Rootfinding with Chebyshev Polynomials in 2 Dimensions

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Outline

The Problem

What are Chebyshev Polynomials and why use them?

The Algorithm

The Problem

2 What are Chebyshev Polynomials and why use them?

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The Problem

Global 2-D Rootfinding Problem

We want to find all solutions to

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

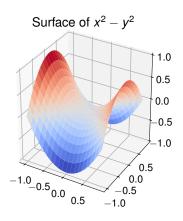
in a given bounded domain Ω

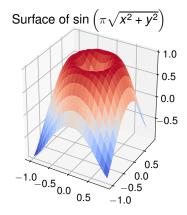
The Big Picture: ChebTools

- ChebTools is a C++ library for working with Chebyshev expansions
- Inspired by the Matlab library Chebfun
- Solving this problem will be a significant feature for ChebTools
- With a higher level Python interface, ChebTools could be useful for a wide range of users

Example

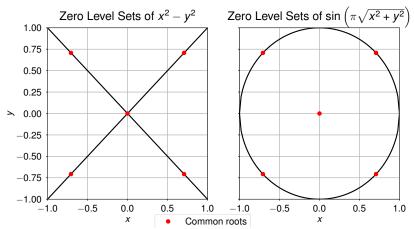
$$f(x,y)=x^2-y^2$$
 and $g(x,y)=\sin\left(\pi\sqrt{x^2+y^2}\right)$ with the square domain $\Omega=[-1,1]^2$





Example (cont.)

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.

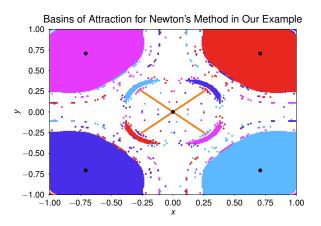


Figure: Note that initial guesses in white areas converged to roots outside our domain and the basin of attraction for (0,0) is relatively small

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
- ullet This may be extremely close for some roots like (0,0) in our example

Goal:

To develop a truly global rootfinding method

The Problem

2 What are Chebyshev Polynomials and why use them?

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What are Chebyshev polynomials?

Chebyshev polynomials

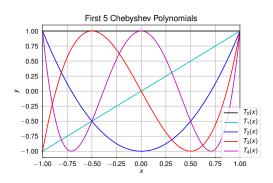
$$T_n(x) = \cos(n \arccos(x)), x \in [-1, 1]$$

Orthogonal under a weighted inner product:

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

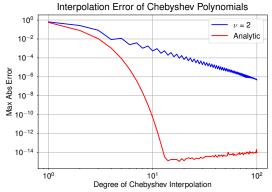
when
$$n \neq k$$

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



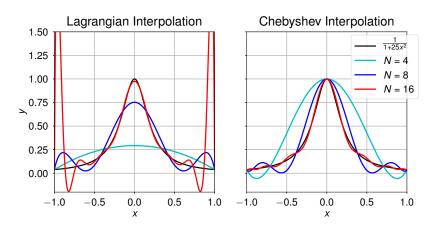
Chebyshev polynomials provide accurate approximations

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



Chebyshev polynomials are numerically stable

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



The Problem

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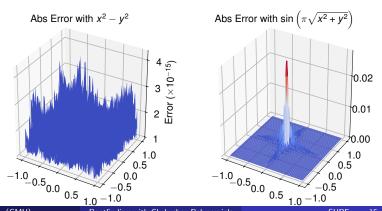
2-D Interpolation

Idea:

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

Our Algorithm Can Provide Accurate Approximations

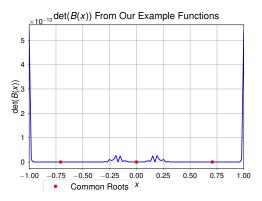
- Almost machine precision accuracy with $x^2 y^2$
- Struggles with $\sin\left(\pi\sqrt{x^2+y^2}\right)$ due to the lack of differentiability at (0,0)



Bézout Matrix Polynomials

We create a matrix polynomial B(x) from our Chebyshevs

- B(x) is a matrix with polynomial entries
- $det(B(x)) = 0 \iff common roots along the specific x value$
- Solving det(B(x)) = 0 is a matrix polynomial eigenvalue problem



1-D Rootfinding and Local Refinement

- We now have the possible x values for where there are common roots
- Employ a well known 1-D rootfinding method again using Chebyshev Polynomials
- Issue: Poor conditioning of matrix polynomial problem ⇒ need for local refinement
- Polish the roots with Newton's method

Results:

Conclusions and Future Work

Key Contributions:

- Made significant progress in replicating the 2-D rootfinding algorithm in chebfun2 with some modifications in C++
- Developed ideas and have a strategy for extending the algorithm to non-rectangular domains

Future Work:

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

Other Contributions 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