Rootfinding with Chebyshev Polynomials in 2 Dimensions

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Outline

The Problem

We want to find all solutions to

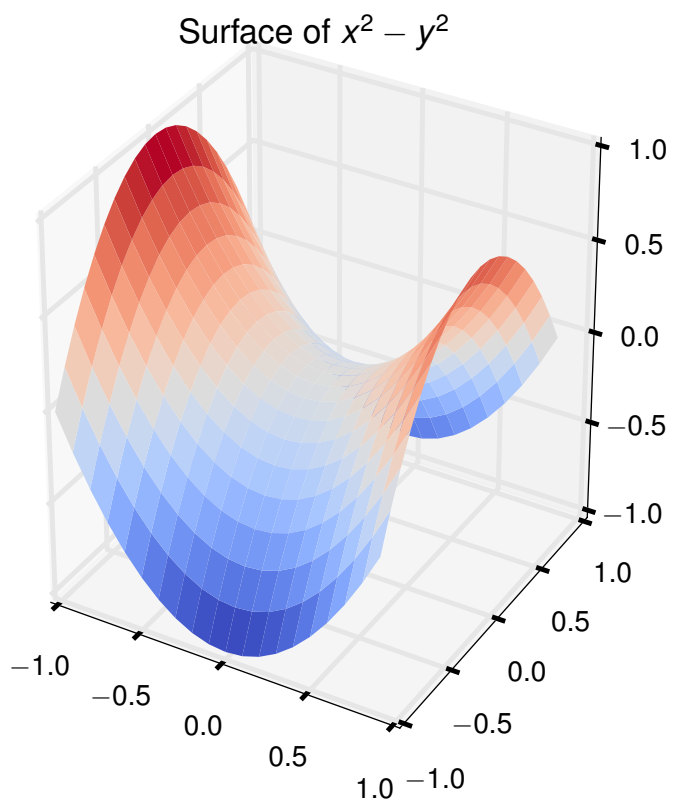
$$\begin{pmatrix} f(x,y) \\ g(x,y) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

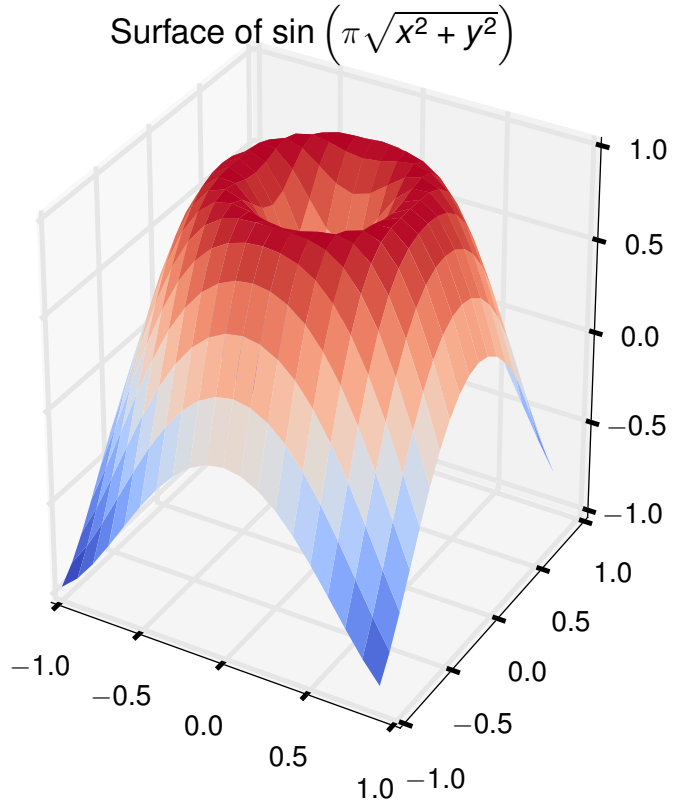
in a given bounded domain Ω

- This is a global rootfinding problem: we want all solutions inside Ω
- rootfinding is has applications in many fields
- An application for NIST would be in making flash calculations to determine properties of a fluid from its equation of state

