The resolution of singularities by rational functions and mesh refinement

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3 March 2025, SIAM CS&E

Outline

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How to model problems with singular solutions?

Two main approaches

1. **Enrich** the approximation space with singular functions
2. **Resolve** the singularity within the approximation space
   - no matter how it is achieved: similar mathematics
   - also leads to new methods

This talk is about the second approach.

First approach: approximation in enriched spaces

Basis + extra functions

- E.g. polynomials + singular functions
- Still a basis? **Redundancy** → **ill-conditioning**
- **well understood** by now from approximation point of view
  - B. Adcock, DH. *Frames and numerical approximation*, SIREV, 2019 [1]
- possible: **stable algorithms**
  - oversampling + regularization → rectangular systems
- possible: **fast algorithms**
  - the AZ algorithm and variants
  - $Ax = b$ where A has block structure
  - like (generalized) Schur complement for rectangular systems
  - A. Herremans, DH. *The AZ algorithm for enriched approximation spaces*, IMAJNA, 2024 [2]

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BUT: need to know the *exact* singularity. Ok in 2D, not in 3D.

Example: 2D Poisson problem on rectangle

Example from: *The AZ algorithm for enriched approximation spaces* [2]

- applied to "Enriched Spectral-Galerkin method" by J. Shen

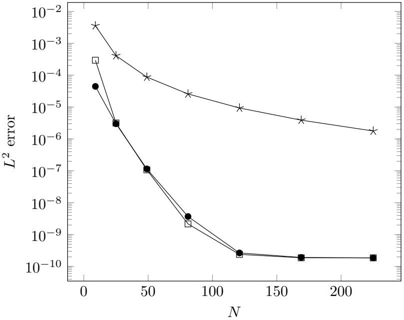
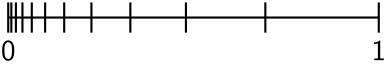


Figure 9: Accuracy of the solution to the 2D Poisson equation in a rectangular domain. Stars: standard Galerkin method without enrichment (i.e. $K = 0$), squares: Galerkin method combined with smoothness constraints (ESG-II) using $K = 1$ and $M_K = 2$, dots: Galerkin method combined with collocation using $K = 1$ and $M_K = 25$. The results for the standard Galerkin method and ESG-II also follow from [6, Fig. 4].

Outline

A model problem for hp-refinement

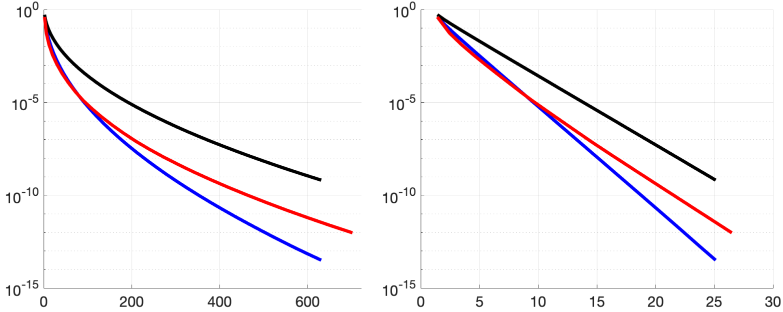
Approximation on $[0,1]$ **with singularity at** 0



- full analysis by Babuska et al, Melenk, Schwab, Devore and Scherer, ... Model problem $f(x) \sim x^\alpha$
- early conclusion: (root-)**exponential convergence** $e^{-c\sqrt{n}}$ (wrt n=ndofs) when using **geometric refinement**
- nodes at η^k for $0 < \eta < k$
- optimal: $\eta = (\sqrt{2}-1)^2 \approx 0.17$ **irrespective of** α
- optimal: p varies with k
  - higher p *further away* from singularity, $p \sim k_{\max} - k$
  - $e^{-d\sqrt{n}}$ possible with p *uniformly large but fixed* ($d = \frac{c}{\sqrt{2}}$)

Numerical illustration

Approximation of $\sqrt{x}$ by piecewise polynomials



- left: plot of **log error versus n**
- right: plot of **log error versus $\sqrt{\mathbf{n}}$**
- BLUE: optimal η. BLACK: $\eta = 0.3$. RED: optimal η, fixed p

Outline

A brief history of the approximation of $|x|$

Approximations of $|x|$ on $[-1,1]$ and $\sqrt{x}$ on $[0,1]$ are equivalent.

