

# CSE276C - Root Finding

Henrik I. Christensen



Computer Science and Engineering  
University of California, San Diego

<http://cri.ucsd.edu>

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# 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
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# Introduction

- 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

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# Braketing

- First problem is to know where to look for roots.
- What would be your strategy?

# Braketing

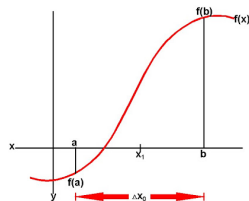
- First problem is to know where to look for roots.
- What would be your strategy?
- Can we identify an interval  $[a, b]$  where  $f(x)$  changes sign, i.e:

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

- 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

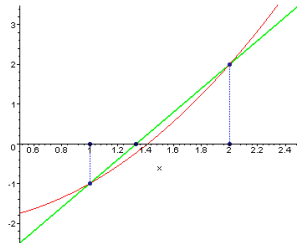
- If you have a smooth function. Take  $a$ ,  $b$ ,  $f(a)$ ,  $f(b)$
- Computer intersection point

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

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

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?

# 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

# Regula Falsi / false position



- 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

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# 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

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

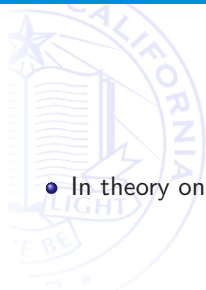
- for a small  $\delta$  and well behaved functions higher order terms are small
- if  $f(x + \delta) = 0$  we have

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

- 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

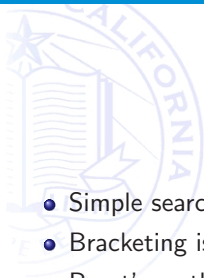
$$\vec{x}_{new} = \vec{x}_{old} + \lambda\delta\vec{x}$$

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

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# 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  $\delta$ ) and when gradient info is available
- Generalization in most cases is relative straight forward



# Questions



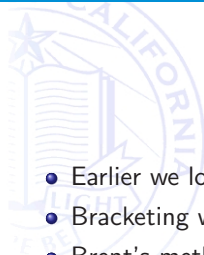
## Roots of Polynomials



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# 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

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# 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

# Quartics

- 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

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



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# 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  $f_0(a), \dots, f_{k1}(a), f_k(a)$  over the number of changes of sign in the sequence  $f_0(b), \dots, f_{k1}(b), f_k(b)$ .

# Sturm - example

- Consider the polynomial

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

The Sturm functions are then

$$f_0(x) = x^5 + 5x^4 - 20x^2 - 10x + 2$$

$$f_1(x) = x^4 + 4x^3 - 8x - 2$$

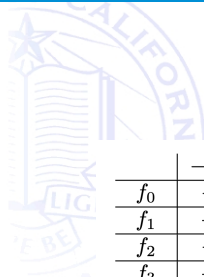
$$f_2(x) = x^3 + 3x^2 - 1$$

$$f_3(x) = 3x^2 + 7x + 1$$

$$f_4(x) = 17x + 11$$

$$f_5(x) = 1$$

# Sturm example (cont)



	$-\infty$	-10	-5	-4	-3	-2	-1	0	1	2	5	10	$\infty$
$f_0$	-	-	-	-	+	-	-	+	-	+	+	+	+
$f_1$	+	+	+	+	-	-	-	-	-	+	+	+	+
$f_2$	-	-	-	-	-	+	+	-	+	+	+	+	+
$f_3$	+	+	+	+	+	-	-	+	+	+	+	+	+
$f_4$	-	-	-	-	-	-	-	+	+	+	+	+	+
$f_5$	+	+	+	+	+	+	+	+	+	+	+	+	+
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  $(1, 2)$

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# Deflation

- 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

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

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# Newton's Method

- 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

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# Müllers Method

- 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  $p(x) = 0$

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# 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