or parabolic problems with implicit time-stepping.

3 Numerical experiments

In this section we illustrate how the RBF pseudospectral approach can be applied in a way completely analogous to standard polynomial pseudospectral methods. Our numerical illustrations consist of two examples taken directly from the book [12] by Trefethen (see Programs 35 and 36 there).

3.1 Example: Allen-Cahn equation

First, we illustrate the solution of a nonlinear reaction-diffusion equation. To be specific we adapt Program 35 of [12] involving the nonlinear Allen-Cahn equation

$$u_t = \mu u_{xx} + u - u^3, \qquad x \in (-1, 1),\ t \geq 0,$$

with parameter μ, initial condition

$$u(x, 0) = 0.53x + 0.47 \sin\left(-\frac{3}{2}\pi x\right), \qquad x \in [-1, 1],$$

and non-homogeneous (time-dependent) boundary conditions $u(-1, t) = -1$ and $u(1, t) = \sin^2(t/5)$. This equation has three steady solutions ($u = -1, 0, 1$) with the two nonzero solutions being stable. The transition between these states is governed by the parameter μ. In our calculations below we use $\mu = 0.01$, and the unstable state should vanish around $t = 30$. Sample Matlab code to solve this problem using an explicit Euler discretization for the time-derivative and a Chebyshev pseudospectral differentiation matrix for the spatial derivative is listed on page 141 of [12].

Essentially, one needs only to form the differentiation matrix for the second spatial derivative (which can be taken as the square of the first derivative matrix, i.e., $D2 = D^2$) and use this within the time-stepping method that incorporates the nonlinearity of the problem.

We can apply the code from [12] almost verbatim for radial basis functions. In [12] the differentiation matrix is obtained by a call to the subroutine `cheb.m` which yields the matrix D for the discretization of the first derivative operation on the Chebyshev points. The only difference is to replace this by a call to a subroutine `DRBF.m` that generates the RBF differentiation matrix $D = A_{\mathcal{L}}A^{-1}$ as explained earlier (see (6)). This can be very easily done by explicitly setting up a first derivative matrix $A_{\mathcal{L}}$ and an evaluation matrix (i.e., interpolation matrix) A and computing its inverse. Note that the majority of the matrix computations are required only once outside the time-stepping procedure. Inside the time-stepping loop we only require matrix-vector multiplication. We point out that this approach is much more efficient than computation of RBF expansion coefficients at every time step (as suggested, e.g., in [6]).

In Figures 1 and 2, respectively, we show the solution obtained via the Chebyshev pseudospectral method and via an RBF pseudospectral approach based on the Matérn function (3) with $\varepsilon = 2.0$. These computations were based on $N = 20$ Chebyshev points in $[-1, 1]$. The solution based on Chebyshev polynomials is slightly more accurate since the transition occurs at the correct time (i.e., at $t \approx 30$) and is a little "sharper".

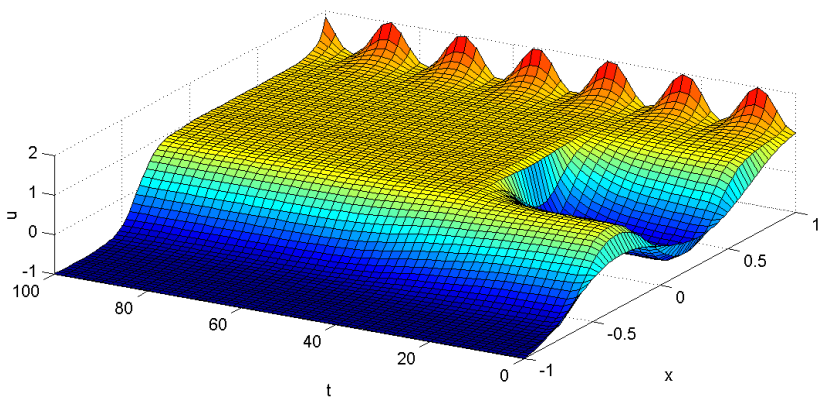

Figure 1: Solution of the Allen-Cahn equation using the Chebyshev pseudospectral method ($N = 20$).

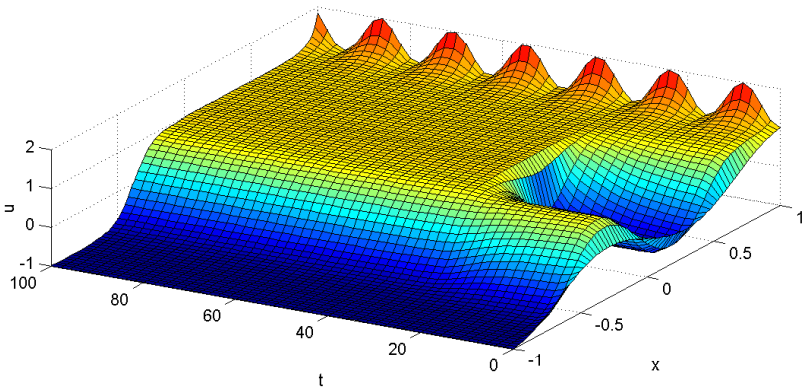

Figure 2: Solution of the Allen-Cahn equation using the Matérn RBF ($N = 20$).

