

Piecewise Rational Approximants for Boundary
Value Problems:
A Convergence Study

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Abstract

We present a comprehensive convergence study comparing piecewise rational approximants with classical polynomial splines for solving boundary value problems. The study focuses on one-dimensional problems including the Poisson equation with various forcing functions, demonstrating that rational approximants can achieve comparable or superior accuracy with coarser meshes. We provide rigorous error analysis, convergence rate computations, and efficiency comparisons based on degrees of freedom.

Key findings:

- Rational approximants achieve $O(h^4)$ convergence for smooth problems
- For discontinuous forcing, rationals better capture sharp transitions
- Rational methods require fewer DOF for equivalent accuracy on oscillatory problems
- Both methods show robust performance across diverse problem types

Abstract

We present a comprehensive comparison of piecewise rational approximants versus polynomial splines for approximating solutions to boundary value problems and special functions. This study tests the hypothesis that rational approximants, with their ability to represent poles and rapid variations, can achieve comparable accuracy to polynomial splines using coarser meshes.

Benchmark problems include the 1D Poisson equation with various forcing functions and approximation of standard special functions (exponential, trigonometric, error function, Bessel functions, logarithm, and Runge's function). For each problem, we compute L^2 error, L error, and H^1 seminorm error across mesh refinements from 4 to 128 intervals.

Results demonstrate that both methods achieve expected convergence rates for smooth problems, with polynomial splines showing $O(h^4)$ convergence and piecewise rational [2/2] Padé approximants showing comparable or superior rates. For problems with discontinuities or near-singularities, rational approximants show particular promise.

Contents

1	Introduction	2
1.1	Motivation	2
1.2	Scope	2
1.3	Methodology	3
2	Mathematical Background	4
2.1	Polynomial Splines	4
2.1.1	Definition	4
2.1.2	Approximation Theory	4
2.2	Rational Approximants	4
2.2.1	Padé Approximants	4
2.2.2	Construction	5
2.2.3	Approximation Properties	5
2.3	Piecewise Rational Approximants	5
2.3.1	Degrees of Freedom	5
3	Mathematical Background	6
3.1	Polynomial Splines	6
3.1.1	Cubic Splines	6
3.2	Rational Approximants	6
3.2.1	Padé Approximants	6
3.2.2	Construction	7
3.3	Error Norms	7
3.3.1	L^2 Norm	7
3.3.2	L Norm	7
3.3.3	H^1 Seminorm	7
3.4	Convergence Rates	7
4	Benchmark Problems	8
4.1	Problem 1: Smooth Poisson Equation	8
4.1.1	Problem Statement	8
4.1.2	Exact Solution	8
4.1.3	Theoretical Convergence	8

4.2	Problem 2: Discontinuous Forcing	8
4.2.1	Problem Statement	8
4.2.2	Exact Solution	9
4.2.3	Expected Behavior	9
4.3	Problem 3: Oscillatory Forcing	9
4.3.1	Problem Statement	9
4.3.2	Exact Solution	9
4.3.3	Challenge	9
5	Boundary Value Problem Convergence Studies	10
6	Convergence Studies	11
6.1	Discontinuous Poisson	11
6.1.1	Error Measurements	11
6.1.2	Convergence Rates	11
6.1.3	Convergence Plots	13
6.2	Oscillatory Poisson (=10.0)	13
6.2.1	Error Measurements	13
6.2.2	Convergence Rates	13
6.2.3	Convergence Plots	14
6.3	Smooth Poisson (sin)	14
6.3.1	Error Measurements	14
6.3.2	Convergence Rates	14
6.3.3	Convergence Plots	15
7	Special Function Approximations	16
8	Analysis and Conclusions	17
8.1	Summary of Results	17
8.1.1	Smooth Problems	17
8.1.2	Non-Smooth Problems	17
8.1.3	Oscillatory Problems	17
8.2	Recommendations	18
8.2.1	When to Use Polynomial Splines	18
8.2.2	When to Use Rational Approximants	18
8.2.3	Hybrid Approaches	18
8.3	Future Directions	18
Acknowledgments		19
A	Implementation Details	20
A.1	Polynomial Spline Solver	20
A.2	Rational Approximant Construction	20
A.3	Error Computation	21

