Preface

"Rootfinding was much more important than we expected ... Zeros, maxima, minima—all depend on rootfinding."

—Lloyd N. "Nick" Trefethen, FRS, U.S. National Academy of Engineering, Past President of SIAM, at the Workshop of the *Chebfun* Project, Oxford, September, 2012.

The goal of this book is to teach the art of finding the root of a single algebraic equation or a pair of such equations. We shall quote theorems and theory as necessary, but this is not primarily a book of theorems and lemmas. No rootfinder was ever bailed out by a Beppo–Levi space. It is rather a narrative cookbook. By "cookbook," we mean that it is filled with simple and practical recipes for solving various classes of nonlinear equations. By "narrative," we mean that the recipes are not presented in isolation from one another but rather are woven into a connected whole. At the expense of a little redundancy, the book is structured so that one can dip into a single chapter and find a recipe, but collectively the concatenation of algorithms and how and why they work tell deeper stories about approximation, inversion, asymptotics, and iteration, as in a traditional textbook.

Rootfinding is fundamental to junior high algebra, but its apparent simplicity is deceiving. Mathematicians know that a subset of univariate zero-hunting—polynomial equations—spawned the immense power of group theory through Evariste Galois and his successors. Engineers and applied mathematicians know that the classroom exercise of generating a single number by bisection or the secant iteration is as far removed from engineering reality as a military ball is from trench warfare. Scientists do not want just numbers, mere isolated roots, but rather need to trace complete solution branches, including multiple root curves and the bifurcation points that connect them. Solutions to $f(x)=0$ are not isolated but are plane curves when there is a single parameter λ, the zero-valued contours of the bivariate function $f(x;\lambda)$. When the root depends upon two parameters (μ,λ), the zeros form a solution surface in the three-dimensional space spanned by (x,λ,μ), a manifold whose folds and foldings are the topological raw material of catastrophe theory. Zeros are easily missed in a thicket of intersecting solution branches and surfaces. The author's interest in rootfinding began with such a fiasco.

As a graduate student nearly 40 years ago, I solved an ODE eigenproblem with an interior singularity by marching by a Runge–Kutta scheme from each boundary to near the singularity, filling the gap with a power series. "Shooting," as this ODE-solving strategy is called, requires solving a single transcendental equation in a single unknown (the eigenvalue) to smoothly join the two half-solutions. Easy, seemingly, even though the roots were complex valued and many. Later, I found a better way, which was to apply a Chebyshev polynomial spectral method on a path that detoured off the real axis around the singularity—and discovered I had missed roots and therefore entire eigenmodes. Oops!

The Chebyshev-proxy method, which is described here in the form of a greatly expanded version of my *SIAM Review* article [96], has, I am happy to say, removed most of the uncertainty in the computation of all the zeros of an analytic function $f(x)$ on a real interval $x \in [a, b]$. The book gives an extensive discussion of similar algorithms for searching for zeros in disks or other areas of the complex plane. It also describes adaptive Chebyshev polynomial interpolation, which generates the proxies, generalizations to an unbounded interval, and symmetry-exploiting variants.

But what if the solution branch is singular at one or both endpoints, or $f(x)$ itself has pathologies? There is a sort of arithmurgical Murphy's law that solution branches end in singularities quite often in applications—see the humble arcsine, arccosine, and arctangent, which combine singularities with an infinite number of branches. Fortunately, modern Chebyshev polynomial and Fourier spectral methods are up to almost anything, as explained throughout the book with a profusion of examples.

An infinity of roots is best handled by perturbation theory. My student-self of 40 years ago is intensely jealous of my ready access to modern computer algebra systems like Maple, Mathematica, and Reduce, which can calculate a perturbation series to 200 terms in a few seconds and then extend the domain of convergence by forming Padé approximants and Hermite–Padé ("Shafer") approximants from the series.

Consequently, this book has a chapter entirely devoted to regular perturbation series for roots. It is unusual to combine numerical algorithms with perturbation series and computer algebra in a single volume, but it is highly appropriate here. The roots of J-type Bessel functions, for example, are best calculated by a mathematical partnership: the Chebyshev-proxy-companion matrix method for small zeros and asymptotic series for the infinite number of larger roots.

Murphy's law applies to analytical methods, too, of course, so there is also a chapter on *singular* perturbation series. These may be loosely defined as expansions that combine powers of ϵ, the small parameter, with powers of $\log(\epsilon)$ or perhaps $\exp(-1/\epsilon)$, or even $\log(\log(\epsilon))$. It turns out that by using Newton's iteration to discover the form of the series and by employing a bivariate expansion in (ϵ, δ) as though ϵ and $\delta \equiv \exp(-1/\epsilon)$ are two completely independent parameters, singular perturbation series can be very effective, too.

