Root Finding with Chebyshev Polynomials: Background and Applications in 2 Dimensions

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Outline

Big Picture

NIST Thermophysical Properties of Fluids Group:

- Mission is to provide reference data for thermophysical properties of fluids
- Provide experimental data
- Developed software to fill in the gaps of experimental data
- End products are libraries like NIST REFPROP[1]and CoolProp[2]
- The computational group fills in the gap with empirical equations of state

[1]E. Lemmon et. al. REFPROP Version 10.0, 2017

[2]I. Bell et. al. *Pure and Pseudo-pure Fluid Thermophysical Property Evaluation and the Open-Source Thermophysical Property Library CoolProp*, 2014.

What is an Equation of State (EOS)?

- Empirical equation that is built to fit the experimental data while holding to physical constraints
- Contains information like melting line, gas liquid transition line, critical point, etc
- Fitting EOS involve hard optimization problems that is a research area of its own

Motivation for Robust Root Finding Methods

- Ian Bell was first interested in root finding methods for EOS to compute an inverse problem[1]
- Useful in applications like fluid and steam in a nuclear reactor[2]
- Older EOS can be solved by finding the roots of a cubic polynomial
- More modern EOS involve transcendental functions and are much harder for the inverse problem
- **Goal:** Compromise between the two.
- **Approach:** Approximate the EOS with a polynomial and find the roots
- This approach has been effective and has led to a software library `ChebTools`[3], which is a variant on `chebfun`[4]

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[1] I. Bell et. al. *Exceptional reliable density solving alg...* 2018.

[2] M. Kunick et. al. *Fast Calculation of Therm...*, 2008.

[3] I. Bell *ChebTools.*, 2018.

[4] T Driscoll. *Chebfun Guide*, 2014.

Polynomial Interpolation

Given

- $n+1$ points $\{x_j\}_{j=1}^{n+1} \subset [a, b]$
- A function, $f : [a, b] \to \mathbb{R}$

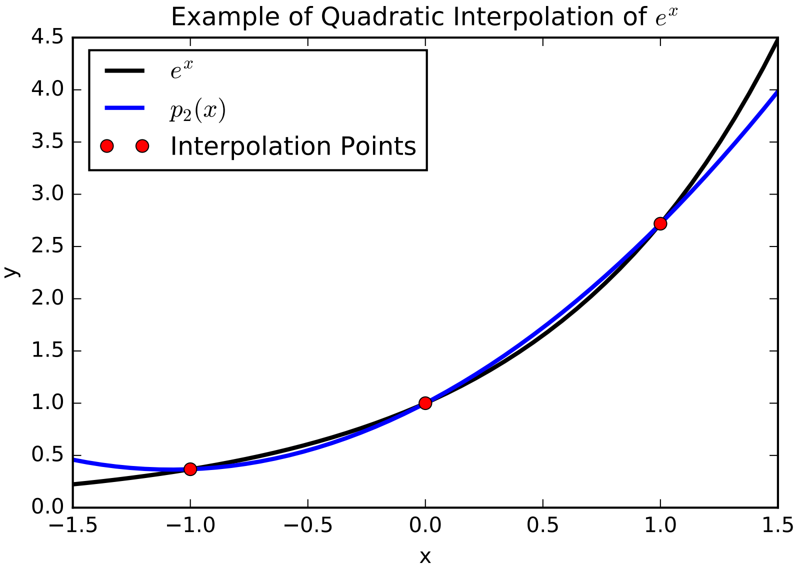
Goal

We want to find a polynomial, p_n, of degree $\leq n$ such that

$$p_n(x_j) = f(x_j), 1 \leq j \leq n+1$$

and provide a good approximation for f

Interpolation Example

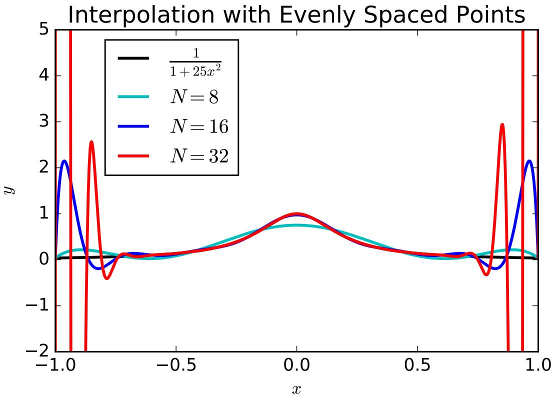


Where Evenly Spaced Interpolation Fails

The classic example is the Runge function

$$f(x) = \frac{1}{1+25x^2}.$$

On evenly spaced points, the polynomial interpolants diverge as $n \to \infty$



Polynomial Interpolation Error

We can actually express the error of polynomial interpolation for a function that is $C^{n+1}[a, b]$:[1]

$$f(x) - p_n(x) = \frac{f^{n+1}(c)}{(n+1)!} \prod_{j=1}^{n+1} (x - x_j),$$

where $c \in [a, b]$. **The Big Question:** What points minimize

$$\max_{x \in [a,b]} \left| \prod_{j=1}^{n+1} (x - x_j) \right| ?$$

For $[-1, 1]$, we'll see that the answer is **The Chebyshev Roots:**

$$x_j = \cos\left(\frac{2j-1}{2(n+1)}\pi\right), 1 \leq j \leq n+1$$

[1] P. Davis *Interpolation and Approximation* 1975. Thm. 3.1.1

Chebyshev Polynomials

Definition

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

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \end{aligned}$$

We can get a recurrence relation for $T_n(x)$ as well.