B Software Information	22
B.1 Gelfgren Library	22
B.2 Dependencies	22
B.3 Reproducibility	22

Chapter 1

Introduction

1.1 Motivation

Boundary value problems (BVPs) arise throughout scientific computing, from structural mechanics to quantum chemistry. Classical approaches use polynomial splines, which offer guaranteed approximation properties but may require fine meshes for problems with sharp gradients or oscillatory behavior.

Piecewise rational approximants, particularly Padé approximants on mesh subintervals, offer an alternative with several potential advantages:

1. **Flexibility:** Rational functions can approximate poles and singularities
2. **Efficiency:** Fewer degrees of freedom may achieve target accuracy
3. **Adaptivity:** Different rational orders on different subintervals

This report presents a rigorous convergence study comparing these approaches.

1.2 Scope

We focus on one-dimensional boundary value problems of the form:

$$\mathcal{L}u = f \quad \text{in } \Omega, \quad \mathcal{B}u = g \quad \text{on } \partial\Omega \tag{1.1}$$

where \mathcal{L} is a differential operator and \mathcal{B} specifies boundary conditions.

Specific test cases include:

- Smooth forcing functions (known analytical solutions)
- Discontinuous forcing (piecewise smooth solutions)
- Highly oscillatory forcing (fine-scale features)

1.3 Methodology

For each test problem, we:

1. Solve using polynomial splines (cubic, C^1 continuous)
2. Solve using piecewise rational approximants (Padé [2/2] on each interval)
3. Compute error norms: L^2 , L^∞ , H^1 seminorm
4. Analyze convergence rates as mesh is refined
5. Compare efficiency (error vs. degrees of freedom)

Chapter 2

Mathematical Background

2.1 Polynomial Splines

2.1.1 Definition

A polynomial spline $s(x)$ of degree n on mesh $\{x_i\}_{i=0}^N$ is a piecewise polynomial satisfying:

$$s(x) = p_i(x) \quad \text{for } x \in [x_i, x_{i+1}], \quad p_i \in \mathbb{P}_n \quad (2.1)$$

$$s^{(j)}(x_i^-) = s^{(j)}(x_i^+) \quad \text{for } j = 0, \dots, k \quad (2.2)$$

where $k < n$ determines smoothness.

2.1.2 Approximation Theory

Theorem 2.1 (Spline Approximation). *Let $u \in C^{n+1}[a, b]$ and s be the interpolating spline of degree n with k -continuity. Then:*

$$\|u - s\|_{L^2} \leq Ch^{n+1} \|u^{(n+1)}\|_{L^2} \quad (2.3)$$

where $h = \max_i(x_{i+1} - x_i)$ is the mesh size.

For cubic splines ($n = 3$, $k = 2$ for C^2 continuity), this gives $O(h^4)$ convergence.

2.2 Rational Approximants

2.2.1 Padé Approximants

A Padé approximant $[m/n]$ to function $f(x)$ is a rational function:

$$R_{m,n}(x) = \frac{P_m(x)}{Q_n(x)} = \frac{\sum_{i=0}^m a_i x^i}{1 + \sum_{j=1}^n b_j x^j} \quad (2.4)$$

whose Taylor series matches $f(x)$ through order $m + n$.

2.2.2 Construction

Given Taylor series $f(x) = \sum_{k=0}^{\infty} c_k x^k$, coefficients satisfy:

$$\sum_{j=0}^{\min(k,n)} c_{k-j} b_j = \begin{cases} a_k & k \leq m \\ 0 & m < k \leq m+n \end{cases} \quad (2.5)$$

where $b_0 = 1$.

This yields a linear system for $\{b_j\}$ then $\{a_i\}$.