Historical developments

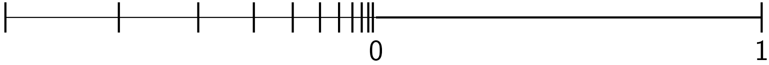
- 1908, de la Vallée-Poussin finds polynomial approximation to $|x|$ with error $O(1/n)$ and asks: is this the best one can do?
- 1912, Bernstein: yes. Mémoire Académie Royale de Belgique.

  La meilleure approximation de $|x|$ *dans l'intervalle* $(-1,+1)$ *par un polynome de degré* $2n > 0$ *est comprise entre* $\frac{\sqrt{2}-1}{4(2n-1)}$ *et* $\frac{2}{\pi(2n+1)}$.
- 1964, Newman: rational approximation with $e^{-c\sqrt{n}}$ accuracy
- 1994, Stahl: study of best rational approximation to $|x|$
- 2018: AAA algorithm for best rational approximants

A. Herremans, DH, L. N. Trefethen, *Resolution of singularities by rational functions*, SINUM, 2023 [3]

Rational approximation to $\sqrt{x}$

Clustering of poles towards 0 (from the left)



- **geometric clustering** of poles: $p_j = -e^{-\sigma j/\sqrt{n}}$
- optimal: *tapered* exponential clustering: $p_j = -e^{-\sigma(\sqrt{n}-\sqrt{j})}$
- stable implementation?
  - use partial fractions with polynomial part:

$$\sqrt{x} \approx \sum_{j=1}^{n_1} a_j \frac{p_j}{z - p_j} + \sum_{j=0}^{n_2} b_j T_j(x)$$

  - compute least squares fit w. oversampling

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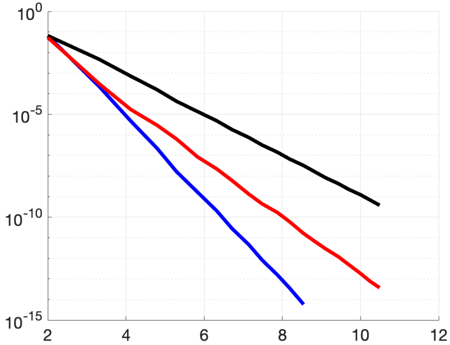
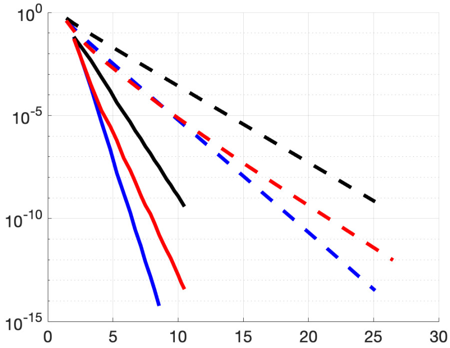


- max-norm error versus $\sqrt{n}$
- BLUE: tapered, optimal $\sigma = \sqrt{8}\pi \approx 8.89$. BLACK: tapered, $\sigma = 0.44$. RED: geometric clustering, optimal σ.

Comparison hp and rational approximations



Convergence rate is $e^{-c\sqrt{n}}$ in both cases, but c differs:

- hp: $c = -\log(\eta)/\sqrt{2} \approx 1.25$
- rat: $c = \sqrt{2}\pi \approx 4.44$
- Best result using $n = 73$ (rat) versus $n = 631$ (hp)

An intermediate observation

Piecewise polynomial approximations are (very) far from optimal when resolving local features.

