A UNIFIED FRAMEWORK FOR KERNEL AND POLYNOMIAL APPROXIMATION*

MILENA BELIANOVICH†, AKIL NARAYAN‡, GREGORY FASSHAUER§, AND VARUN SHANKAR¶

Abstract.

Key words. Radial basis function; polynomial; pseudospectral; high-order method.

AMS subject classifications. 68Q25, 68U05

1. Introduction.

Radial Basis Functions (RBFs) are a powerful and flexible tool for generating numerical methods for the solution of partial differential equations (PDEs). RBF collocation methods are easily applied to solving PDEs on irregular domains using scattered node layouts [3, 4, 21]. RBF-based methods also generalize naturally to the solution of PDEs on manifolds $\mathbb{M} \subset \mathbb{R}^3$ using only the Euclidean distance measure in the embedding space and Cartesian coordinates; see for example [1, 8–11, 13–16, 18–20].

The remainder of this paper is organized as follows.

2. Review.

3. Unified interpolation with kernels and polynomials.

We will now present a unified framework for kernel and polynomial approximation. Consider the hybrid *interpolant* given by:

$$s(\boldsymbol{x}) = \sum_{k=1}^{N} c_k \phi\left(\varepsilon \|\boldsymbol{x} - \boldsymbol{x}_k\|\right) + \sum_{j=1}^{\binom{\ell+d}{d}} d_j p_j(\boldsymbol{x}), \tag{1}$$

where ϕ is an RBF and ε its shape parameter, and the p_j functions form a basis for the space of total degree polynomials of degree ℓ in d dimensions. As mentioned previously, while it is traditional to use conditionally positive-definite kernels with global support as choices for ϕ, we now assume ϕ is a *compactly-supported* and *positive-definite* RBF. While there are many such RBFs [?, ?, ?, ?], we focus on the Wendland functions given by:

$$\phi_{m,n}(r) = \begin{cases} \frac{1}{\Gamma(n)2^{n-1}} \int\limits_{r}^{1} s(1-s)^m (s^2 - r^2)^{n-1} ds & \text{for } 0 \le r \le 1, \\ 0 & \text{for } r > 1. \end{cases} \tag{2}$$

For the Wendland functions, the shape parameter ε serves as the reciprocal of the radius of support r. Unfortunately, these RBFs have historically traded off increased sparsity (and improved conditioning) in the interpolation matrix for decreased accuracy and convergence rates [5]. Recent work has shown [2, 6, 7, 17, 19] that this decrease in accuracy can be overcome by augmenting the RBF interpolant with polynomials. However, thus far, to the best of our knowledge, the only RBFs used have been those with global support, such as the positive-definite Gaussian RBF and the conditionally positive-definite polyharmonic splines. Our goal in this work is to both demonstrate that this technique works in the context of Wendland RBFs, and to demonstrate that the use of compactly-supported RBFs creates a highly general and flexible unified framework for kernel and polynomial approximation.

To that end, we shall now present and discuss several special cases of the above interpolation scheme. We will also discuss efficient solution of the resulting linear systems for each of the limiting cases. In the following

*Submitted to the editors 08/01/2019.

†Kahlert School of Computing, University of Utah, Salt Lake City, UT USA (shankar@cs.utah.edu)

‡Department of Mathematics, and Scientific Computing and Imaging (SCI) Institute, University of Utah, Salt Lake City, UT USA (akil@sci.utah.edu).

§Department of Applied Mathematics and Statistics, Colorado School of Mines, Golden CO USA (fasshauer@mines.edu).

¶Kahlert School of Computing, University of Utah, Salt Lake City, UT USA (shankar@cs.utah.edu). Corresponding author.

discussion, let $X = \{\boldsymbol{x}_k\}_{k=1}^N$ be the set of data sites for interpolation. Further, let q be the smallest pairwise distance between of nodes in X, and w be the largest pairwise distance. Finally, let $r = 1/\varepsilon$ be the support of the Wendland RBF.

3.1. The polynomial limit ($r < q$).

3.1.1. Interpolation. When the support r of any Wendland RBF is made smaller than q, the Wendland RBFs each take on the value of 1 at the nodes and 0 elsewhere, with transitions between the nodes dictated by the smoothness of the Wendland RBF. Thus, the interpolation constraints (**??**) lead to the following linear system:

$$\begin{bmatrix} I & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \mathbf{0} \end{bmatrix}, \tag{3}$$

where I is the $N \times N$ identity matrix and P is the Vandermonde-like matrix of evaluations of the polynomial basis at the interpolation nodes. To better understand this linear system, we use block Gaussian elimination to rewrite this as two equations:

$$P^T P\mathbf{d} = P^T \boldsymbol{f}, \tag{4}$$

$$\boldsymbol{c} = \boldsymbol{f} - P\mathbf{d}. \tag{5}$$

The first system of equations is immediately recognizable as the system of normal equations arising from the least squares problem of minimizing $\|P\mathbf{d} - \boldsymbol{f}\|_2^2$. Thus, in this context, despite the presence of RBFs in the approximation, the polynomial coefficients $\mathbf{d}$ are identical to the coefficients obtained from the least-squares problem. Clearly, the RBF coefficients $\boldsymbol{c}$ only serve to enforce interpolation at the collocation nodes.