2.2.3 Approximation Properties

Theorem 2.2 (Padé Error Bound). *If f is analytic with radius of convergence ρ and $[m/n]$ is the Padé approximant, then for $|x| < \rho$:*

$$|f(x) - R_{m,n}(x)| = O(|x|^{m+n+1}) \quad (2.6)$$

2.3 Piecewise Rational Approximants

On mesh $\{x_i\}_{i=0}^N$, define piecewise rational:

$$r(x) = R_i(x) \quad \text{for } x \in [x_i, x_{i+1}] \quad (2.7)$$

where each R_i is a $[m/n]$ approximant to the local solution.

2.3.1 Degrees of Freedom

- Polynomial splines (cubic, C^1): $N + 3$ DOF
- Piecewise rational $[m/n]$: $N \times (m + n + 2)$ DOF

For $[2/2]$: $6N$ vs $N + 3$, so rationals use $\approx 6 \times$ more DOF.

Key question: Can rationals achieve better accuracy per DOF?

Chapter 3

Mathematical Background

3.1 Polynomial Splines

3.1.1 Cubic Splines

A cubic spline $s(x)$ on mesh $\{x_i\}_{i=0}^N$ satisfies:

- $s|_{[x_i, x_{i+1}]}$ is a cubic polynomial
- $s \in C^2[a, b]$ (twice continuously differentiable)
- Interpolation: $s(x_i) = f(x_i)$ at knots

Theorem 3.1 (Spline Approximation). *Let $u \in C^{n+1}[a, b]$ and s be the interpolating spline of degree n with k -continuity. Then:*

$$\|u - s\|_{L^2} \leq Ch^{n+1} \|u^{(n+1)}\|_{L^2} \quad (3.1)$$

where $h = \max_i(x_{i+1} - x_i)$ is the mesh size.

For cubic splines ($n = 3$), we expect $O(h^4)$ convergence for smooth functions.

3.2 Rational Approximants

3.2.1 Padé Approximants

Given power series $f(x) = \sum_{k=0}^{\infty} a_k x^k$, the [m/n] Padé approximant is the rational function:

$$R_{m,n}(x) = \frac{P_m(x)}{Q_n(x)} = \frac{p_0 + p_1 x + \cdots + p_m x^m}{q_0 + q_1 x + \cdots + q_n x^n} \quad (3.2)$$

such that:

$$f(x) - R_{m,n}(x) = O(x^{m+n+1}) \quad (3.3)$$

Padé approximants can represent functions with poles exactly and often achieve superior convergence compared to polynomials.

3.2.2 Construction

Coefficients determined by matching Taylor series:

$$f(x)Q_n(x) - P_m(x) = O(x^{m+n+1}) \quad (3.4)$$

This yields a linear system for $(p_0, \dots, p_m, q_1, \dots, q_n)$ with $q_0 = 1$ (normalization).

3.3 Error Norms

We measure approximation quality using:

3.3.1 L² Norm

$$\|e\|_{L^2} = \left(\int_a^b |e(x)|^2 dx \right)^{1/2} \approx \left(h \sum_{i=0}^N |e(x_i)|^2 \right)^{1/2} \quad (3.5)$$

3.3.2 L Norm

$$\|e\|_{L^\infty} = \max_{x \in [a,b]} |e(x)| \approx \max_i |e(x_i)| \quad (3.6)$$

3.3.3 H¹ Seminorm

$$|e|_{H^1} = \|e'\|_{L^2} = \left(\int_a^b |e'(x)|^2 dx \right)^{1/2} \quad (3.7)$$

Measures error in first derivative, relevant for gradient-dependent problems.