Let $\theta = \arccos(x)$ and $n \geq 1$.

$$\begin{aligned} T_{n+1}(x) + T_{n-1}(x) =& \cos((n+1)\theta) + \cos((n-1)\theta) \\ =& \cos(n\theta)\cos(\theta) - \sin(n\theta)\sin(\theta) \\ & + \cos(n\theta)\cos(-\theta) - \sin(n\theta)\sin(-\theta) \\ =& 2\cos(n\theta)\cos(\theta) = 2xT_n(x) \\ \implies T_{n+1}(x) =& 2xT_n(x) - T_{n-1}(x) \end{aligned}$$

Figure: First 5 Chebyshev Polynomials

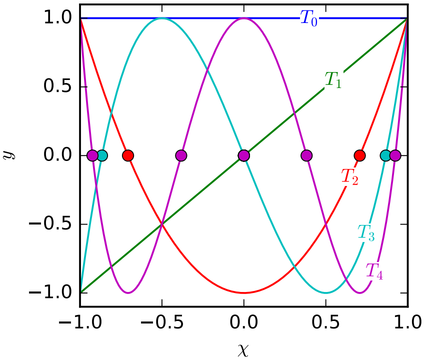
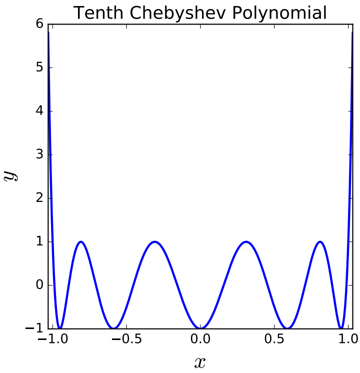


Figure: $T_{10}(x)$



Connection with Error Formula

Recall $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$ for $n \geq 1$.

- The leading coefficient for $T_n(x)$ is 2^{n-1}.
- Therefore, the polynomial $2^{1-n}T_n(x)$ is monic and we can express

$$2^{1-n}T_n(x) = \left|\prod_{i=1}^{n}(x - x_i)\right|$$

- $\max_{x\in[-1,1]} |2^{1-n}T_n(x)| = 2^{1-n}$
- All monic polynomials have a larger maximum than 2^{1-n}.[1]

Therefore, the Chebyshev roots are the best for our error formula.

[1] P. Davis *Interpolation and Approximation* 1975. Thm. 3.3.4

Error Estimate for Chebyshev Roots Points

We can now have an error estimate for interpolating through the Chebyshev points for $n \geq 1$

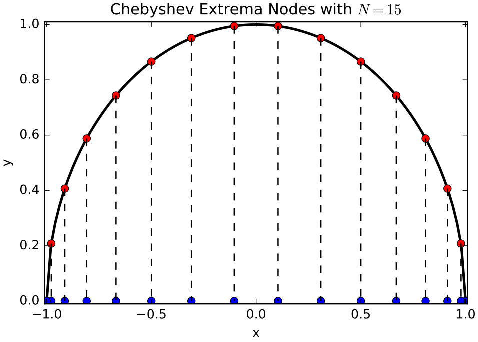
$$\|f(x) - p_n(x)\|_\infty \leq \max_{x\in[-1,1]} \left| \frac{f^{n+1}(c)}{(n+1)!} \prod_{i=1}^{n+1} n(c - x_i) \right|$$
$$\leq \frac{1}{2^n (n+1)!} \max_{c\in[-1,1]} \left| f^{n+1}(c) \right|$$

Other Useful Points

The Chebyshev Extrema Points

$$x_j = \cos\left(\frac{j\pi}{n}\right), 0 \le j \le n$$

are also useful for interpolation. They can be thought of as the x components of points evenly spaced on the unit circle:



The Chebyshev Extrema Points

The Chebyshev Extrema Points $x_j = \cos\left(\frac{j\pi}{n}\right)$ are used by us in `ChebTools` and also are the points used in `chebfun`. It isn't hard to

interpolate with these points because there is a matrix A where

$$\begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix} = A \begin{pmatrix} f(x_0) \\ \vdots \\ f(x_n) \end{pmatrix}$$ [1],

This gives us the advantage of having the coefficients a_j, which we'll need for root finding methods with polynomials.