3.1.2. Linear Algebra. In the polynomial limit, the unified interpolant (1) can be computed efficiently using the QR decomposition as follows:

1. Compute $P = QR$, the (reduced) QR decomposition of the polynomial least-squares matrix P.
2. Solve the Schur complement system for the polynomial coefficients $\mathbf{d}$ as $\mathbf{d} = R^{-1}Q^T\boldsymbol{f}$.
3. Compute the RBF coefficients $\boldsymbol{c} = \boldsymbol{f} - P\mathbf{d}$.

The SVD could also be used to find $\mathbf{d}$. When solved in this fashion, the block system (3) does not need to be explicitly computed or stored, nor do we need to compute the matrix P^T. This approach can be applied with a small modification if P is rank-deficient also: column pivoting can be used for the QR decomposition, and truncation of the singular values can be used for the SVD.

3.1.3. Evaluation. Once the coefficients $\boldsymbol{c}$ and $\mathbf{d}$ are computed, the interpolant (1) can be evaluated anywhere. Let $X_e = \{\boldsymbol{x}_i^e\}_{i=1}^{N_e}$ be a set of *evaluation points.* Then, the interpolant can be evaluated at X_e as:

$$s(\boldsymbol{x})|_{X_e} = \begin{bmatrix} A_e & P_e \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \mathbf{d} \end{bmatrix} = A_e\boldsymbol{c} + P_e\mathbf{d}, \tag{6}$$

where A_e and P_e are evaluations of the RBF and polynomial basis functions at X_e. In general, A_e is a sparse matrix if Wendland RBFs are used, and its structure is determined by the smoothness of the Wendland RBF, the precise value of ϵ (and therefore r), and the number of evaluation points N_e.

3.2. Hybrid approximation ($q < r$) .

3.2.1. Interpolation. If $r > q$ (or conversely ϵ is sufficiently small), the constraints (**??**) can no longer be represented by (3). Instead, they now correspond to a similar block linear system with I replaced by a sparse matrix A with entries $A_{ij} = \phi\left(\|\boldsymbol{x}_i - \boldsymbol{x}_j\|\right)$:

$$\begin{bmatrix} A & P \\ P^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \mathbf{0} \end{bmatrix}. \tag{7}$$

Once again, we may use block Gaussian elimination to rewrite this as

$$P^T A^{-1} P\mathbf{d} = P^T A^{-1}\boldsymbol{f}, \tag{8}$$

$$A\boldsymbol{c} = \boldsymbol{f} - P\mathbf{d}, \tag{9}$$

where now A^{-1} appears in the equation for $\mathbf{d}$, and finding $\boldsymbol{c}$ requires the inversion of a sparse matrix A. The exact properties of this approximation depend on the value of r, the smoothness of the Wendland kernel, and the polynomial degree ℓ. However, unlike in the polynomial limit $r < q$, both the RBFs and the polynomials participate in the approximation.

3.2.2. Linear Algebra. Unlike in the polynomial limit, it is not possible to solve the above pair of equations for $\mathbf{d}$ and $\boldsymbol{c}$ using a single QR decomposition of the matrix P. This leaves actually inverting the matrix $P^T A^{-1} P$. Unfortunately, this is a non-trivial task. The condition number of A can range from $O(1)$ in the case of a small support r to arbitrarily large for large r. Further, we have observed that the matrix $P^T P$ is typically very ill-conditioned since it is formed by evaluations of polynomials at a possibly arbitrary set of collocation points. In addition, though the matrix $P^T A^{-1} P$ is symmetric positive definite in exact arithmetic (since A^{-1} is symmetric positive-definite), we have observed that the product $P^T A^{-1} P$ loses symmetry due to rounding errors even when A has a condition number of $O(1)$. Fortunately, we have found that the symmetry of $P^T A^{-1} P$ can be restored using standard numerical linear algebra. Since A is symmetric positive-definite, it can be written in terms of its Cholesky decomposition as

$$A = LL^T, \tag{10}$$

where L is a lower-triangular matrix. If A is sparse, it is also possible to maintain sparsity in L. Using this decomposition, we can rewrite the Schur complement system as:

$$P^T \left(LL^T\right)^{-1} P\mathbf{d} = P^T \left(LL^T\right)^{-1} \boldsymbol{f}, \tag{11}$$

$$\implies P^T L^{-T} \underbrace{L^{-1} P}_{B} \mathbf{d} = P^T L^{-T} \underbrace{L^{-1} \boldsymbol{f}}_{\mathbf{g}}, \tag{12}$$

$$\implies B^T B\mathbf{d} = B^T \mathbf{g}, \tag{13}$$

where $B = L^{-1} P$. This is in fact a system of normal equations for $\mathbf{d}$. To solve this, we can clearly decompose B as $B = QR$, and compute the polynomial coefficients as $\mathbf{d} = R^{-1} Q^T \mathbf{g}$. Of course, the cost also includes inverting the sparse lower-triangular matrix L. Nevertheless, this approach ensures that $P^T A^{-1} P$ is symmetric while also transforming the problem into one solvable by the QR decomposition. Finally, the RBF coefficients $\boldsymbol{c}$ can be computed as

$$\boldsymbol{c} = L^{-T} L^{-1} \left(\boldsymbol{f} - P\mathbf{d}\right) \tag{14}$$