- sizable difference in 1D
- bigger difference in 2D, 3D, . . . ?

$\Rightarrow$ multivariate rational approximations!

How do rational functions resolve a singularity?

DH, L. N. Trefethen, *Sigmoid functions, multiscale resolution of singularities and hp-mesh refinement*, SIREV, 2024 [4]

Answer: the same way hp-methods (and other schemes) do

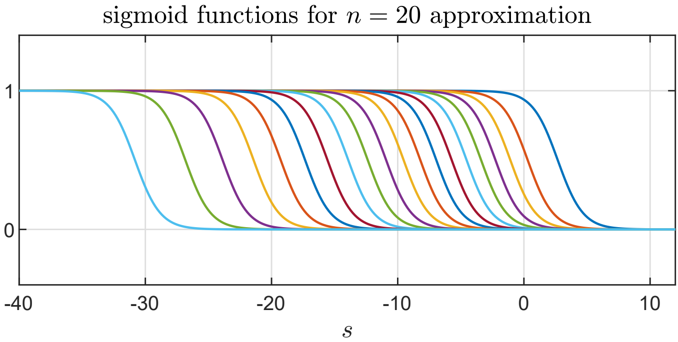
- everything makes sense after a change of variables

$$s = \log x$$

- $\sqrt{x}$ is **singular on** $[0, 1]$, $\sqrt{e^s} = e^{s/2}$ is **smooth on** $(-\infty, 0)$
- **equispaced** scheme in s $\rightarrow$ **exponential clustering** in x
- in s-space every method for smooth functions works, **including radial basis functions**
- for bounded singular functions: tapering effect

What do rational functions look like?

Plot of partial fractions $\frac{p_j}{x-p_j}$ in s-space with clustering poles



- partial fractions are **active** in geometrically graded intervals
- how to choose spacing parameter σ? Make these functions look like B-splines and RBF's do

The tapering effect

Manifests itself in two ways:

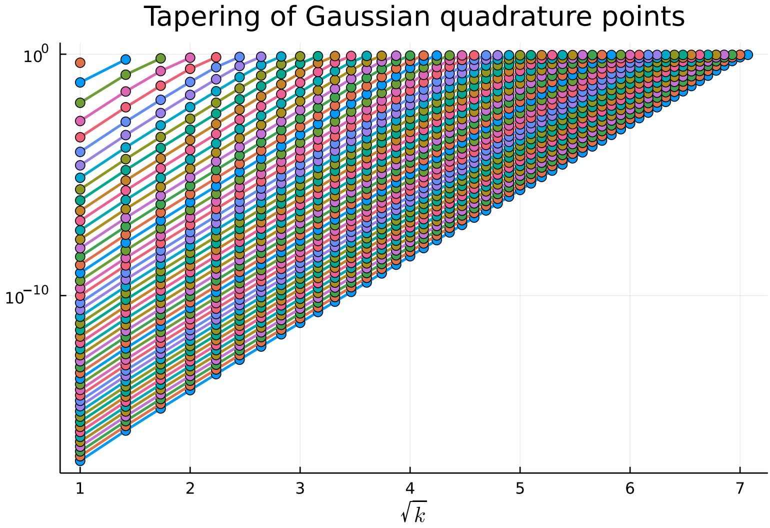
- polynomial degree can decrease towards singularity
- poles can tend to zero slightly faster than exponentially: $p_j = -e^{-\sigma(\sqrt{n}-\sqrt{j})}$

Simple reason

- approximation of $\sqrt{x}$ on $[1/2, 1]$ is the same as approximation of $\sqrt{2x}$ on $[1/4, 1/2]$
- so approximation of $\sqrt{x}$ on $[1/4, 1/2]$ is the same problem too, but with an **accuracy criterion loosened** by a factor $\sqrt{2}$
- exponentially accurate scheme on each scale: constant factor $\sqrt{2}$ yields fixed reduction in degrees of freedom