[1] JP Boyd *Finding the Zeros of a Univariate Equation: Proxy Rootfinders, Chebyshev Interpolation, and the Companion Matrix*, 2013. Appendix A.

An Orthogonal View of Chebyshev Polynomials

Chebyshev polynomials are orthogonal with respect to a weight:

$$\langle T_n, T_m \rangle = \int_{-1}^{1} \frac{T_n(x) T_m(x)}{\sqrt{1-x^2}} \mathrm{d}x = \begin{cases} 0, n \neq m \\ \frac{\pi}{2}, n = m > 0 \\ \pi, n = m = 0 \end{cases}$$

We can approximate a function $f : [-1, 1] \to \mathbb{R}$ as

$$f(x) = \sum_{n=0}^{N} a_n T_n(x), \qquad a_n = \frac{\langle f, T_n \rangle}{\langle T_n, T_n \rangle},$$

which is we'll call a Chebyshev projection of f.

Uniform Convergence[1]

If f is Lipschitz continuous on $[-1, 1]$, then the Chebyshev projections converge uniformly to f on $[-1, 1]$

[1] L. N. Trefethen, *Approximation Theory and Approximation Practice*, 2013. Theorem 3.1

Convergence Properties

Differentiable Functions[1]

Let $f \in C^{\nu-1}[-1,1]$ and have f^{ν} be of bounded variation. Then the interpolating Chebyshev polynomial, p_n, satisfies:

$$\|f - p_n\|_\infty = \mathcal{O}(n^{-\nu})$$

Analytic Functions[2]

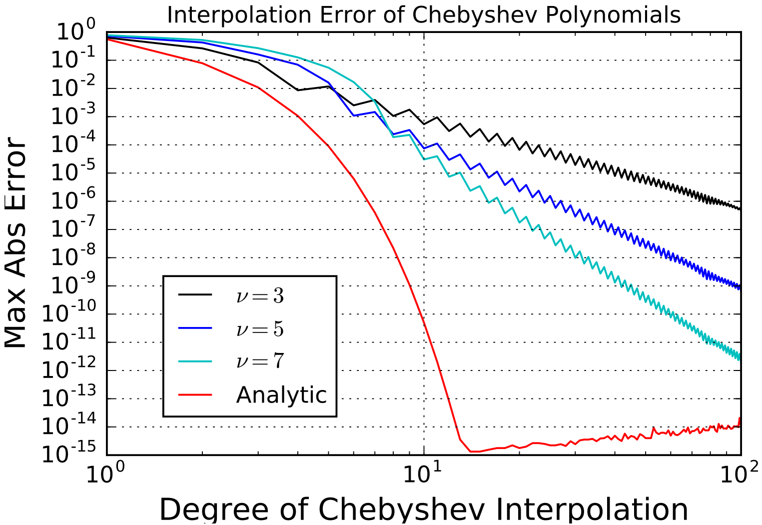
Let f be analytic on $[-1,1]$. Then the interpolating Chebyshev polynomial, p_n, satisfies:

$$\|f - p_n\| = \mathcal{O}(\rho^{-n}),$$

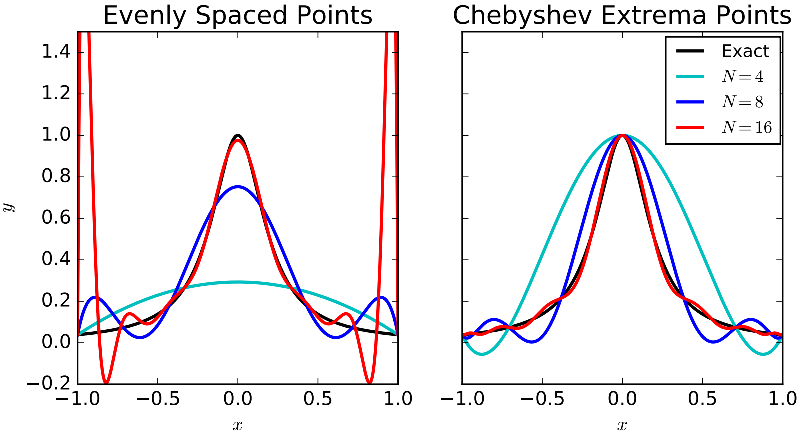
[1] L. N. Trefethen, *Approximation Theory and Approximation Practice*, 2013. Theorem 7.2

[1] Theorem 8.2

Convergence Examples



Chebyshev Interpolation Can Handle the Runge Function



Root Finding: The Companion Matrix Method[1]

Idea: Convert a root x to an eigenvalue of a matrix.
First we start with

$$xT_0(x) = T_1(x)$$

and

$$xT_n(x) = \frac{1}{2}T_{n+1}(x) + \frac{1}{2}T_{n-1}(x), n \geq 1$$

We can arrange the above equation as a matrix equation

$$\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \ddots & \frac{1}{2} \\ 0 & 0 & \cdots & \frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} = x \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{1}{2}T_n(x) \end{pmatrix}$$