3.2 Example: 2-D Laplace equation

Our second example is an elliptic equation. For such a problem inversion of the differentiation matrix is required. Even though this may not be warranted theoretically, we compare an RBF pseudospectral method based on the non-symmetric Kansa *Ansatz* with a Chebyshev pseudospectral method. As in the previous example, the Matérn RBF (3) is used (this time with $\varepsilon = 2.4$), and the (inverse of the) differentiation matrix is computed using standard Matlab routines.

We consider the 2-D Laplace equation

$$u_{xx} + u_{yy} = 0, \quad x, y \in (-1, 1)^2,$$

with boundary conditions

$$u(x, y) = \begin{cases} \sin^4(\pi x), & y = 1 \text{ and } -1 < x < 0, \\ \frac{1}{5}\sin(3\pi y), & x = 1, \\ 0, & \text{otherwise.} \end{cases}$$

This is the same problem as used in Program 36 of [12].

Figure 3 shows the solution obtained via the RBF PS method. Now the spatial discretization consists of a tensor product of $N = 24 \times 24$ Chebyshev points. The qualitative behavior of the RBF solution is very similar to that of the Chebyshev PS method (for a nearly identical graph see Output 36 on page 142 of [12]).

While there is no advantage in going to arbitrarily irregular grid points for any of the problems presented here, there is nothing that prevents us from doing so for

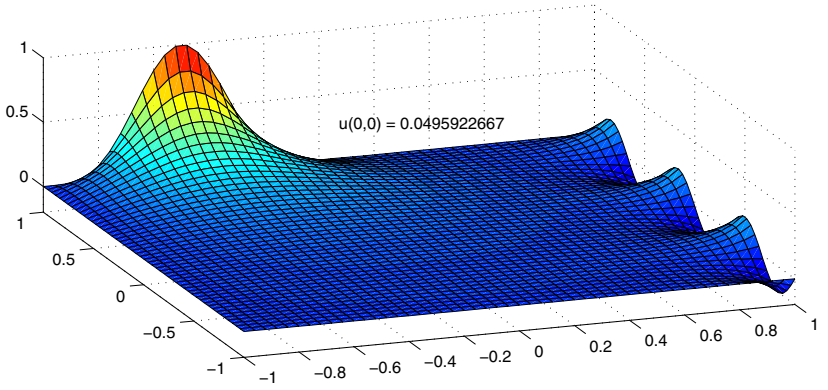

Figure 3: Solution of the Laplace equation using the Matérn RBF ($\varepsilon = 2.4, N = 24 \times 24$).

the RBF approach. In particular, we are not limited to using tensor product grids for higher-dimensional spatial discretizations. This is a potential advantage of the RBF pseudospectral approach over the standard polynomial methods.

4 Summary

In this paper we illustrated a connection between RBF collocation methods and standard (polynomial) pseudospectral methods. Our numerical experiments relied on the fact that for the non-symmetric (Kansa) *Ansatz* we can always formulate the discrete differential operator

$$L_\Gamma = \begin{bmatrix} \tilde{A}_{\mathcal{L}} \\ \tilde{A} \end{bmatrix} A^{-1}.$$

However, we cannot ensure in general the invertibility of L_Γ. This implies that the non-symmetric RBF pseudospectral approach is justified for time-dependent PDEs (with explicit time-stepping methods).

In the RBF literature (see, e.g., [2]) there is also a symmetric collocation *Ansatz*. For that approach we can in general ensure the solution of $\mathcal{L}u = f$. However, it is not possible in general to even formulate the corresponding discrete differential operator (for details see [3]). This suggests that we should use the symmetric approach for time-independent PDEs as well as for time-dependent PDEs with implicit time-stepping.

The theoretical difficulties with both approaches can be attributed to the possible singularity of Kansa's matrix which appears as discretized differential operator for

the non-symmetric approach, and (via its transpose) as the evaluation matrix in the symmetric approach (see [3] for details).

Since the non-symmetric approach is quite a bit easier to implement than the symmetric approach, and since the grid configurations for which the Kansa matrix is singular seem to be very rare (see [7]) many researchers (include ourselves) often prefer to use the non-symmetric approach – even under questionable circumstances (such as with implicit time-stepping procedures, or for elliptic problems). In [3] we discuss a connection to polynomials in the limiting case $\varepsilon = 0$ which justifies this point of view at least for 1-D problems.

Overall, the coupling of RBF collocation and pseudospectral methods obtained here has provided a number of new insights. For example, it should now be clear that we can apply many standard pseudospectral procedures to RBF solvers. However, with RBF expansions we can also take advantage of scattered (multivariate) grids as well as spatial domains with non-rectangular geometries. Thus, we now have "standard" procedures for solving time-dependent PDEs with RBFs.

Future challenges include the problem of dealing with larger problems in an efficient and stable way. Thus, such issues as preconditioning and FFT-type algorithms need to be studied in the context of RBF pseudospectral methods. Some first results in this directions have been reported very recently in [10].

Another possible avenue opened up by the use of RBFs instead of polynomials is the study of pseudospectral methods with moving (adaptive) grids. This will be computationally much more involved, but the use of RBFs should imply that there is no major restriction imposed by moving (scattered) grids.

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