

CSE276C - Root Finding

Henrik I. Christensen



Computer Science and Engineering
University of California, San Diego
<http://cri.ucsd.edu>

October 2024

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

- Root finding or detection of zero-crossings, i.e., $f(x) = 0$
- Numerous applications in robotics
 - 1 Numerical solution to inverse kinematics
 - 2 Collision detection in planning and navigation
 - 3 Detection of optimal control strategies
- Two main cases:
 - 1 Non-linear systems
 - 2 Polynomial systems - factorization

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Braketing

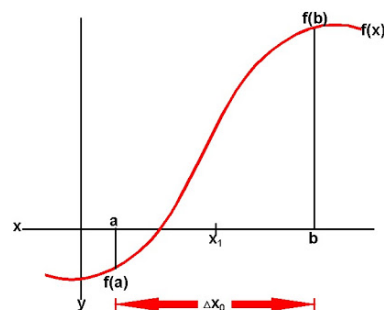
- First problem is to know where to look for roots.
- What would be your strategy?
- Can we identify an interval $[a, b]$ where $f(x)$ changes sign, i.e:

$$f(a)f(b) < 0$$

- Once we have an interval/bracket we can refine the strategy
- Good strategies?
 - Hill climbing/decent
 - Sampling
 - Model information

Bracketing

- Consider this function, what would be your strategy?



Bisection

- Given $a, b, f(a), f(b)$ evaluate f at

$$c = \frac{a + b}{2}$$

decision

$$f(a)f(c) < 0 \quad ? \quad \begin{cases} \text{Yes} & I_{\text{new}} = [a, c] \\ \text{No} & I_{\text{new}} = [c, b] \end{cases}$$

Bisection convergence

- The interval size is changing

$$s_{n+1} = \frac{s_n}{2}$$

- number of evaluations is

$$n = \log_2 \frac{s_0}{s}$$

- Convergence is considered **linear** as

$$s_{n+1} = \text{const } s_n^m$$

with $m = 1$.

- When $m > 1$ convergence is termed super linear

Secant Method

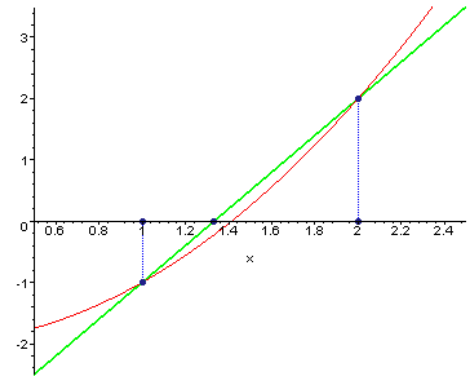
- If you have a smooth function. Take $a, b, f(a), f(b)$
- Computer intersection point

$$\Delta = \frac{f(a) - f(b)}{a - b}$$

$$c\Delta + f(a) = 0 \Leftrightarrow c = \frac{-f(a)}{\Delta}$$

so $d = a + c$

repeat for convergence



Secant Method

- The Secant Method is not guaranteed to pick the two points with opposite sign
- Secant is super-linear with a convergence rate of

$$\lim_{k \rightarrow \infty} |s_{k+1}| = \text{const} |s_k|^{1.618}$$

- When could we be in trouble?
- When you have major changes in the 2nd derivative close to root

- Principle similar to Secant
- Always choose the interval with end-point of opposite sign
- Regula-falsi also has super-linear convergence, but harder to show

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Brent's Method

- We can leverage methods from interpolation theory
- Assume we have three points $(a, f(a))$, $(b, f(b))$, $(c, f(c))$
- We can leverage Lagrange's method

$$x = \frac{(y-f(a))(y-f(b))c}{(f(c)-f(a))(f(c)-f(b))} + \frac{(y-f(b))(y-f(c))a}{(f(a)-f(b))(f(a)-f(c))} + \frac{(y-f(c))(y-f(a))b}{(f(b)-f(c))(f(b)-f(a))}$$

- if we set $y = 0$ and solve for x we get

$$x = b + \frac{P}{Q}$$

Brent's Method (cont)

- such that

$$P = S(T(R - T)(c - b) - (1 - R)(b - a))$$
$$Q = (T - 1)(R - 1)(S - 1)$$

- where $R = f(b)/f(c)$, $S = f(b)/f(a)$, $T = f(a)/f(c)$
- So b is expected to be “the estimate” and $\frac{P}{Q}$ is a correction term.
- When $\frac{P}{Q}$ is too small it is replaced by a bi-section step
- Brent is generally considered the recommended method.

