RBFs Over Near-Flat Surfaces

APPM 5480 Asymptotics

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Introduction/Background

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Radial Basis Functions

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Type of basis function	Radial function $\phi(r)$
Gaussian (GA)	$e^{-(\varepsilon r)^2}$
Multiquadric(MQ)	$\sqrt{1+(\varepsilon r)^2}$
Inverse Multiquadric (IMQ)	$1/\sqrt{1+(\varepsilon r)^2}$
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$$S(\mathbf{x}) = \sum_{i=1}^{n} \lambda_{i} \phi_{\varepsilon}(\|\mathbf{x} - \mathbf{x}_{i}\|)$$

where λ_i can be found by solving

$$\underbrace{\begin{pmatrix} \phi_{\varepsilon}(\|\mathbf{x}_{1} - \mathbf{x}_{1}\|) & \phi_{\varepsilon}(\|\mathbf{x}_{1} - \mathbf{x}_{2}\|) & \cdots & \phi_{\varepsilon}(\|\mathbf{x}_{1} - \mathbf{x}_{n}\|) \\ \phi_{\varepsilon}(\|\mathbf{x}_{2} - \mathbf{x}_{1}\|) & \phi_{\varepsilon}(\|\mathbf{x}_{2} - \mathbf{x}_{2}\|) & \cdots & \phi_{\varepsilon}(\|\mathbf{x}_{2} - \mathbf{x}_{n}\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_{\varepsilon}(\|\mathbf{x}_{n} - \mathbf{x}_{1}\|) & \phi_{\varepsilon}(\|\mathbf{x}_{n} - \mathbf{x}_{2}\|) & \cdots & \phi_{\varepsilon}(\|\mathbf{x}_{n} - \mathbf{x}_{n}\|) \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} \lambda_{1} \\ \lambda_{2} \\ \vdots \\ \lambda_{n} \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} f_{1} \\ f_{2} \\ \vdots \\ f_{n} \end{pmatrix}}_{F}.$$

Introduction/Background

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RBF Contour Padé (RBF-CP) (precursor to RBF-RA)

RBF Rational Approximations (RBF-RA) (circa 2017) [3]

RBF-RA issues

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However, RBF-RA breaks down when the data is on a near-flat surface (i.e. surface with small curvature).

So, we would like understand/explore why RBF-RA breaks on near flat surfaces.

Enter Asymptotics!

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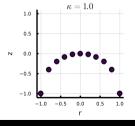
A perturbation problem

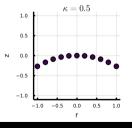
Suppose we have the pairs of points $\{(x_i, y_i)\}_{i=1}^n$ in the *unit disk*. Then, define our interpolation nodes as

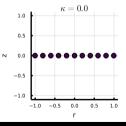
$$\mathbf{x}_i = \left\langle x_i, y_i, \sqrt{\frac{1}{\kappa^2} - r_i^2} - \frac{1}{\kappa} \right\rangle, \quad r_i = \sqrt{x_i^2 + y_i^2}.$$

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Then, the difference between two nodes is given as

$$\|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + \left(\sqrt{\frac{1}{\kappa^2} - r_i^2} - \sqrt{\frac{1}{\kappa^2} - r_j^2}\right)^2$$

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Further, each entry of the collocation matrix A will be

$$A_{ij} = \phi_{\varepsilon}(\|\mathbf{x}_i - \mathbf{x}_j\|_2) = e^{-(\varepsilon\|\mathbf{x}_i - \mathbf{x}_j\|_2)^2} = e^{-\varepsilon^2\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}$$

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$$= e^{-\varepsilon^{2}\left((x_{i} - x_{j})^{2} + (y_{i} - y_{j})^{2} + \left(\sqrt{\frac{1}{\kappa^{2}} - r_{i}^{2}} - \sqrt{\frac{1}{\kappa^{2}} - r_{j}^{2}}\right)^{2}\right)}$$

$$= e^{-\varepsilon^{2}\left((x_{i} - x_{j})^{2} + (y_{i} - y_{j})^{2}\right)} e^{-\varepsilon^{2}\left(\sqrt{\frac{1}{\kappa^{2}} - r_{i}^{2}} - \sqrt{\frac{1}{\kappa^{2}} - r_{j}^{2}}\right)^{2}}$$

$$= e^{-\varepsilon^{2}\left((x_{i} - x_{j})^{2} + (y_{i} - y_{j})^{2}\right)} \left(1 - \frac{1}{4}\varepsilon^{2}\kappa^{2}(r_{i}^{2} - r_{j}^{2})^{2} + \cdots\right)$$

$$= e^{-\varepsilon^{2}\left((x_{i} - x_{j})^{2} + (y_{i} - y_{j})^{2}\right)} - \kappa^{2}\frac{1}{4}\varepsilon^{2}(r_{i}^{2} - r_{j}^{2})^{2}e^{-\varepsilon^{2}\left((x_{i} - x_{j})^{2} + (y_{i} - y_{j})^{2}\right)} + \mathcal{O}(\kappa^{4}).$$

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$$A = A_{0} + \kappa^{2}A_{1} + \mathcal{O}(\kappa^{4})$$

With the expansion of A

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our perturbed interpolant problem is then given by

$$A\lambda = F \implies (A_0 + \kappa^2 A_1 + \cdots)\lambda = F, \quad 0 < \kappa \ll 1.$$

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Note, A_0 is just the standard collocation matrix if our data was on a flat surface. We know

 A_0 is nonsingular for $\varepsilon \in \mathbb{R}, \varepsilon \neq 0$.