We'll denote C to be the LHS matrix

[1] JP Boyd *Finding the Zeros of a Univariate Equation...*, 2013. Appendix C

Now add and subtract away the interpolant, $p_n(x)$

$$C \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} = x \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{1}{2} T_n(x) \end{pmatrix}$$
$$+ \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \gamma \end{pmatrix} \left(a_n T_n(x) + \sum_{j=0}^{n-1} a_j T_j(x) - p_n(x) \right)$$

Setting $\gamma = \frac{1}{2a_n}$ we get:

$$C \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} = x \begin{pmatrix} T_0(x) \\ T_1(x) \\ \vdots \\ T_{n-1}(x) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{1}{2a_n} \end{pmatrix} \left(\sum_{j=0}^{n-1} a_j T_j(x) - p_n(x) \right)$$

The Companion Matrix

Rearranging and setting x to be a root of $p_n(x)$, we end with

$$\begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \ddots & \frac{1}{2} \\ \frac{-a_0}{2a_n} & \frac{-a_1}{2a_n} & \cdots & \frac{1}{2} - \frac{a_{n-2}}{2a_n} & -\frac{a_{n-1}}{2a_n} \end{pmatrix} \mathbf{v} = x\mathbf{v},$$

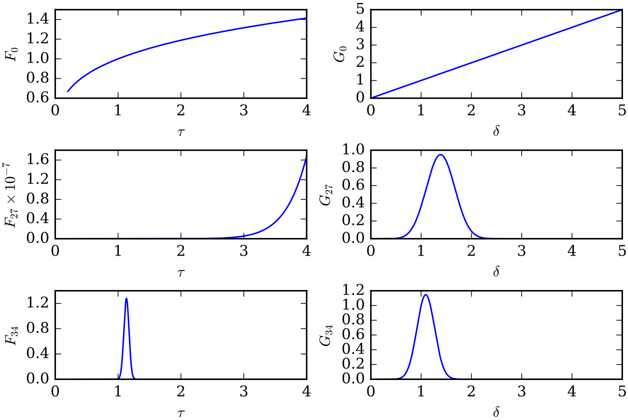
which is an eigenvalue problem whose eigenvalues are the roots of $p_n(x)$. We can now eigenvalue solve to get all roots of $p_n(x)$.

(Boyd, 2013)[1] Shows how to derive companion matrices for a general basis.

[1] JP Boyd *Finding the Zeros of a Univariate Equation...*, 2013. Appendix C

Example EOS

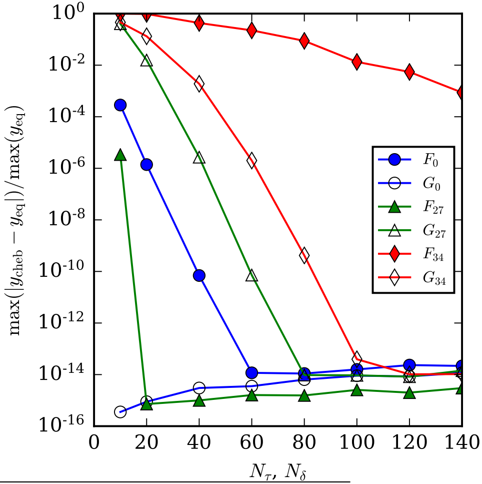
Figure: Example EOS terms for Nitrogen[1]



[1] I. Bell et. al. *Exceptional reliable density solving algorithms for multi parameter mixture models from Chebyshev expansion root finding* 2018.

Effectiveness of Chebyshev Interpolants for Our Application

Figure: Accuracy of Chebyshev Approximations[1]



Speed:

- Have been able to use root finding techniques to get comparable speeds to other options[1]

[1] I. Bell et. al. *Exceptional reliable density solving algorithms for multi parameter mixture models from Chebyshev expansion root finding* 2018.

Why go to Two Dimensions?

- So far we have assumed that we know 1 proprerty
- For Ian Bell's density solver, we assumed we knew the temperature
- The more general problem is finding the temperature and pressure at which two desired thermophysical properties hold