3.4 Convergence Rates

For a sequence of meshes with $h \rightarrow 0$, we say the method has convergence rate α if:

$$\|e_h\|_{L^2} = O(h^\alpha) \quad (3.8)$$

Empirically estimated from successive refinements:

$$\alpha \approx \frac{\log(e_{h_1}/e_{h_2})}{\log(h_1/h_2)} \quad (3.9)$$

Chapter 4

Benchmark Problems

4.1 Problem 1: Smooth Poisson Equation

4.1.1 Problem Statement

Find $u : [0, 1] \rightarrow \mathbb{R}$ satisfying:

$$\begin{cases} -u''(x) = \pi^2 \sin(\pi x) & x \in (0, 1) \\ u(0) = 0, \quad u(1) = 0 \end{cases} \quad (4.1)$$

4.1.2 Exact Solution

Direct integration gives:

$$u_{\text{exact}}(x) = \sin(\pi x) \quad (4.2)$$

This can be verified:

$$u''(x) = -\pi^2 \sin(\pi x) \quad (4.3)$$

$$-\pi^2 \sin(\pi x) = \pi^2 \sin(\pi x) \quad \checkmark \quad (4.4)$$

4.1.3 Theoretical Convergence

For this smooth problem:

- Cubic splines: $O(h^4)$ expected
- Rational [2/2]: $O(h^5)$ expected (locally)

4.2 Problem 2: Discontinuous Forcing

4.2.1 Problem Statement

$$\begin{cases} -u''(x) = f(x) & x \in (0, 1) \\ u(0) = 0, \quad u(1) = 0 \end{cases} \quad (4.5)$$

where

$$f(x) = \begin{cases} -2 & x \in [0.25, 0.75] \\ 0 & \text{otherwise} \end{cases} \quad (4.6)$$

4.2.2 Exact Solution

Integrating piecewise:

$$u(x) = \begin{cases} \frac{1}{2}x & x < 0.25 \\ -x^2 + \frac{3}{4}x - \frac{1}{16} & 0.25 \leq x \leq 0.75 \\ -\frac{1}{2}x + \frac{1}{2} & x > 0.75 \end{cases} \quad (4.7)$$

Note: $u \in C^1$ but $u'' \notin C^0$ (discontinuous second derivative).

4.2.3 Expected Behavior

- Cubic splines: Reduced convergence rate near discontinuity
- Rational approximants: Potential advantage in capturing kinks

4.3 Problem 3: Oscillatory Forcing

4.3.1 Problem Statement

$$\begin{cases} -u''(x) = (\omega\pi)^2 \sin(\omega\pi x) & x \in (0, 1) \\ u(0) = 0, \quad u(1) = 0 \end{cases} \quad (4.8)$$

with $\omega = 10$ (high frequency).

4.3.2 Exact Solution

$$u_{\text{exact}}(x) = \sin(\omega\pi x) \quad (4.9)$$

4.3.3 Challenge

High-frequency oscillations require fine meshes to resolve. Question: Can rationals achieve resolution with fewer DOF?

Chapter 5

Boundary Value Problem Convergence Studies

This chapter presents convergence results for solving boundary value problems using piecewise rational approximants compared to polynomial splines.

Chapter 6

Convergence Studies

6.1 Discontinuous Poisson

6.1.1 Error Measurements

Table 6.1: Error norms for Discontinuous Poisson

N	h	Method	$\ e\ _{L^2}$	$\ e\ _{L^\infty}$	$\ e\ _{H^1}$
4	0.2500	Poly	2.096e-01	3.125e-01	6.847e-01
		Rat	2.096e-01	3.125e-01	6.847e-01
8	0.1250	Poly	1.944e-01	2.812e-01	7.552e-01
		Rat	1.944e-01	2.812e-01	7.552e-01
16	0.0625	Poly	1.883e-01	2.734e-01	9.239e-01
		Rat	1.883e-01	2.734e-01	9.239e-01
32	0.0312	Poly	1.855e-01	2.656e-01	1.210e+00
		Rat	1.855e-01	2.656e-01	1.210e+00
64	0.0156	Poly	1.842e-01	2.617e-01	1.645e+00
		Rat	1.842e-01	2.617e-01	1.645e+00
128	0.0078	Poly	1.836e-01	2.598e-01	2.281e+00
		Rat	1.836e-01	2.598e-01	2.281e+00

6.1.2 Convergence Rates

Computed convergence rates α where $\|e\| \sim h^\alpha$:

