Rootfinding with Chebyshev Polynomials in 2 Dimensions

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Outline

The Problem

Global 2-D Rootfinding Problem

We want to find all solutions to

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

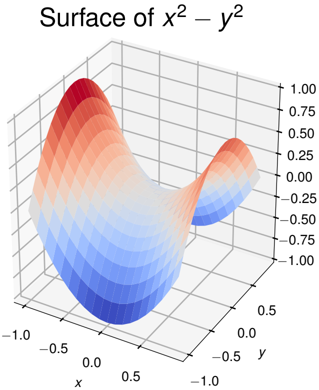
in a given bounded domain Ω

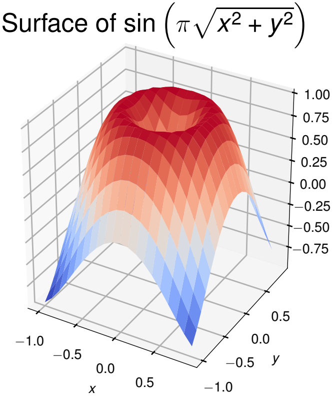
The Big Picture: `chebtools`

- `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 $\Omega = [-1,1]^2$





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.

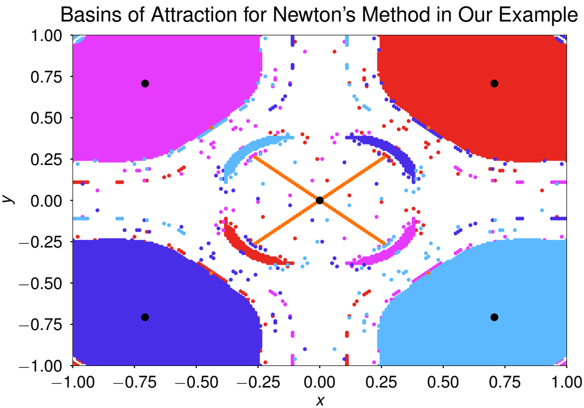


Figure: Initial guesses in white areas did not converge to roots in Ω

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

What are Chebyshev polynomials?

Chebyshev polynomials

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

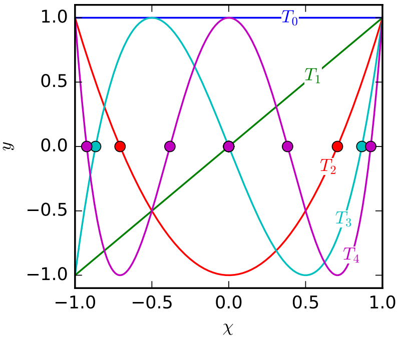
Orthogonal under a weighted inner product:

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

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

Numerically stable for interpolating functions

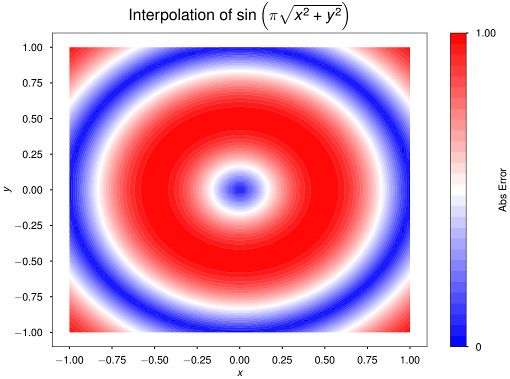
Figure: First 5 Chebyshev Polynomials



2-D Interpolation

Idea:

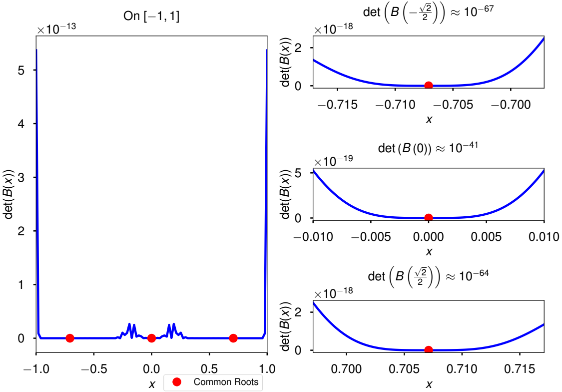
- Pick point of maximum error
- Do 1-D interpolations in x and y directions



Bézout Matrix Polynomials

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

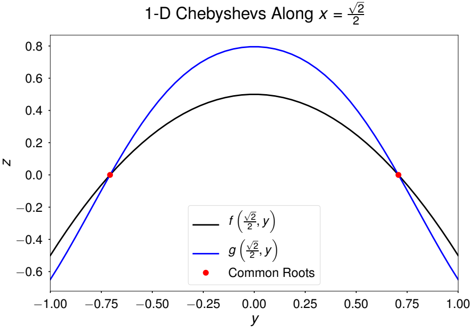
- $B(x)$ is a matrix with polynomial entries
- $\det(B(x)) = 0 \iff$ common roots along the specific x value
- Solving $\det(B(x)) = 0$ is a **matrix polynomial eigenvalue problem**



1-D Rootfinding and Local Refinement

1-D Rootfinding

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



Problem: Poor conditioning of matrix polynomial problem

- Need for local refinement of roots
- Refine the roots with Newton's method

Results:

	chebtools		chebfun	
Functions	Error	Time (s)	Error	Time (s)
$F_1(x,y), F_2(x,y)$	6.97×10^{-32}	0.004268	7.7×10^{-16}	0.522
$G_1(x,y), G_2(x,y)$	6.21×10^{-16}	214.059	2.92×10^{-10}	0.294
$H_1(x,y), H_2(x,y)$	3.24×10^{-16}	195.903	2.77×10^{-11}	0.296

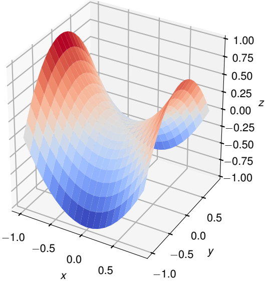
$$F_1(x,y) = T_3(x) - 13T_1(x)$$
$$F_2(x,y) = T_3(y) - 13T_1(y)$$
$$G_1(x,y) = \cos(\pi x)(y-2)$$
$$G_2(x,y) = (y-.9)(x-2)$$
$$H_1(x,y) = \cos\left(\pi x - \frac{\pi}{10}\right)(y-2)$$
$$H_2(x,y) = (y-.1)(y-.9)(x-2)$$

Back to Our First Example

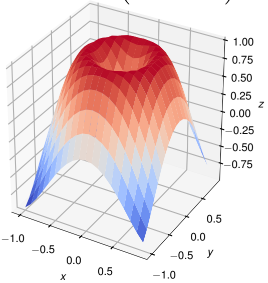
chebfun also struggled

- Found 4 of the roots with an error of $5.55 \times 10^{-}16$
- Took 208.8 seconds
- Missed the root at $(0, 0)$

Surface of $x^2 - y^2$



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



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

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[3] L. N. Trefethen, *Approximation Theory and Approximation Practice*, SIAM, Philadelphia, 2013.