Tapering is a small optimization

Tapering: illustration



Gaussian quadrature points for rational quadrature on $[0, 1]$

Outline

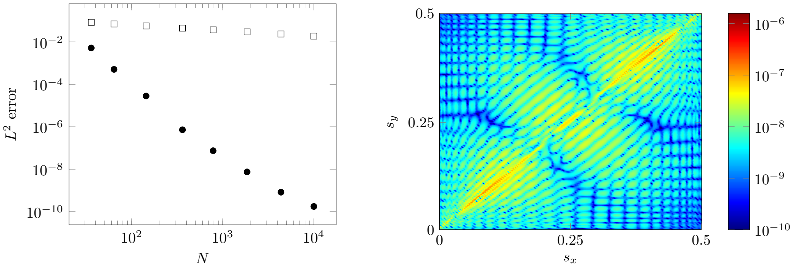
Example: Green's function of gravity Helmholtz equation

A. Barnett et al, *High-order boundary integral equation solution of high frequency wave scattering from obstacles in an unbounded linearly stratified medium*, JCP, 2015 [5]

Approximation in enriched space

$$G(\mathbf{x},\mathbf{y}) = A(\mathbf{x},\mathbf{y})\log(\mathbf{x}-\mathbf{y}) + B(\mathbf{x},\mathbf{y})$$

with $\mathbf{x},\mathbf{y}$ varying along a 1D curve in 2D



Left: convergence with and without singular terms. Right: error

Multivariate rational approximation

In 1D: poles are points. In 2D: “poles” can be 2D manifolds in 4D complex coordinate space. *But that should not stop us.*

For general *singularity curve* $Q(x, y) = 0$:

$$r(x, y) = \sum_{j=1}^{N_q} \sum_{0 \leq k, \ell \leq N_p} a_{jkl} \frac{p_j P_k(x) P_\ell(y)}{Q(x, y) - p_j} + \sum_{0 \leq k, \ell \leq N_s} b_{kl} P_k(x) P_\ell(y),$$

Generalization of partial fractions representation to 1D:

- For a diagonal singularity $Q(x, y) = x - y = 0$.
- p_j can be chosen to be **complex numbers** exponentially clustering towards zero

N. Boullé, A. Herremans, DH, *Multivariate rational approximation of functions with curves of singularities*, SISC, 2024 [6]

Multivariate rational approximation of Green's function

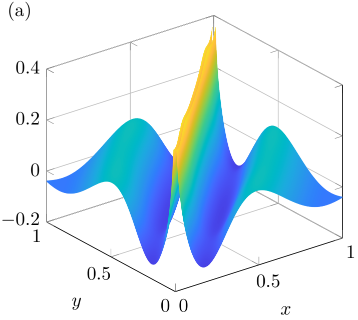


Fig. 11: Approximation of the Green's function $G(\mathbf{x}, \mathbf{y})$ of the gravity Helmholtz equation (as defined in [6]). The function is singular on the diagonal and has wavelike behavior in the tangential and normal directions. The left panel shows the function for $\mathbf{x}$ and $\mathbf{y}$ varying along a semi-circle, leading to a bivariate function on the square $[0, 1]^2$. The right panel shows uniformly high accuracy of the approximation in a dense grid of points, including points close to but excluding the diagonal.

References

1 B. Adcock, DH. *Frames and numerical approximation*, SIREV, 2019

2 A. Herremans, DH. *The AZ algorithm for enriched approximation spaces*, IMAJNA, 2024

3 A. Herremans, DH, L. N. Trefethen, *Resolution of singularities by rational functions*, SINUM, 2023

4 DH, L. N. Trefethen, *Sigmoid functions, multiscale resolution of singularities and hp-mesh refinement*, SIREV, 2024

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