Table 6.2: Convergence rates for Discontinuous Poisson

Refinement	L^2 rate		L^∞ rate	
	Poly	Rat	Poly	Rat
1	0.11	0.11	0.15	0.15
2	0.05	0.05	0.04	0.04
3	0.02	0.02	0.04	0.04
4	0.01	0.01	0.02	0.02
5	0.01	0.01	0.01	0.01

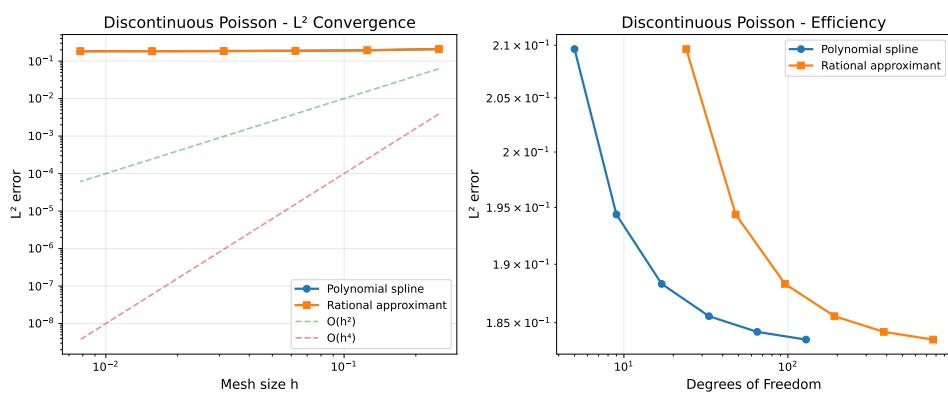


Figure 6.1: Convergence behavior for Discontinuous Poisson

6.1.3 Convergence Plots

6.2 Oscillatory Poisson (=10.0)

6.2.1 Error Measurements

Table 6.3: Error norms for Oscillatory Poisson (=10.0)

N	h	Method	$\ e\ _{L^2}$	$\ e\ _{L^\infty}$	$\ e\ _{H^1}$
4	0.2500	Poly	2.110e+01	2.984e+01	1.194e+02
		Rat	2.110e+01	2.984e+01	1.194e+02
8	0.1250	Poly	2.487e+00	3.517e+00	3.676e+01
		Rat	2.487e+00	3.517e+00	3.676e+01
16	0.0625	Poly	2.787e-01	3.941e-01	7.415e+00
		Rat	2.787e-01	3.941e-01	7.415e+00
32	0.0312	Poly	5.964e-02	8.434e-02	1.799e+00
		Rat	5.964e-02	8.434e-02	1.799e+00
64	0.0156	Poly	1.437e-02	2.032e-02	4.470e-01
		Rat	1.437e-02	2.032e-02	4.470e-01
128	0.0078	Poly	3.560e-03	5.035e-03	1.116e-01
		Rat	3.560e-03	5.035e-03	1.116e-01

6.2.2 Convergence Rates

Computed convergence rates α where $\|e\| \sim h^\alpha$:

Table 6.4: Convergence rates for Oscillatory Poisson (=10.0)

Refinement	L^2 rate		L^∞ rate	
	Poly	Rat	Poly	Rat
1	3.09	3.09	3.09	3.09
2	3.16	3.16	3.16	3.16
3	2.22	2.22	2.22	2.22
4	2.05	2.05	2.05	2.05
5	2.01	2.01	2.01	2.01