Example

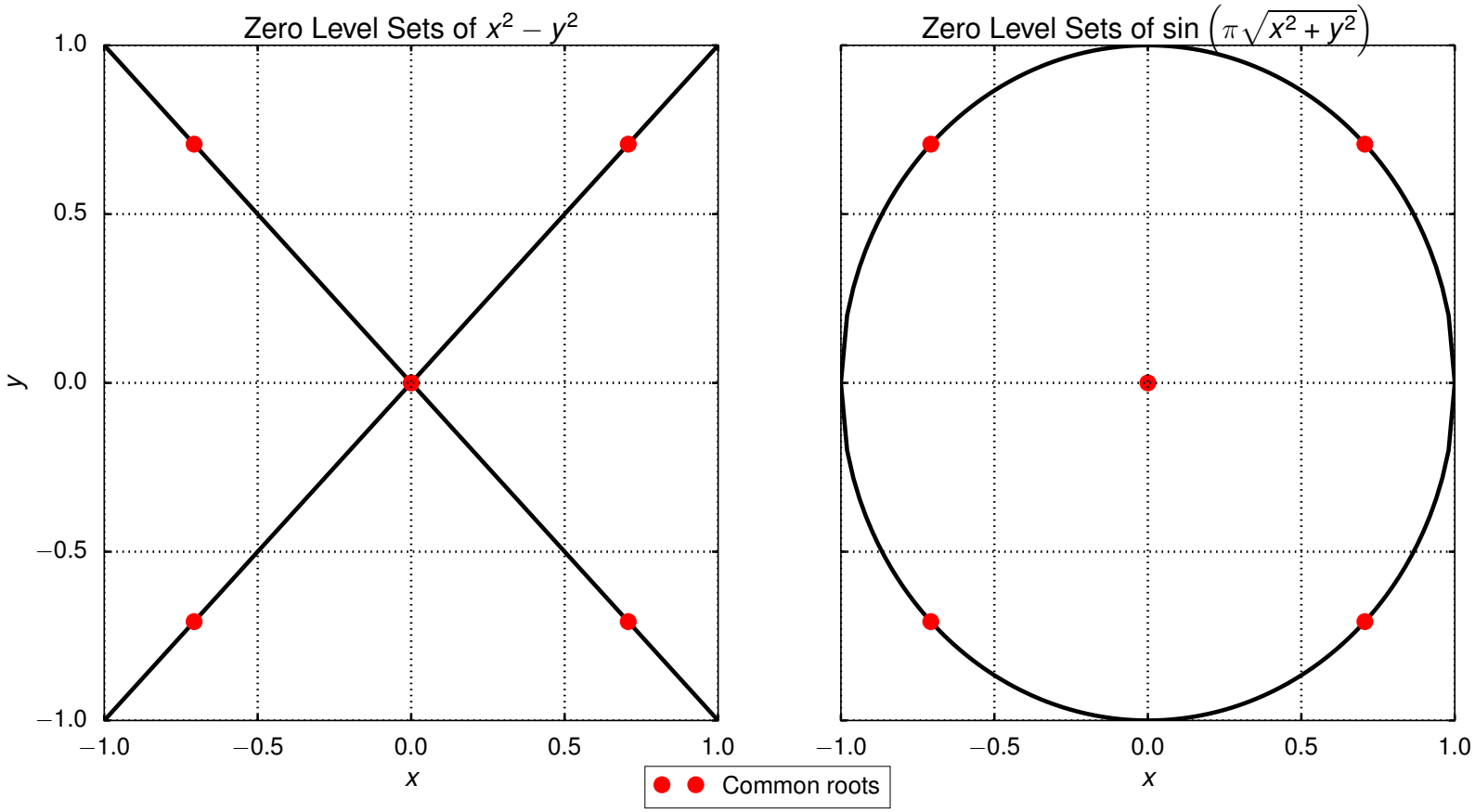
$f(x, y) = x^2 - y^2$ and $g(x, y) = \sin\left(\pi\sqrt{x^2 + y^2}\right)$ with the square domain $\Omega = [-1, 1]^2$





Example

Another view: We are finding where f and g's zero level sets intersect inside Ω



Local Methods May Not Be Good for Global rootfinding

There are actually infinitely many roots outside Ω in our example. Local methods may converge to roots outside the domain of interest.