The Problem

Global 2-D Root Finding Problem

We want to find all solutions $\mathbf{x} \in \Omega \subset \mathbb{R}^2$ to

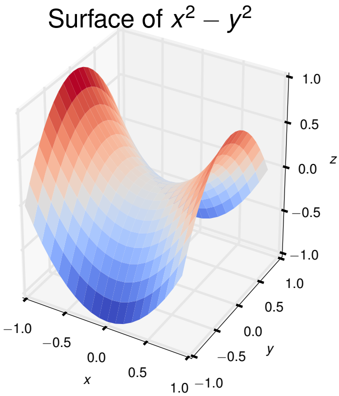
$$\mathbf{F}(\mathbf{x}) = \mathbf{0}$$

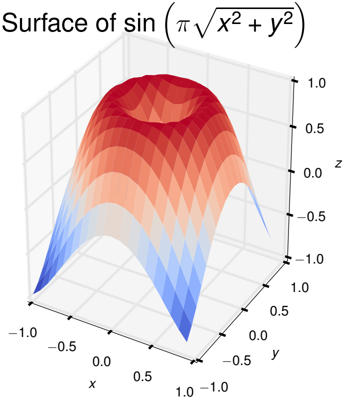
Additional assumptions

- Ω will be a bounded domain and rectangular for now
- Treat **F** as $\begin{pmatrix} f(x,y) \\ g(x,y) \end{pmatrix}$, where $x, y \in \mathbb{R}$ and f, g are scalar functions
- Assume f, g are smooth enough (more on this later)
- Assume finitely many roots

Example

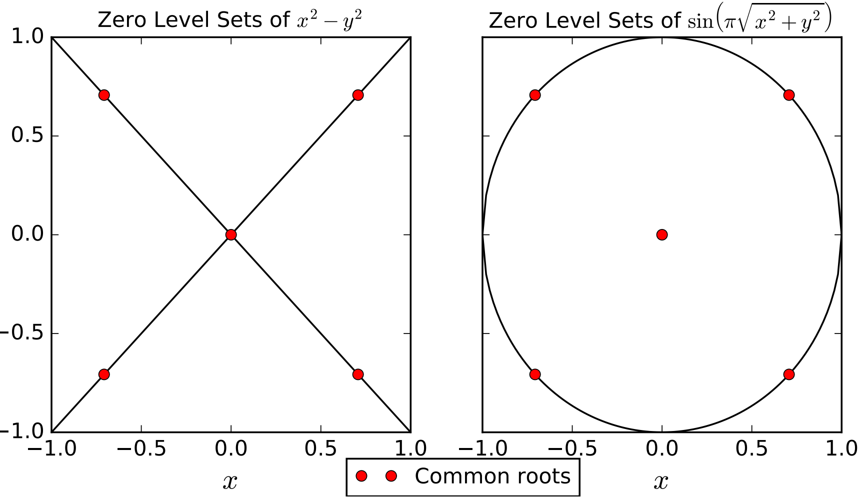
$f(x,y) = x^2 - y^2$ and $g(x,y) = \sin\left(\pi\sqrt{x^2+y^2}\right)$ with the square domain $\Omega = [-1,1]^2$





Example (cont.)

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



A Need for a Method to Find All Roots

- Iterative methods may take multiple runs to find all roots.
- We need a method to find all solutions at once, just like the companion matrix methods in 1-D

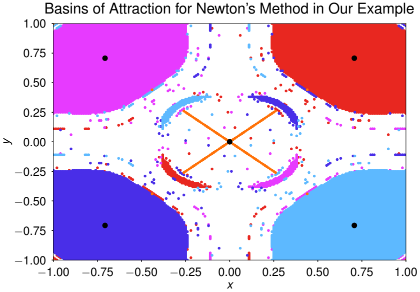


Figure: Initial guesses in white areas did not converge to roots in Ω

Townsend's 2-D Interpolation Idea[1]

Want to express

$$f(x,y) \approx \sum_{i=0}^{n} \sum_{j=0}^{m} T_i(x) T_j(y)$$

in as few 1-D interpolations as possible. One way to do it is express

$$f(x,y) \approx \sum_{i=0}^{K} p_i(x) q_i(y)$$

where p_i, q_i are 1-D Chebyshev expansions K is as small as we can make it to get desired accuracy.

When is K is relatively small compared to the degree of polynomials, Townsend calls it a **Low Rank Approximation** of f

[1] A. Townsend. *Computing with Functions in Two Dimensions*, 2014.

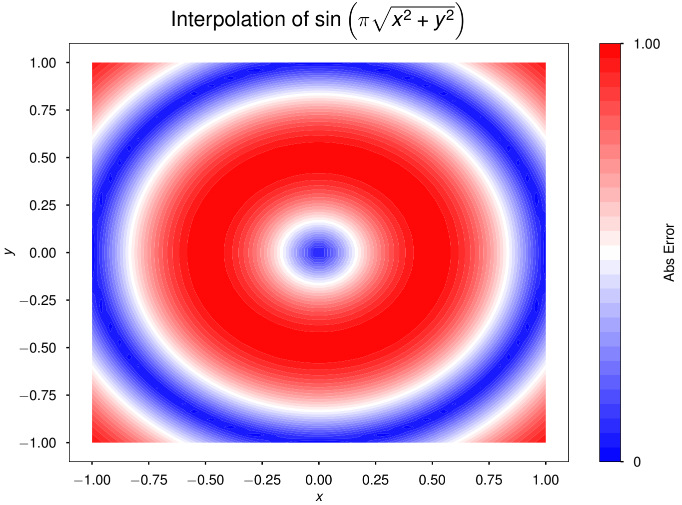
Townsend's 2-D Interpolation Algorithm

- Define our first error function as $e_0(x, y) = f(x, y)$
- Define later error functions as $e_k(x, y) \coloneqq e_{k-1}(x, y) - P_{k-1}(x, y)$ where P_{k-1} is our approximation

