

Rootfinding with Chebyshev Polynomials in 2 Dimensions

Lucas C. Bouck

George Mason University
Department of Mathematical Sciences

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Collaborator: Ian H. Bell (NIST Division 647)

- 1 The Problem
- 2 What are Chebyshev Polynomials and why use them?
- 3 The Algorithm

1 The Problem

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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

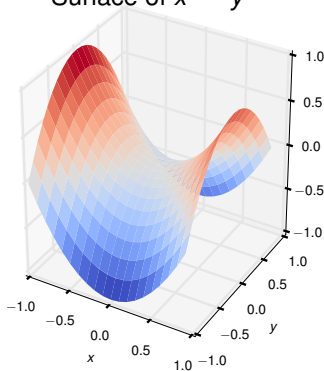
The Big Picture: `chebtools`

- `chebtools` is a C++ library for working with Chebyshev expansions developed by Ian Bell
- 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

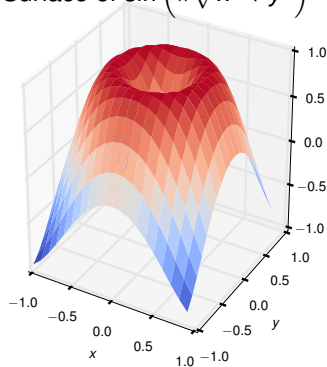
Example

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

Surface of $x^2 - y^2$

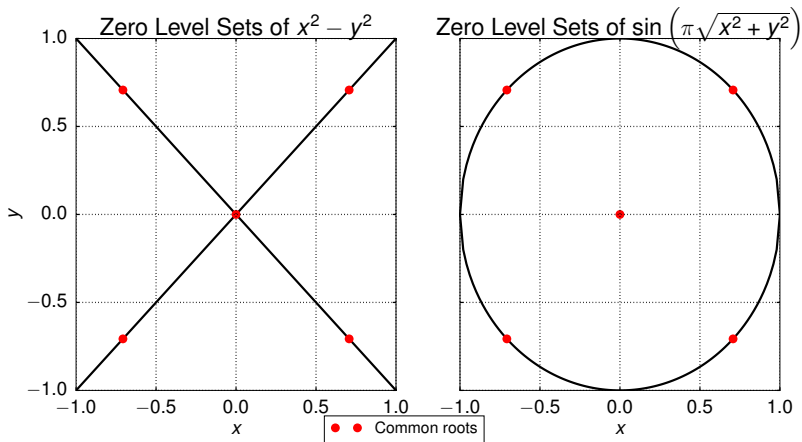


Surface of $\sin\left(\pi\sqrt{x^2 + y^2}\right)$



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.

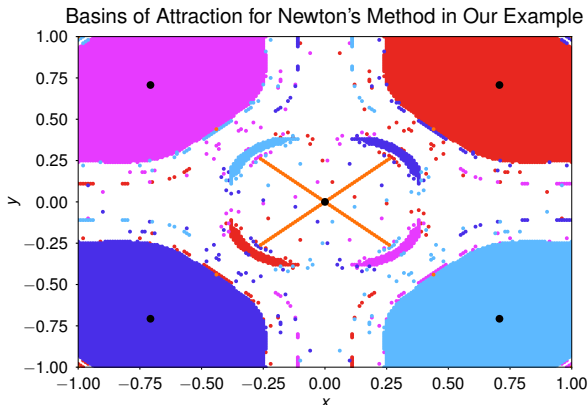


Figure: Initial guesses in white areas did not converge to roots in Ω

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

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What are Chebyshev polynomials?