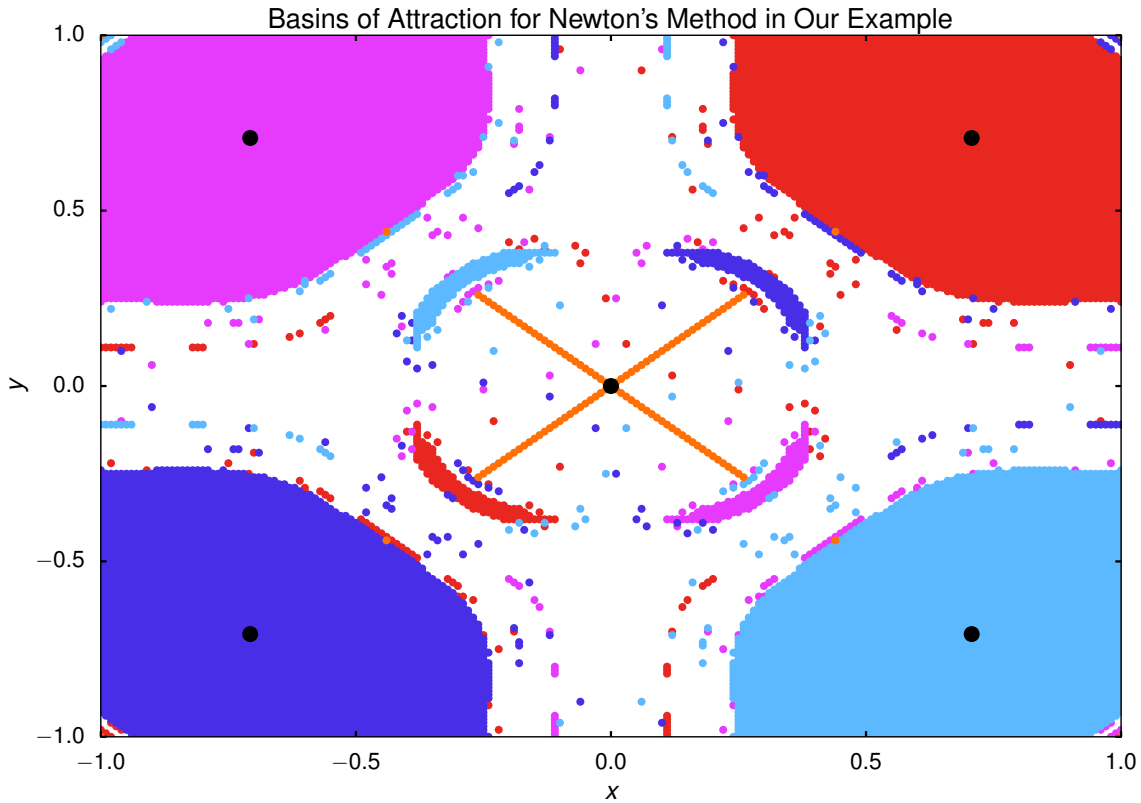


Figure: Note that initial guesses in white areas converged to roots outside our domain and the basin of attraction for $(0, 0)$ is relatively small

A Need for a Global Method

Our example illustrates a few lessons

- Many iterative and local methods like Newton's method can only guarantee convergence to a root if the initial guess is sufficiently close
- Sufficiently close depends on the problem
- This may be extremely close for some roots like $(0, 0)$ in our example

Goal:

To develop a truly global rootfinding method

1 The Problem

2 What are Chebyshev Polynomials and why use them?

3 The Algorithm

What are Chebyshev polynomials?