Algorithm Outline

- Find (x_k, y_k) s.t. $|e_k(x_k, y_k)| = \max |e_k(x, y)|$
- Do 1-D interpolations of $e_k(x, y_k)$ and $e_k(x_k, y)/e_k(x_k, y_k)$ denoted $p_x(x)$ and $p_y(y)$
- Compute new approximation $P_k(x, y) = P_{k-1}(x, y) + p_x(x)p_y(y)$

Interpolation From Our Example



The Advantage of The Low Rank Approximation

The pivots below are for a 64×64 grid of Chebyshev nodes. Note we do less interpolations than if we used all 64^2 points

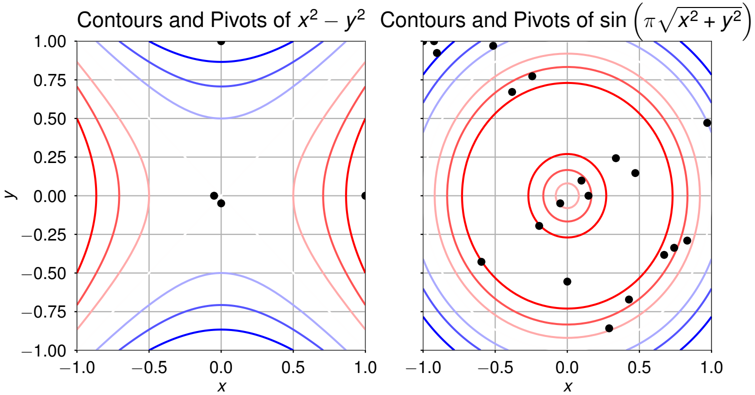
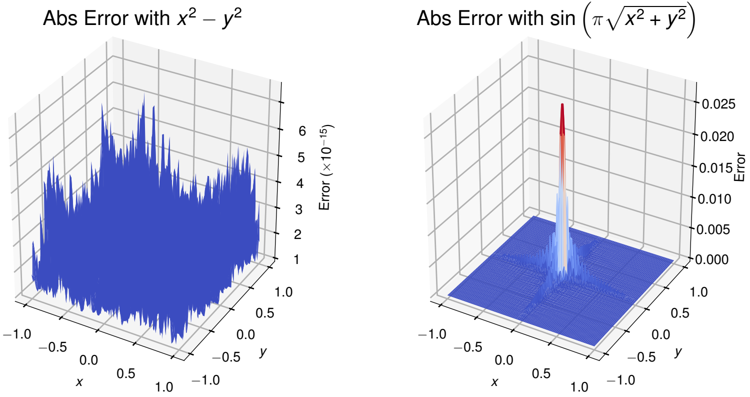


Figure: Plot of the contours of our example functions with pivots from the algorithm

Approximations of Our Example Functions

- 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 Resultant Method

- From our Chebyshev approximations $p_f(x, y), p_g(x, y)$, we can construct a Bézout matrix polynomial $B(x)$
- $\det(B(x_0)) = 0 \iff p_f(x_0, \cdot)$ and $p_g(x_0, \cdot)$ have common root

If p_f, p_g are of degree $(m_f, n_f), (m_g, n_g)$ respectively, then the resulting form of the matrix polynomial of degree M is

$$B(x) = \sum_{i=0}^{M} B_i T_i(x)$$

- B_i are square matrices of size $n = \max(n_f, n_g)$ and $M \leq m_f + m_g$.
- Solving $\det(B(x_0)) = 0$ involves linearizing $B(x)$[1]

[1] Y. Nakatsukasa *Computing the Common Zeros of Two Bivariate Functions Via Beout Resultants* 2014.

Solving the Matrix Polynomial Eigenvalue Problem[1]

Expressing $B(x) = \sum_{i=0}^{M} B_i T_i(x)$, then we can solve $\det\left(B(x)\right) = 0$ by solving the generalized eigenvalue problem

$$\frac{1}{2}\begin{pmatrix} -B_{M-1} & I_n - B_{M-2} & -B_{M-3} & \cdots & -B_0 \\ I_n & 0 & I_n & & \\ & \ddots & \ddots & \ddots & \\ & & I_n & 0 & I_n \\ & & & 2I_n & 0 \end{pmatrix}\mathbf{v}$$