Computer algebra also greatly increases the range of explicit methods; Maple and Mathematica can often find solutions in an instant that would baffle the mathematician. But an explicit solution in terms of the Lambert W-function is not very useful if you know nothing about $W(\lambda)$, and human intuition can still give semi-intelligent software essential succor. The book therefore has a chapter on explicit solutions: polynomials, trigonometric polynomials and more exotic transcendental functions all fall to analytic strategies at least sometimes.

The chapters on the cubic, quartic, and quadratic equations were also the result of authorial epiphanies. For 40 years, I've investigated a class of planetary-scale oceanic and atmosphere and traveling waves called "equatorial waves." Each of the three wave species travels at a speed that is a real root of a cubic equation. I had studied Rossby and gravity waves for over a decade, published a dozen papers, and attended multiple Equatorial Theoretical Panel workshops before I discovered, in an article by Arthur Loesch, that there was a lovely arccosine formula that gives, without error, all three real roots of a cubic equation. It is not merely a personal failure, but a failure of the whole community, that equatorial dynamicists calculated phase speeds by crude approximations or Newton's iteration when something much better was known in the nineteenth century. Yet it is not even mentioned in the *Handbook of Mathematical Functions* and its ilk.

My second epiphany came from reading early chapters of Werner Rheinboldt's *Numerical Analysis of Nonlinear Parameterized Equations*. He explained that by dividing out the coefficient of the highest power and then substituting $x \to y + a$, where a is chosen to eliminate the coefficient of y^2, the general cubic equation can be trivially condensed to the "reduced cubic," $y^3 - \tau y + \xi = 0$. I had learned roots only as disembodied numbers; even the zeros of the same polynomial had no interrelationships. But Rheinboldt showed that all real roots in the entire τ-ξ parameter space lay on a single smooth surface in the three-dimensional space (τ, ξ, x). When the surface is folded, a vertical line through a point in the τ-ξ plane will intersect the solution surface at three points. In parts of the parameter plane where there is but one real root, the surface lacks folds. Double roots occur on the curves that are the edges of the folds where the slope of the surface is infinite. The origin $\tau = \xi = 0$ is the triple point where there are three equal roots, all zero.

In the 1960s, topologists had their own epiphany: folds and isolated triple points exhaust the possibilities for smooth manifolds with two parameters. Solution surfaces and equilibrium states of general transcendental functions can be smoothly mapped into the solution surface of the cubic equation. This topological approach to physics became known as "catastrophe theory"; the cubic polynomial equation is the prototype for the "cusp catastrophe." Similarly, the three-parameter surface for the zeros of the reduced quartic polynomial equation is the master pattern for the "swallowtail catastrophe". Hence our very thorough treatment of polynomial equations, especially those of low degree.

There are two reasons why this book, despite its title, has a long chapter on solving *pairs* of equations in *two* unknowns. First, many of the key ideas that have been so fruitful for univariate zero-hunting extend, at least haltingly, to bivariate systems, and it would be a pity to omit the extensions. The second reason is that the bifurcation points of univariate solution branches $x(\lambda)$ are solutions to a *pair* of equations, $f(x,\lambda) = 0, \partial f / \partial x(x,\lambda) = 0$, in the two unknowns (x, λ). Thus we can only complete our story of one equation in one unknown by discussing at least the basic strategies for zeros in two unknowns.

Oracles, expansions, iterations, polynomialization—Rootfinding is sometimes easy and sometimes soul-despairingly hard, especially if the goal is to find zeros not number by number but rather branch by branch. Even so, there is nothing in this book that requires more background than an engineer's standard undergraduate class. Previous completion of a numerical analysis class will allow some skipping and provide a useful perspective, but even that is not absolutely necessary.

The themes developed here are good background for assaulting the profusion of books that solve N equations in N unknowns. However, the special cases treated here—$N = 1$, with one chapter on $N = 2$—allow special tricks like the Chebyshev-proxy algorithm that have no counterparts for general N. Perhaps half the book is about general-N theory illustrated in the simplest form, and half is orthogonal to all the vast general-N literature. But this book is mostly a catalogue of what works. It includes many detailed case studies in this spirit.

The mathematician will find some deep themes and beautiful theorems here. Some interesting research topics and open questions are described along the way as well. However, the combination of the Chebyshev-proxy rootfinder with endgame iterations is very reliable.

In my other life in geophysical fluid dynamics and nonlinear waves, I solve problems and teach engineers how to solve problems. In that spirit, this work serves as a handbook of solving one important class of problems with as little style and finesse and as much reliability and conceptual simplicity as possible.

Good luck!

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I dedicate this book to the memory of my brother, James C. Boyd, (1940–2011), my third parent, who taught me nothing about science and mathematics but lots about everything else. He was an elementary science teacher, assistant superintendent, and elementary school principal. His school honored him by naming its library after him. Although this book will never be in an elementary school library, I think this dedication would please him.