Newton Rapson's Method

- How can we use access to 1st order gradient information?
- For well behaved functions we can use a Taylor approximation

$$f(x + \delta) \approx f(x) + f'(x)\delta + \frac{f''(x)}{2}\delta^2 + \dots$$

- for a small δ and well behaved functions higher order terms are small
- if $f(x + \delta) = 0$ we have

$$\begin{aligned} f(x) + f'(x)\delta &= 0 \Leftrightarrow \\ \delta &= -\frac{f(x)}{f'(x)} \end{aligned}$$

- A search strategy is then

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Newton-Raphson - Notes

- In theory one can approximate the gradient

$$f'(x) = \frac{f(x + dx) - f(x)}{dx}$$

- For many cases this may not be a good approach
 - 1 for $\delta \gg 0$ the linearity assumption is weak
 - 2 For $\delta \approx 0$ the numerical accuracy can be challenging

Multi-variate Newton Raphson

- What is we have to solve

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

- A simple example

$$f_i(x_0, x_1, \dots, x_{n-1}) \quad i = 0, \dots, n-1$$

we get

$$f_i(\vec{x} + \delta\vec{x}) = f_i(\vec{x}) + \sum_{j=0}^{n-1} \frac{\partial f_i}{\partial x_j} \delta x_j + O(\delta\vec{x}^2)$$

Multi-variate case

- The matrix of partial derivatives

$$J_{ij} = \frac{\partial f_i}{\partial x_j}$$

- is termed the Jacobian.
- We can now formulate

$$f_i(\vec{x} + \delta\vec{x}) = f_i(\vec{x}) + J\delta\vec{x} + O(\delta\vec{x}^2)$$

- we can then as before rewrite

$$J\delta\vec{x} = -f \text{ solve w. LU}$$

or

$$\vec{x}_{new} = \vec{x}_{old} + \delta\vec{x}$$

for some cases an improved strategy is

$$\vec{x}_{new} = \vec{x}_{old} + \lambda\delta\vec{x}$$

where $\lambda \in [0, 1]$ to control convergence

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Search Summary

- Simple search strategies for detect zeros / roots
- Bracketing is essential to determine the locations to search
- Brent's method in general robust strategy for root finding
- Newton-Raphson effective (for small δ) and when gradient info is available
- Generalization in most cases is relative straight forward

Questions

Roots of polynomials

Roots of Polynomials

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Introduction

- Earlier we looked at direct search for roots
- Bracketing was the way to limit the search domain
- Brent's method was a simple strategy to do search
- What if we have a polynomial?
 - 1 Can we find the roots?
 - 2 Can we simplify the polynomial?
- Lets explore this

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Low order polynomials

- We have closed form solutions to roots of polynomials up to degree 4
- Quadratics

$$ax^2 + bx + c = 0, \quad a \neq 0$$

has two roots

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

we have real unique, dual or imaginary solutions

Cubics

- The cubic equation

$$x^3 + px^2 + qx + r = 0$$

can be reduced using substitution

$$x = y - \frac{p}{3}$$

to the form

$$y^3 + ay + b = 0$$

where

$$\begin{aligned} a &= \frac{1}{3}(3q - p^2) \\ b &= \frac{1}{27}(2p^3 - 9pq + 27r) \end{aligned}$$

the condensed form has 3 roots

$$\begin{aligned} y_1 &= A + B \\ y_2 &= -\frac{1}{2}(A + B) + \frac{i\sqrt{3}}{2}(A - B) \\ y_3 &= -\frac{1}{2}(A + B) - \frac{i\sqrt{3}}{2}(A - B) \end{aligned}$$

where

$$A = \sqrt[3]{-\frac{b}{2} + \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}} \quad B = \sqrt[3]{-\frac{b}{2} - \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}}$$