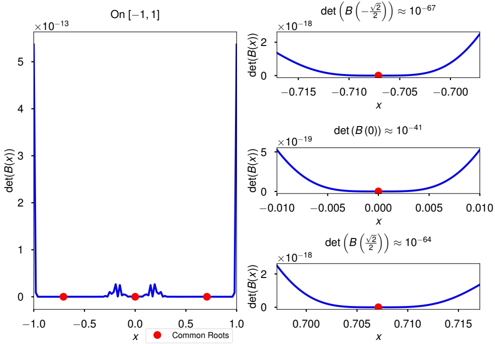
$$= \lambda \begin{pmatrix} B_M & & & \\ & I_n & & \\ & & \ddots & \\ & & & I_n \end{pmatrix}\mathbf{v}$$

Has computational complexity of $\mathcal{O}\left(M^3 n^3\right)$

[1] Y. Nakatsukasa *Computing the Common Zeros of Two Bivariate Functions Via Bezout Resultants* 2014.

Conditioning of the Bézout Matrix Polynomials

- The Bézout matrix polynomial technique can square the condition number of the common root.[1]
- The `chebfun` algorithm refines the roots by recomputing the matrix polynomial problem on a zoomed in region of the root

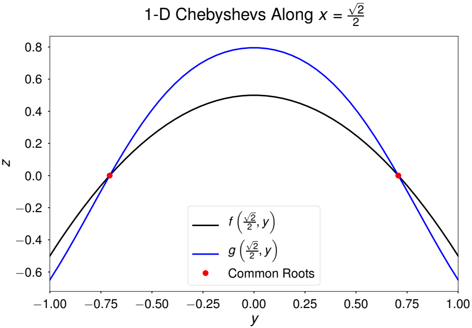


[1] Y. Nakatsukasa *Computing the Common Zeros of Two Bivariate Functions Via Bezout Resultants* 2014.

1-D Root Finding

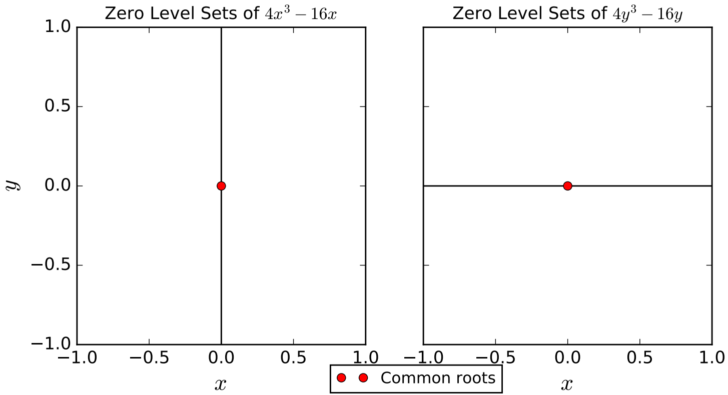
1-D Root Finding

- We now have the possible x values for where there are common roots
- Employ a companion matrix method finding the roots of 1-D Chebyshev polynomials



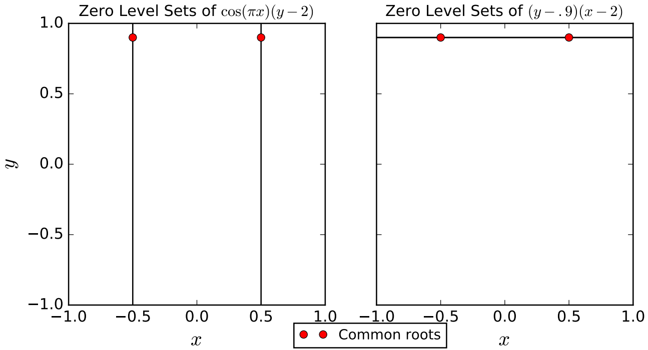
Example 1

	$\|\cdot\|_2$ Error	Time (s)
`ChebTools`	6.97×10^{-32}	0.004268
`chebfun`	7.7×10^{-16}	0.522



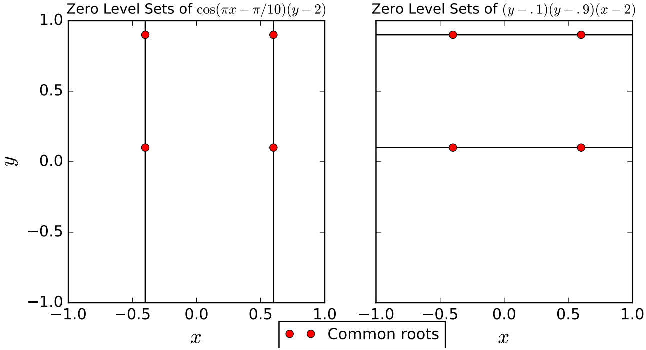
Example 2

	$\|\cdot\|_2$ Error	Time (s)
`ChebTools`	6.21×10^{-16}	214.059
`chebfun`	2.92×10^{-10}	0.294