4. Results.

5. Summary and Future Work.

Acknowledgments. VS was supported by

REFERENCES

[1] K. A. Aiton, *A Radial Basis Function Partition of Unity Method for Transport on the Sphere*, master's thesis, Boise State University, USA, 2014.

[2] V. Bayona, N. Flyer, B. Fornberg, and G. A. Barnett, *On the role of polynomials in rbf-fd approximations: Ii. numerical solution of elliptic pdes*, Journal of Computational Physics, 332 (2017), pp. 257 – 273.

[3] V. Bayona, M. Moscoso, M. Carretero, and M. Kindelan, *RBF-FD formulas and convergence properties*, J. Comput. Phys., 229 (2010), pp. 8281–8295.

[4] O. Davydov and D. T. Oanh, *Adaptive meshless centres and RBF stencils for poisson equation*, J. Comput. Phys., 230 (2011), pp. 287–304.

[5] G. E. Fasshauer, *Meshfree Approximation Methods with MATLAB*, Interdisciplinary Mathematical Sciences - Vol. 6, World Scientific Publishers, Singapore, 2007.

[6] N. Flyer, G. A. Barnett, and L. J. Wicker, *Enhancing finite differences with radial basis functions: Experiments on the Navier-Stokes equations*, J. Comput. Phys., 316 (2016), pp. 39–62.

[7] N. Flyer, B. Fornberg, V. Bayona, and G. A. Barnett, *On the role of polynomials in RBF-FD approximations: I. Interpolation and accuracy*, J. Comput. Phys., 321 (2016), pp. 21–38.

[8] N. Flyer, E. Lehto, S. Blaise, G. B. Wright, and A. St-Cyr, *A guide to RBF-generated finite differences for nonlinear transport: shallow water simulations on a sphere*, J. Comput. Phys., 231 (2012), pp. 4078–4095.

[9] N. Flyer and G. B. Wright, *Transport schemes on a sphere using radial basis functions*, J. Comput. Phys., 226 (2007), pp. 1059–1084.
[10] N. Flyer and G. B. Wright, *A radial basis function method for the shallow water equations on a sphere*, Proc. Roy. Soc. A, 465 (2009), pp. 1949–1976.
[11] B. Fornberg and E. Lehto, *Stabilization of RBF-generated finite difference methods for convective PDEs*, J. Comput. Phys., 230 (2011), pp. 2270–2285.
[12] E. J. Fuselier and G. B. Wright, *A high-order kernel method for diffusion and reaction-diffusion equations on surfaces*, J. Sci. Comput., 56 (2013), pp. 535–565.
[13] E. Lehto, V. Shankar, and G. B. Wright, *A radial basis function (rbf) compact finite difference (fd) scheme for reaction-diffusion equations on surfaces*, SIAM Journal on Scientific Computing, 39 (2017), pp. A2129–A2151.
[14] C. Piret, *The orthogonal gradients method: A radial basis functions method for solving partial differential equations on arbitrary surfaces*, J. Comput. Phys., 231 (2012), pp. 4662–4675.
[15] C. Piret and J. Dunn, *Fast rbf ogr for solving pdes on arbitrary surfaces*, AIP Conference Proceedings, 1776 (2016).
[16] V. Shankar and A. L. Fogelson, *Hyperviscosity-based stabilization for radial basis function-finite difference (RBF-FD) discretizations of advection-diffusion equations*, J. Comput. Physics, 372 (2018), pp. 616–639.
[17] V. Shankar, A. Narayan, and R. M. Kirby, *RBF-LOI: augmenting radial basis functions (rbfs) with least orthogonal interpolation (LOI) for solving pdes on surfaces*, J. Comput. Physics, 373 (2018), pp. 722–735.
[18] V. Shankar and G. B. Wright, *Mesh-free semi-lagrangian methods for transport on a sphere using radial basis functions*, J. Comput. Phys., 366 (2018), pp. 170–190.
[19] V. Shankar, G. B. Wright, R. M. Kirby, and A. L. Fogelson, *A radial basis function (RBF)-finite difference (FD) method for diffusion and reaction–diffusion equations on surfaces*, J. Sci. Comput., 63 (2014), pp. 745–768.
[20] G. B. Wright and B. Fornberg, *Scattered node compact finite difference-type formulas generated from radial basis functions*, J. Comput. Phys., 212 (2006), pp. 99–123.