Cubic (cont)

- We have three cases:

- 1 $\frac{b^2}{4} + \frac{a^3}{27} > 0$: one real root and two conjugate roots
- 2 $\frac{b^2}{4} + \frac{a^3}{27} = 0$: three real roots of which at least two are equal
- 3 $\frac{b^2}{4} + \frac{a^3}{27} < 0$: three real roots and unequal roots

- For the equation

$$x^4 + px^3 + qx^2 + rx + s = 0$$

we can apply a similar trick

$$x = y - \frac{p}{4}$$

to get

$$y^4 + ay^2 + by + c = 0$$

where

$$\begin{aligned} a &= q - \frac{3p^2}{8} \\ b &= r + \frac{p^3}{8} - \frac{pq}{2} \\ c &= s - \frac{4p^4}{256} + \frac{p^2q}{16} - \frac{pr}{4} \end{aligned}$$

Quartics (cont.)

- The reduced equation can be factorized into

$$z^3 - qz^2 + (pr - 4s)z + (4sq - r^2 - p^2s) = 0$$

if we can estimate z_1 of the above cubic then

$$\begin{aligned} x_1 &= -\frac{p}{4} + \frac{1}{2}(R + D) \\ x_2 &= -\frac{p}{4} + \frac{1}{2}(R - D) \\ x_3 &= -\frac{p}{4} - \frac{1}{2}(R + E) \\ x_4 &= -\frac{p}{4} - \frac{1}{2}(R - D) \end{aligned}$$

where

$$\begin{aligned} R &= \sqrt{\frac{1}{4}p^2 - q + z_1} \\ D &= \sqrt{\frac{3}{4}p^2 - R^2 - 2Q + \frac{1}{4}(4pq - 8r - p^3)R^{-1}} \\ E &= \sqrt{\frac{3}{4}p^2 - R^2 - 2Q - \frac{1}{4}(4pq - 8r - p^3)R^{-1}} \end{aligned}$$

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

Root Counting

- Consider a polynomial of degree n :

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

- if a_i are real the roots are real or complex conjugate pairs.
- $p(x)$ has n roots
- Descartes rules of sign:
 - “The number of positive real zeroes in a polynomial function $p(x)$ is the same or less than by an even numbers as the number of changes in the sign of the coefficients. The number of negative real zeroes of the $p(x)$ is the same as the number of changes in sign of the coefficients of the terms of $p(-x)$ or less than this by an even number”

- Consider

$$p(x) = x^5 + 4x^4 - 3x^2 + x - 6$$

- So it must have 3 or 1 positive root and
- and it must have 2 or 0 negative roots

Sturms theorem

- We can derive a sequence of polynomials
- Let $f(x)$ be a polynomial. Denote the original $f_0(x)$ and the derivative $f'(x) = f_1(x)$. Consider

$$\begin{aligned}f_0(x) &= q_1(x)f_1(x) - f_2(x) \\f_1(x) &= q_2(x)f_2(x) - f_3(x) \\&\vdots \\f_{k-2}(x) &= q_{k-1}(x)f_{k-1}(x) - f_k(x) \\f_{k-1}(x) &= q_k(x)f_k(x)\end{aligned}$$

- The theorem
 - The number of distinct real zeros of a polynomial $f(x)$ with real coefficients in (a, b) is equal to the excess of the number of changes of sign in the sequence $f_0(a), \dots, f_{k-1}(a), f_k(a)$ over the number of changes of sign in the sequence $f_0(b), \dots, f_{k-1}(b), f_k(b)$.