Example 3

	$\|\cdot\|_2$ Error	Time (s)
`ChebTools`	3.24×10^{-16}	195.903
`chebfun`	2.77×10^{-11}	0.296



Application Motivates Current Work

Subdivision for Non-rectangular Domains

- Right now, we don't have a subdivision technique to reduce the size of the matrix polynomials
- We want a subdivision technique that will be able to handle non-rectangular domains
- Empirical equations of state in thermodynamics have ranges of validity which are not rectangular domains
- Solutions outside the domain will not make physical sense
- Some properties are not defined at certain points (ex: Critical Point)
- The work done by Townsend can not handle this problem in general

Example Domains for Water

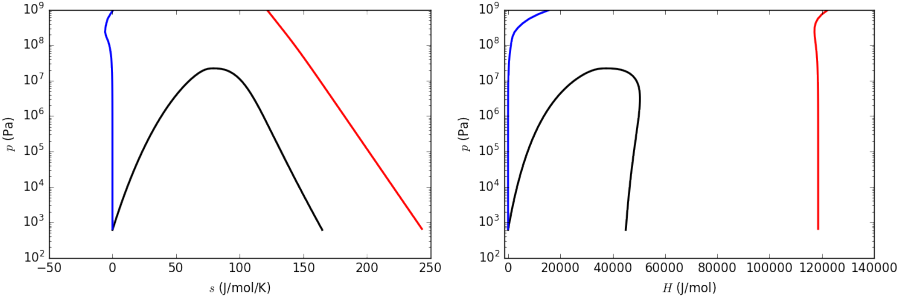


Figure: Examples of liquid/vapor equilibrium region for water.

Domain with Critical Point

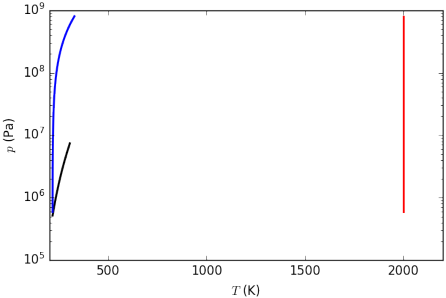


Figure: Example Domain with CO_2 that has a critical point

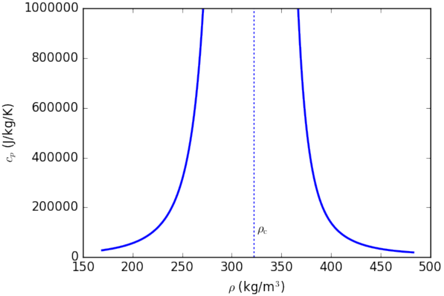


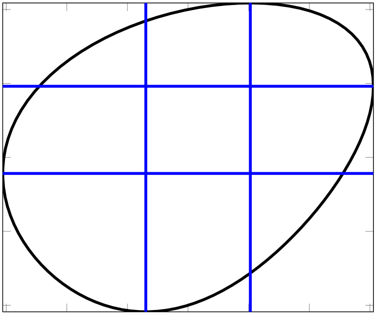
Figure: The specific heat of water becomes undefined at the critical point

Our Subdivision Idea

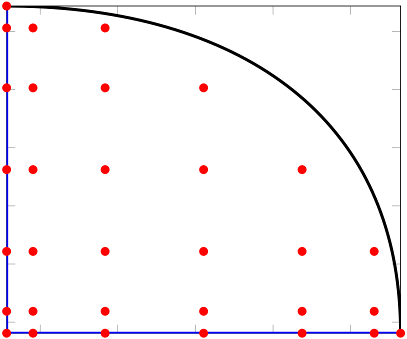
- Subdivide where the boundary is flat, vertical, or has a discontinuity in the derivative
- Our boundary curve can then be represented as a 1 variable function
- Will allow for quick checking of whether points are inside the domain
- Easy to do coordinate transformations to a rectangle

Subdivision Example

Interior of the closed curve $(1.5\cos t + .15\sin 2t, \sin t + .3\cos t)$ with $t \in [0, 2\pi]$



(a) Boundary in black and initial subdivisions in blue.



(b) Interior 7x7 Chebyshev nodes in red.

Figure: Example domain on the left and the upper right subdomain on the right

Future Work

For Non-Rectangular Domains

- Further develop ideas for subdivision methods, such as stopping criterion
- Look into root finding techniques for Chebyshev polynomials other than Bézout Resultant Method
    - Root finding in higher dimensions is needed for mixture EOS
    - Resultant methods will not generalize well for high dimensions[1]
    - Undergrad group at BYU working on applying algebraic geometry ideas to the root finding process

Software:

- Introduce GPU and parallel computing to the `ChebTools` library
- Add other features to the library
- We are looking for more developers
- Link: https://github.com/usnistgov/ChebTools

[1] V. Noferini *Numerical Instability of Resultant Methods for Multidimensional Rootfinding* 2016.

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Questions?