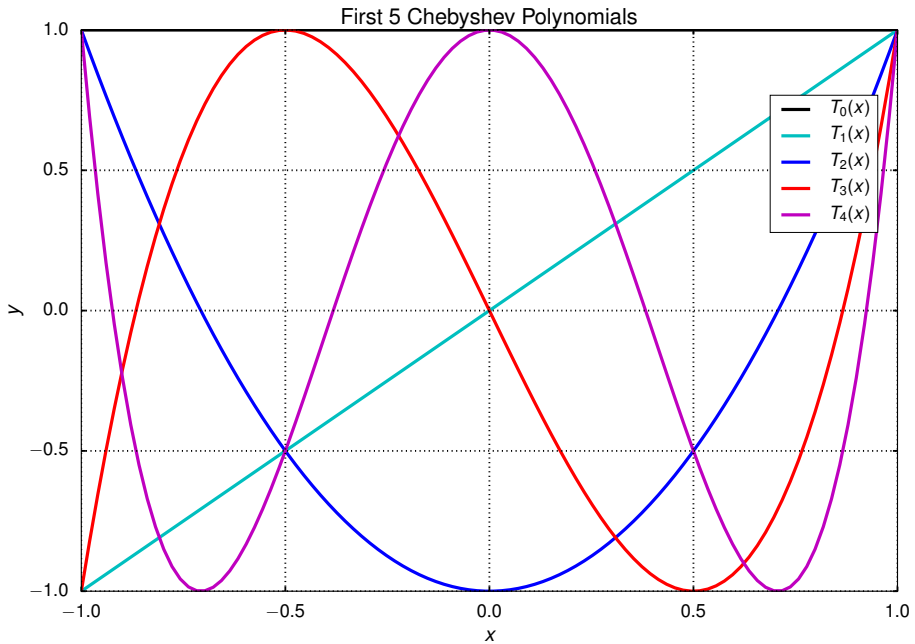
Chebyshev polynomials

$$T_n(x) = \cos\left(n \arccos(x)\right), \; x \in [-1, 1]$$

They are orthogonal under a weighted inner product:

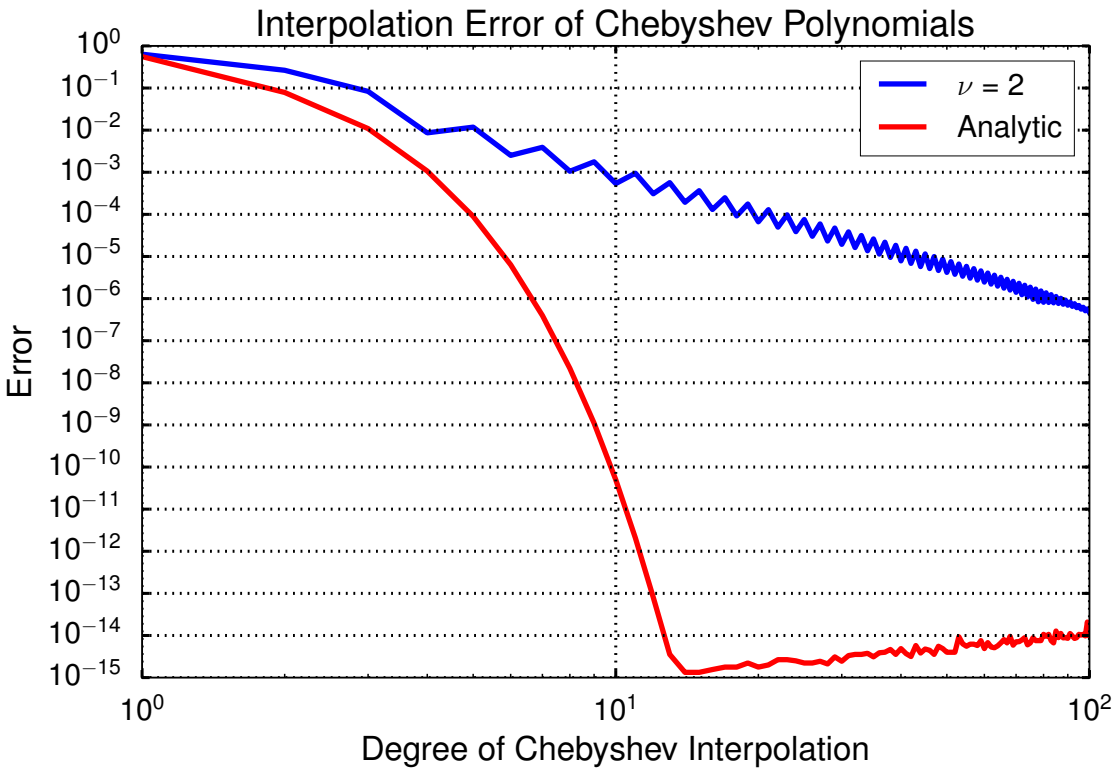
$$\int_{-1}^{1} T_n(x) T_k(x) w(x)\, dx = 0$$