Chebyshev polynomials

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

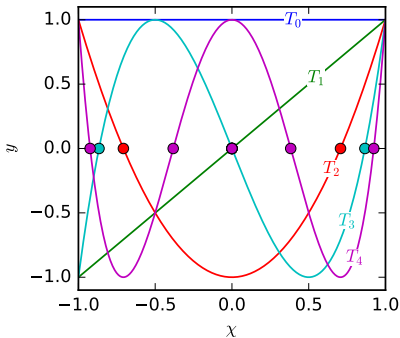
Orthogonal under a weighted inner product:

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

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

Numerically stable for interpolating functions

Figure: First 5 Chebyshev Polynomials



Chebyshev polynomials are numerically stable

- Interpolation on evenly spaced points is susceptible to the **Runge phenomenon**
- Chebyshev interpolation minimizes this effect.

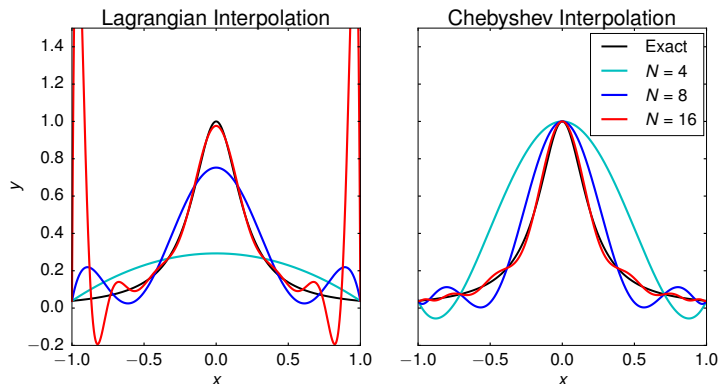


Figure: Interpolating $\frac{1}{1+25x^2}$

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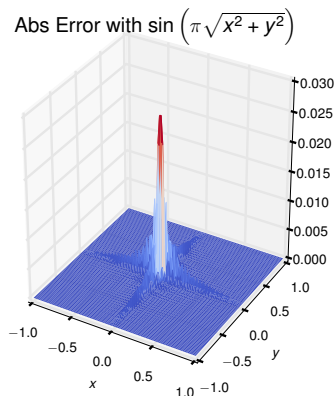
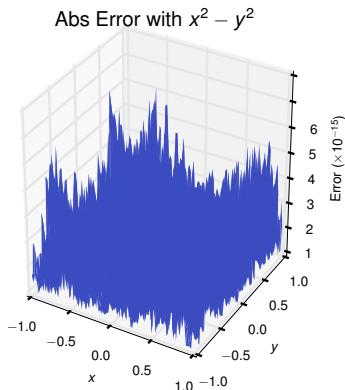
2-D Interpolation

Idea:

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

Our Algorithm Can Provide Accurate Approximations

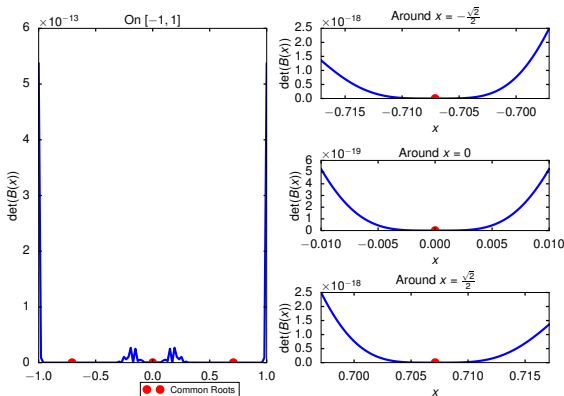
- Almost machine precision accuracy with $x^2 - y^2$
- Struggles with $\sin\left(\pi\sqrt{x^2 + y^2}\right)$ due to the lack of differentiability at $(0,0)$



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
- **Problem:** Poor conditioning of matrix polynomial problem \implies need for local refinement of roots
- Refine the roots with Newton's method

Results:

Conclusions and Future Work

Key Contributions:

- Made significant progress in replicating the 2-D rootfinding algorithm in `chebfun` with some modifications in C++11, which will be fully open source
- 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