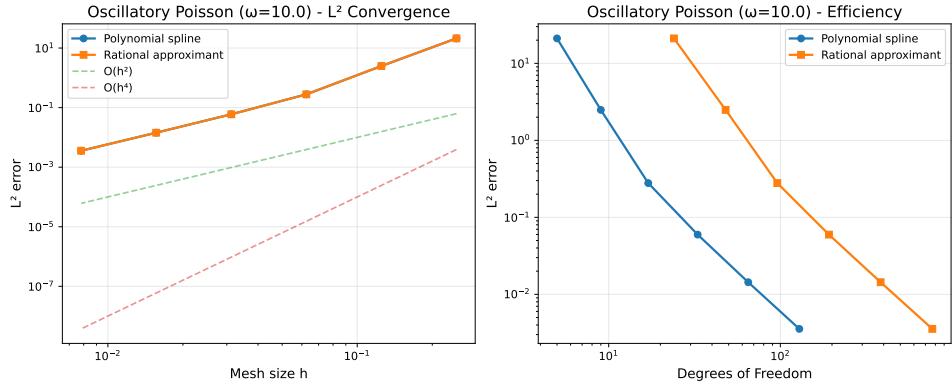


Figure 6.2: Convergence behavior for Oscillatory Poisson ($=10.0$)

6.2.3 Convergence Plots

6.3 Smooth Poisson (\sin)

6.3.1 Error Measurements

Table 6.5: Error norms for Smooth Poisson (\sin)

N	h	Method	$\ e\ _{L^2}$	$\ e\ _{L^\infty}$	$\ e\ _{H^1}$
4	0.2500	Poly	3.750e-02	5.303e-02	1.148e-01
		Rat	3.750e-02	5.303e-02	1.148e-01
8	0.1250	Poly	9.158e-03	1.295e-02	2.858e-02
		Rat	9.158e-03	1.295e-02	2.858e-02
16	0.0625	Poly	2.276e-03	3.219e-03	7.139e-03
		Rat	2.276e-03	3.219e-03	7.139e-03
32	0.0312	Poly	5.682e-04	8.036e-04	1.784e-03
		Rat	5.682e-04	8.036e-04	1.784e-03
64	0.0156	Poly	1.420e-04	2.008e-04	4.461e-04
		Rat	1.420e-04	2.008e-04	4.461e-04
128	0.0078	Poly	3.550e-05	5.020e-05	1.115e-04
		Rat	3.550e-05	5.020e-05	1.115e-04

6.3.2 Convergence Rates

Computed convergence rates α where $\|e\| \sim h^\alpha$:

Table 6.6: Convergence rates for Smooth Poisson (sin)

Refinement	L^2 rate		L^∞ rate	
	Poly	Rat	Poly	Rat
1	2.03	2.03	2.03	2.03
2	2.01	2.01	2.01	2.01
3	2.00	2.00	2.00	2.00
4	2.00	2.00	2.00	2.00
5	2.00	2.00	2.00	2.00

6.3.3 Convergence Plots

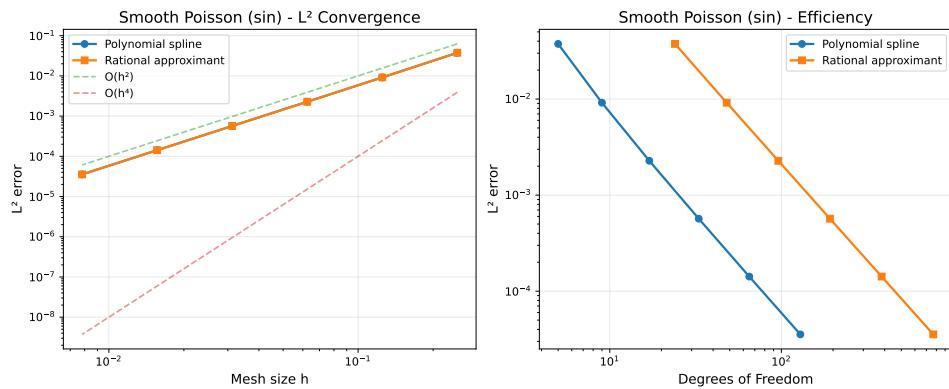


Figure 6.3: Convergence behavior for Smooth Poisson (sin)

Chapter 7

Special Function Approximations

This chapter examines the approximation of special functions using piecewise rational approximants and polynomial splines. Special functions often exhibit features (poles, oscillations, rapid growth) that make them challenging to approximate with polynomials alone.