when $n \neq k$
and $w(x) = \frac{1}{\sqrt{1-x^2}}$



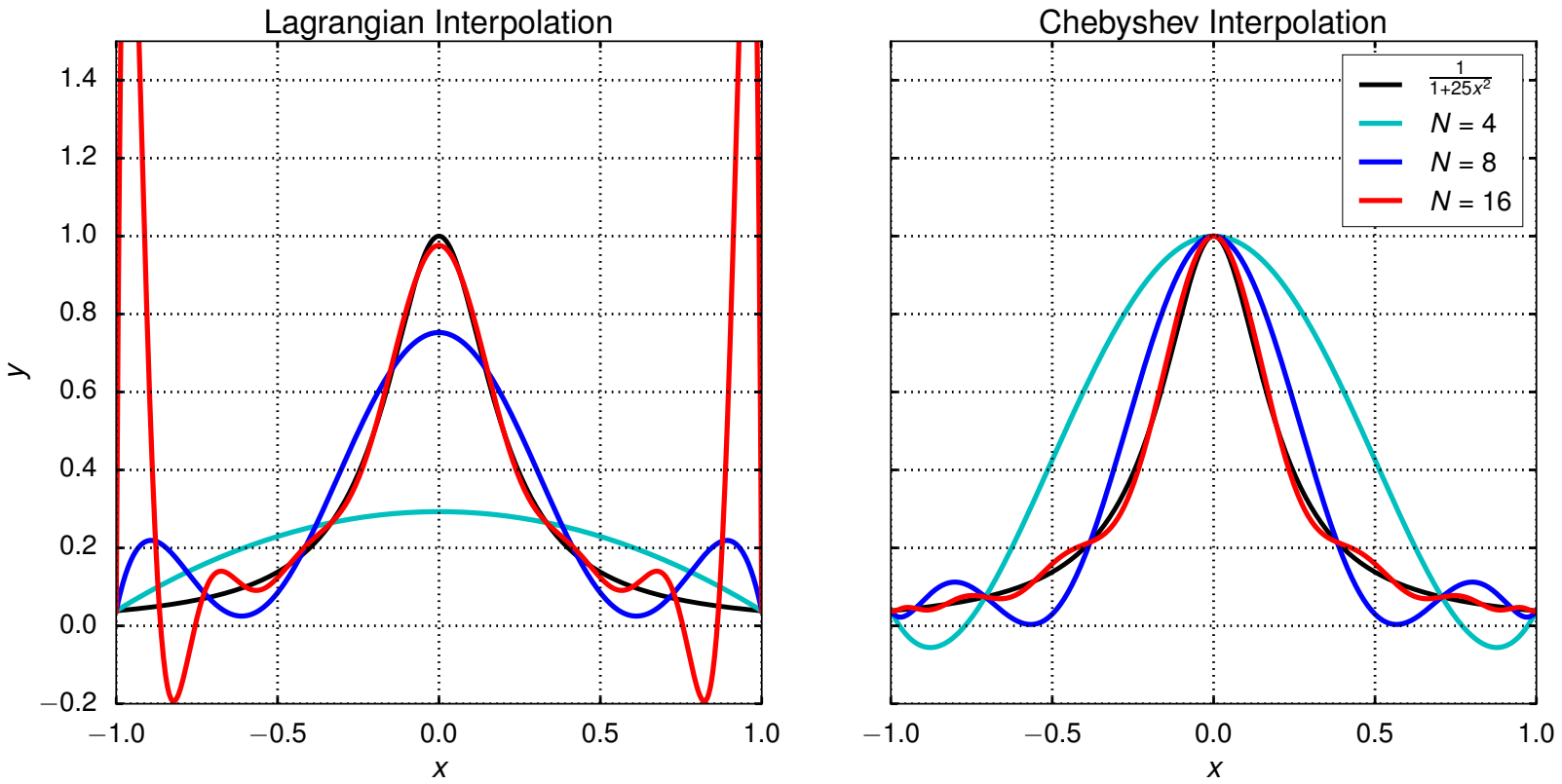
Chebyshev polynomials provide accurate approximations

