A Numerical Mercer Method for Radial Basis Function Interpolation

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Introduction

Radial basis function (RBF) methods have been used successfully for a variety of interpolation problems as well as problems involving partial differential equations on complex domains. A radial basis function is a function of the distance between two points. The class of radial basis functions we will consider also accepts as an argument a positive value ε called the shape parameter. RBF methods are theoretically most accurate when ε is small, but the direct implementation suffers from an ill-conditioned linear system for small ε, which significantly reduces accuracy. In recent years, a few methods have been devised which attempt to bypass this ill-conditioned linear system.

Mercer Method

A common approach to solve this ill-conditioning problem is to perform the interpolation in an alternate manner which results in a well-conditioned linear system. One recent method uses the fact that an RBF may be viewed as a symmetric positive-definite kernel $K(x, y)$ for an integral operator

$$T[f] = \int_a^b K(x, y) f(x) \mathrm{d}x$$

on the space $L^2[a, b]$ of square-integrable functions. By Mercer's Theorem, this symmetric positive-definite kernel may be represented as an infinite series

$$K(x, y) = \sum_{n=1}^{\infty} \lambda_n \varphi_n(x) \varphi_n(y),$$

where λ_n is the n^{th} eigenvalue and φ_n is the n^{th} normalized eigenfunction of the associated integral operator T. Furthermore, the eigenvalues are positive and converge to zero as $n \to \infty$. [1]

Numerical Mercer Expansion

The Mercer method uses only RBFs with known Mercer series expansions, which does not include common RBFs such as the multiquadric RBF $K(x, y) = \sqrt{1 + \varepsilon^2 \|x - y\|^2}$ and the inverse quadratic RBF $K(x, y) = \frac{1}{1+\varepsilon^2 \|x-y\|^2}$. However, a numerical Mercer expansion may be obtained by the following process:

1. Given one-dimensional interpolation points $\{x_n\}_{n=1}^N$, choose M, the number of eigenvalues and eigenfunctions to use in the approximate Mercer expansion, with $M \geq N$.
2. For the Legendre-Gauss points $\{y_m\}_{m=1}^M$ on $[x_0, x_N]$, form the $M \times M$ matrix B with $B_{i,j} = K(y_i, y_j)$, $1 \leq i, j \leq M$.
3. Solve the eigensystem $B\mathbf{u}_m = \lambda_m^* \mathbf{u}_m$ for the matrix eigenvalues λ_m^* and the matrix eigenvectors $\mathbf{u}_m$, and normalize each $\mathbf{u}_m$.
4. Approximate the kernel eigenvalues λ_m as $\lambda_m \approx \frac{\lambda_m^*}{M}$ for $1 \leq m \leq M$.
5. Approximate the kernel eigenfunctions as $\varphi_i(y_j) \approx \sqrt{M}(\mathbf{u}_i)_j$ for $1 \leq i, j \leq M$.
6. The Nyström method gives the approximate value of the m^{th} eigenfunction at any value y as
$$\varphi_m(y) \approx \frac{\sqrt{M}}{\lambda_m^*} \mathbf{k}(y)^T \mathbf{u}_m,$$
where $\mathbf{k}(y)^T = (K(y_1, y), \ldots, K(y_M, y))$. [2]
7. Using the approximate values of the eigenfunctions at the interpolation points, we may factor the $N \times N$ matrix B with $B_{i,j} = K(x_i, x_j)$ as $B = \Phi \Lambda \Phi^T$, where $\Phi_{i,j} = \varphi_j(x_i)$, $1 \leq i \leq N$, $1 \leq j \leq M$, and $\Lambda_{i,i} = \lambda_i$, $1 \leq i \leq M$.

Results

After factoring the system matrix as $B = \Phi \Lambda \Phi^T$, the interpolation problem may be solved using the QR method as outlined in [1]. Below are the results for interpolating the function $f(x) = \mathrm{e}^{\sin(\pi x)}$ on the interval $[0, 1]$ with $N = 25$ uniformly spaced interpolation points and $N_e = 50$ uniformly spaced evaluation points using the inverse quadratic RBF with varying shape parameter. The parameter M is set at $M = N$, and the eigensystem in the numerical Mercer expansion is solved in quad precision.

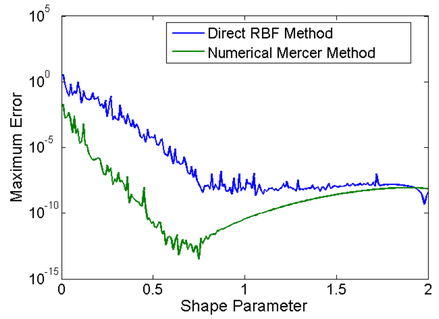

Figure 1: Maximum interpolation error versus shape parameter ε. The maximum error is decreasing until approximately $\varepsilon = 0.8$, at which point the method becomes unstable and the maximum error begins to increase. The numerical Mercer method outperforms the direct RBF method when implemented in double precision (besides the eigensystem solution) in this example.

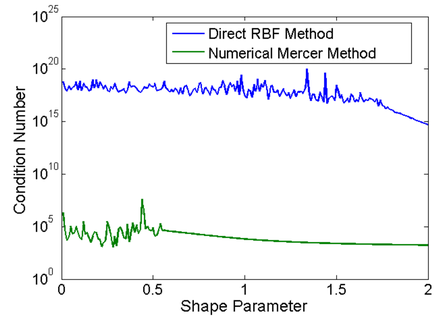

Figure 2: Condition number of the new system matrix versus shape parameter ε. Compared to the direct RBF method, the condition number for the numerical Mercer method remains relatively constant when the method is stable. For $\varepsilon = 0.5$, the condition number for the direct RBF method is actually above 10^{35}, so the numerical Mercer method succeeds in significantly improving conditioning.

Conclusion

From Figures 1 and 2, we see that the numerical Mercer method is effective at reducing the condition number of the linear system, but it fails to reduce the maximum error for all values of the shape parameter. The reason for the method's success in improving the conditioning is that the ill-conditioning is contained in the eigenvalues, and the QR method is able to bypass that ill-conditioning. However, isolating the ill-conditioning in the eigenvalues leads to a problem in the numerical Mercer expansion itself. The eigenvalues decay geometrically, and the rate of decay is greater for small ε, so the eigenvalues quickly become too small to be accurately approximated with double or quad precision. As a result, the eigenfunctions are not approximated in a stable manner and significant error is introduced. The only remedy for this problem is to implement the eigensystem solution in higher precision.

References

[1] G. E. Fasshauer and M. McCourt. Stable evaluation of Gaussian RBF interpolants. *SIAM J. Sci. Comput.*, 34(2):A737–A762, 2012.

[2] C. E. Rasmussen and C. K. I. Williams. *Gaussian Processes for Machine Learning*. MIT Press, 2006.

Future Research

Despite its failure to obtain stability for all values of ε, the numerical Mercer method in higher precision may be used to study the eigenfunctions of important radial basis functions for which the Mercer expansion is not known analytically. Other future research includes quantifying the relationship between the shape parameter and the eigenvalue rate of decay in an effort to estimate the amount of precision required to approximate the Mercer expansion for a given radial basis function.

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