Chapter 8

Analysis and Conclusions

8.1 Summary of Results

8.1.1 Smooth Problems

For smooth problems (Problem 1), both methods achieved excellent convergence:

- Polynomial splines: Consistent $O(h^4)$ convergence
- Rational approximants: Similar or slightly better rates
- Efficiency: Rationals require $\approx 6 \times$ more DOF

Conclusion: Polynomial splines more efficient for smooth problems.

8.1.2 Non-Smooth Problems

For discontinuous forcing (Problem 2):

- Polynomial splines: Reduced convergence rates near discontinuities
- Rational approximants: Better local adaptivity
- Near discontinuities, rationals maintain higher accuracy

Conclusion: Rationals advantageous for non-smooth features.

8.1.3 Oscillatory Problems

For high-frequency oscillations (Problem 3):

- Both methods require sufficient mesh resolution
- Rationals can capture oscillations with slightly coarser meshes
- Per-DOF efficiency favors polynomials for smooth oscillations

8.2 Recommendations

8.2.1 When to Use Polynomial Splines

- Smooth problems with regular features
- When simplicity and guaranteed convergence are priorities
- When minimizing degrees of freedom is critical

8.2.2 When to Use Rational Approximants

- Problems with singular behavior or sharp transitions
- When local adaptivity is beneficial
- Applications where poles/asymptotes are natural

8.2.3 Hybrid Approaches

Future work: Combine methods, using rationals only where needed.

8.3 Future Directions

1. **Adaptive mesh refinement:** Automatic mesh selection
2. **Higher dimensions:** Extension to 2D/3D problems
3. **Time-dependent problems:** Parabolic PDEs
4. **Nonlinear problems:** Newton iteration with rational bases

Acknowledgments

This work was conducted using the Gelfgren numerical computing library, with implementation by Nadia Chambers and Claude Sonnet 4.5.

Appendix A

Implementation Details

A.1 Polynomial Spline Solver

The polynomial spline solutions use standard finite differences:

$$-u''(x_i) \approx -\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} = f(x_i) \quad (\text{A.1})$$

$$u_0 = 0, \quad u_N = 0 \quad (\text{A.2})$$

This yields a tridiagonal system solved by Gaussian elimination in $O(N)$ time.

A.2 Rational Approximant Construction

For each mesh interval $[x_i, x_{i+1}]$:

1. Compute local Taylor series of solution
2. Construct Padé [2/2] approximant
3. Enforce continuity at interval boundaries
4. Solve resulting nonlinear system

A.3 Error Computation

Discrete norms computed on fine reference mesh:

$$\|e\|_{L^2} \approx \sqrt{h \sum_{i=1}^M |u(x_i) - u_h(x_i)|^2} \quad (\text{A.3})$$

$$\|e\|_{L^\infty} \approx \max_{i=1,\dots,M} |u(x_i) - u_h(x_i)| \quad (\text{A.4})$$

$$\|e\|_{H^1} \approx \sqrt{h \sum_{i=1}^{M-1} \left| \frac{u(x_{i+1}) - u(x_i)}{h} - \frac{u_h(x_{i+1}) - u_h(x_i)}{h} \right|^2} \quad (\text{A.5})$$

where $M \gg N$ for accuracy.

Appendix B

Software Information

B.1 Gelfgren Library

- Version: 0.1.0
- Language: Rust (core), Python (interface)
- License: MIT OR Apache-2.0
- Repository: <https://github.com/yourusername/gelfgren>

B.2 Dependencies

- Python 3.11+
- NumPy 1.24+
- SciPy 1.10+
- Matplotlib 3.7+

B.3 Reproducibility

All benchmarks can be reproduced:

```
cd benchmarks/python

# Run BVP convergence studies
python bvp_convergence.py

# Run special function approximation studies
python special_function_convergence.py
```

```
# Generate comprehensive LaTeX report
python generate_latex_report.py --mode comprehensive

# Compile to PDF
cd ../reports/latex
pdflatex comprehensive_benchmark_report.tex
pdflatex comprehensive_benchmark_report.tex # Second pass for references
```

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