- Lipschitz continuity $\implies$ uniform convergence of Chebyshev interpolations
- $\nu - 1$ continuous derivatives and a νth derivative of bounded variation $\implies$ Chebyshev interpolation converges like $\mathcal{O}(n^{-\nu})$
- Analytic function $\implies$ geometric convergence



Chebyshev polynomials are accurate and numerically stable

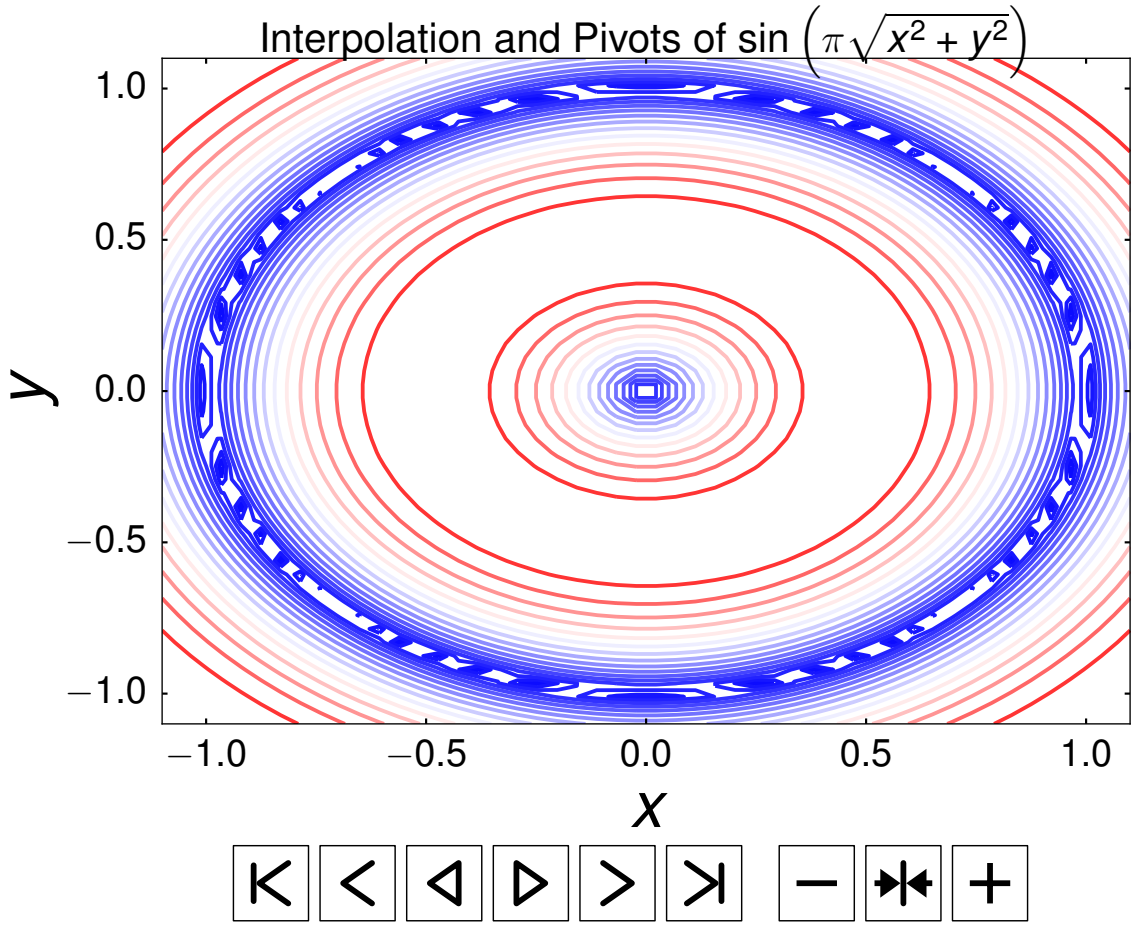
- Typical interpolation is susceptible to the **Runge phenomenon**
- Chebyshev interpolation minimizes this effect.