Sturm - example

- Consider the polynomial

$$x^5 + 5x^4 - 20x^2 - 10x + 2 = 0$$

The Sturm functions are then

$$\begin{aligned}f_0(x) &= x^5 + 5x^4 - 20x^2 - 10x + 2 \\f_1(x) &= x^4 + 4x^3 - 8x - 2 \\f_2(x) &= x^3 + 3x^2 - 1 \\f_3(x) &= 3x^2 + 7x + 1 \\f_4(x) &= 17x + 11 \\f_5(x) &= 1\end{aligned}$$

Sturm example (cont)

	$-\infty$	-10	-5	-4	-3	-2	-1	0	1	2	5	10	∞
f_0	-	-	-	-	+	-	-	+	-	+	+	+	+
f_1	+	+	+	+	-	-	-	-	-	+	+	+	+
f_2	-	-	-	-	-	+	+	-	+	+	+	+	+
f_3	+	+	+	+	+	-	-	+	+	+	+	+	+
f_4	-	-	-	-	-	-	-	+	+	+	+	+	+
f_5	+	+	+	+	+	+	+	+	+	+	+	+	+
var.	5	5	5	5	4	3	3	2	1	0	0	0	0

- So roots between $(-4, -3)$, $(-3, -2)$, $(-1,0)$, $(0,1)$ and $(1,2)$

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

- Once you have a root r you can deflate a polynomial

$$p(x) = (x - r)q(x)$$

- As the degree decreases the complexity of root finding is simplified.
- One can use Horner's scheme

$$p(x) = b_0 + (x - r)(b_n x^{n-1} + \dots + b_2 x + b_1)$$

as r is a root $b_0 = 0$ so

$$q(x) = b_n x^{n-1} + \dots + b_2 x + b_1$$

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

- Remember we can do root search/refinement

$$x_{k+1} = x_k - \frac{p(x_k)}{p'(x_k)}$$

we know that

$$p(x) = p(t) + (x - t)q(x)$$

So $p'(t) = q(t)$ or

$$q(x) = \frac{p(x)}{x - t}$$

- If $p(x)$ has double roots it could be a challenge

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

- Newton's Method is local and sensitive to seed guess
- Müllers method is more global
- Based on a quadratic interpolation
- Assume you have three estimates of the root: x_{k-2}, x_{k-1}, x_k
- Interpolation polynomial

$$p(x) = f(x_k) + f[x_{k-1}, x_k](x - x_k) + f[x_{k-2}, x_{k-1}, x_k](x - x_k)(x - x_{k-1})$$

- Using the equality

$$(x - x_k)(x - x_{k-1}) = (x - x_k)^2 + (x - x_k)(x_k - x_{k-1})$$

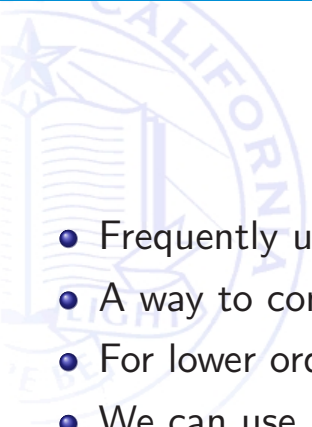
we get

$$p(x) = f(x_k) + b(x - x_k) + a(x - x_k)^2$$

which we can solve for $p(x) = 0$

Outline

- 1 Introduction
- 2 Bracketing
 - Bi-section
 - Secant
 - Regula Falsi / False Position
- 3 Root Finding
 - Brent's Method
 - Newton-Raphson's Method
- 4 Search Summary
- 5 Polynomial Roots - Introduction
- 6 Roots of Low Order Polynomials
- 7 Root Counting
- 8 Deflation
- 9 Newton's Method
- 10 Müller's Method
- 11 Summary

- 
- Frequently using a polynomial refactorization is more stable
 - A way to compress data into a semantic form
 - For lower order polynomials we have closed for solutions
 - We can use Descartes rules, ... to bracket roots
 - We can find roots and reduce polynomials
 - Newton's method is a simple local rule, but could be noisy
 - Mullers method is a way to solve it more generally
 - Lots of methods available for special cases