 A_0 is symmetric [1].

RBF-RA is able to stably work with A_0 .

Enter Asymptotics!

Perturbed solution

Perturbed interpolation weights problem

$$(A_0 + \kappa^2 A_1 + \cdots) \lambda = \mathbf{F}, \quad 0 < \kappa \ll 1$$

Assume λ has the regular expansion

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}_0 + \kappa^2 \boldsymbol{\lambda}_1 + \cdots.$$

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$$\mathcal{O}(1): A_0 \boldsymbol{\lambda}_0 = \boldsymbol{F} \implies \boldsymbol{\lambda}_0 = A_0^{-1} \boldsymbol{F}$$

$$\mathcal{O}(\kappa^2): A_0 \boldsymbol{\lambda}_1 + A_1 \boldsymbol{\lambda}_0 = 0 \implies \boldsymbol{\lambda}_1 = -A_0^{-1} A_1 \boldsymbol{\lambda}_0$$

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So in general,

$$\boldsymbol{\lambda}_n = -A_0^{-1}(A_1\boldsymbol{\lambda}_{n-1} + A_2\boldsymbol{\lambda}_{n-2} + \cdots + A_n\boldsymbol{\lambda}_0).$$

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Solution remarks

Putting everything together, our interpolation weights can be written as

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We can use this asymptotic expansion to bypass the small curvature issue in RBF-RA.

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Modified RBF-RA Algorithm

- (a) Compute κ estimate of data using desired algorithm
- (b) Use RBF-RA to stably compute needed λ_i
- (c) Compute λ using $\lambda = \lambda_0 + \kappa^2 \lambda_1 + \cdots$ up to desired term.

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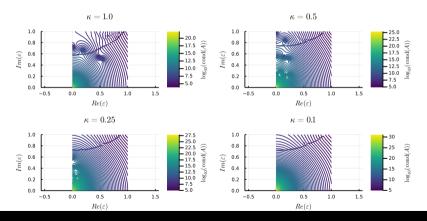
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Patching an algorithm like this is not ideal. Instead, we would like to understand why the algorithm breaks and then fix the algorithm at the fundamental level.

What's Next

A closer look at conditioning

The conditioning of the collocation matrix at various κ and ε in the complex plane can be seen below



A perturbed eigenvalue problem

Using the same perturbed collocation matrix as before, we can pose a perturbed eigenvalue problem as

$$(A_0 + \kappa^2 A_1 + \cdots) \mathbf{x} = \lambda \mathbf{x}.$$

Now, because A depends on arbitrary, real life data, it is reasonable to assume that A has all distinct eigenvalues. So, finding a perturbed eigenvalue/eigenvector solution to this is readily found using our formulas derived early on in our course or in *Hinch* [2]. In this case, the eigenvalues all have regular perturbations

$$\lambda(\varepsilon;\kappa) = \lambda_0(\varepsilon) + \kappa^2 \lambda_2(\varepsilon) + \cdots$$

A perturbed root finding problem

The A matrix is normal and so

$$\operatorname{cond}(A) = \frac{|\lambda_{\mathsf{max}}|}{|\lambda_{\mathsf{min}}|}.$$

So, to understand when the condition number blows up, we want to know when $\lambda(\varepsilon;\kappa)=0$ for any of the eigenvalues λ . So, an interesting perturbed root finding problem is find ε such that

$$\lambda_0(\varepsilon) + \kappa^2 \lambda_2(\varepsilon) + \dots = 0, \quad 0 < \kappa \ll 1.$$

Even for simple node-sets, $\lambda_i(\varepsilon)$ can be very nonlinear making this perturbed root finding problem quite difficult.

References

- [1] B. FORNBERG AND N. FLYER, A primer on radial basis functions with applications to the geosciences, vol. 87 of CBMS-NSF regional conference series in applied mathematics. SIAM, 2015.
- [2] E. J. HINCH, Perturbation Methods, Cambridge Texts in Applied Mathematics. Cambridge University Press. 1991.
- [3] G. B. Wright and B. Fornberg. Stable computations with flat radial basis functions using vector-valued rational approximations, Journal of Computational Physics, 331 (2017), pp. 137–156.

THANK YOU

ANY QUESTIONS?