2-D Interpolation

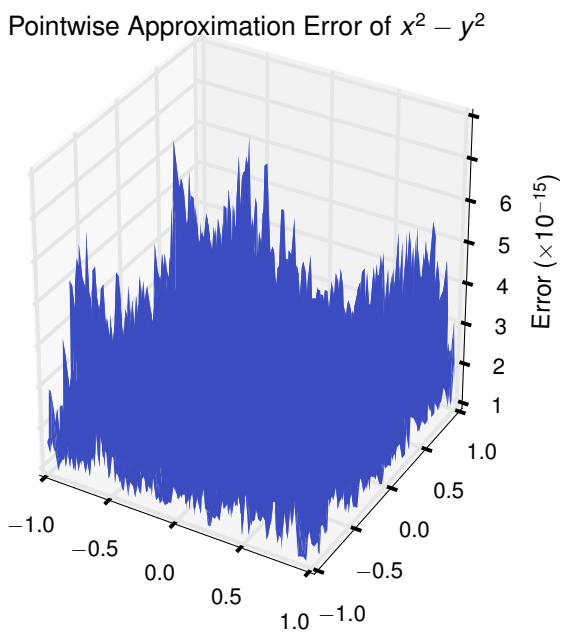
Idea:

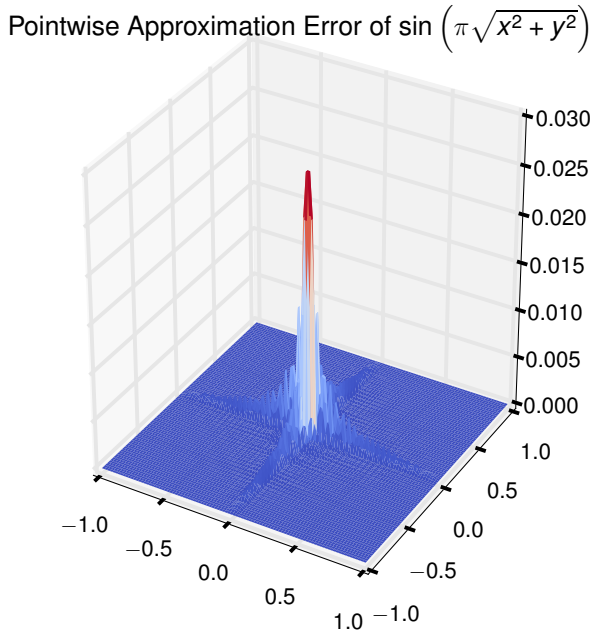
- Pick point of maximum error
- Do 1-D interpolations in x and y directions



Our Algorithm Can Provide Accurate Approximations

- Almost machine precision accuracy with $x^2 - y^2$
- Struggles with $\sin\left(\pi\sqrt{x^2+y^2}\right)$ due to the lack of differentiability at $(0,0)$





Bézout Matrix Polynomials

- We can create Bézout matrices at each Chebyshev node along the x or y axis
- Interpolating the Bézout matrices gives us a matrix polynomial $B(x)$

The matrix polynomial can be expressed as

$$B(x) = \sum_{k=0}^{M} B_k T_k(x)$$

where B_k are $N \times N$ matrices.

- $\det(B(x)) = 0 \iff$ common roots along the specific x value
- Solving $\det(B(x)) = 0$ is a **matrix polynomial eigenvalue problem**
- The most computational intensive part of the algorithm

1-D rootfinding

- We now have the possible x (or y) values for where there are common roots
- Employ a well known 1-D rootfinding method again using Chebyshev Polynomials

We do the following:

- Find the 1-D Chebyshev polynomials $p_f(y), p_g(y)$ at the specific x values
- Utilize 1-D Chebyshev rootfinding techniques
- Polish the roots with Newton's method

Conclusions and Future Work

Key Contributions:

- Replicated Alex Townsend's algorithm in chebfun2 with some modifications in C++
- Developed ideas and have a strategy for extending the algorithm to non-rectangular domains

Future Work:

- Introduce GPU/parallel computing to the rootfinding process
- Further develop ideas on non-rectangular domains and subdivision strategies

Other ideas while at NIST:

- Idea for using Gram-Schmidt process to create orthogonal terms for developing equations of state

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References

References here