CSE276C - Root Finding

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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. Summary

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

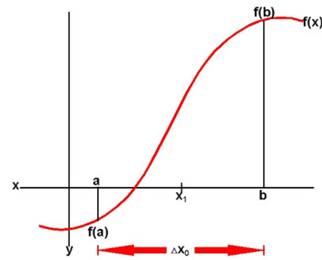
- First problem is to know where to look for roots.
- What would be your strategy?
- Can we identify an interval $[a, b]$ where f(x) changes sign, i.e:

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

- 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

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

Bisection convergence

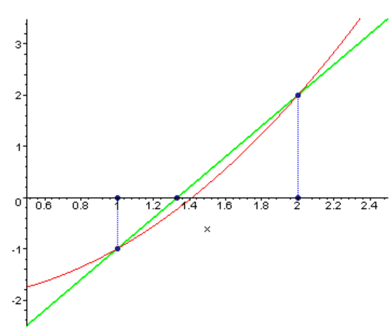
- The interval size is changing
$$s_{n+1} = \frac{s_n}{2}$$
- number of evaluations is
$$n = \log_2 \frac{s_0}{s}$$
- Convergence is considered **linear** as
$$s_{n+1} = \text{ const } s_n^m$$
with m = 1.
- When $m > 1$ convergence is termed super linear

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 gauranteed to pick the two points with opposite sign
- Secant is super-linear with a convergence rate of

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

- When could we be in trouble?

Secant Method

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- Secant is super-linear with a convergence rate of

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

- 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

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

- where R = f(b)/f(c), S = f(b)/f(a), T = f(a)/f(c)

Brent's Method (cont)

- such that

$$\begin{aligned} P &= S(T(R-T)(c-b)-(1-R)(b-a)) \\ Q &= (T-1)(R-1)(S-1) \end{aligned}$$

- 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

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

- 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 $\delta >> 0$ 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

$$f_i(x_0, x_1, \ldots, x_{n-1}) \; i = 0, ..., n-1$$

we get

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

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

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

- 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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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

CSE276C - Roots of Polynomials

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Introduction

- Last time 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

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

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
$$\begin{aligned} a &= \tfrac{1}{3}(3q - p^2) \\ b &= \tfrac{1}{27}(2p^3 - 9pq + 27r) \end{aligned}$$
the condensed form has 3 roots
$$\begin{aligned} y_1 &= A + B \\ y_2 &= -\tfrac{1}{2}(A+B) + \tfrac{i\sqrt{3}}{2}(A-B) \\ y_3 &= -\tfrac{1}{2}(A+B) - \tfrac{i\sqrt{3}}{2}(A-B) \end{aligned}$$
where
$$A = \sqrt[3]{-\frac{b}{2} + \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}} \qquad B = \sqrt[3]{-\frac{b}{2} - \sqrt{\frac{b^2}{4} + \frac{a^3}{27}}}$$

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

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

Quartics (cont.)

- The reduced equation can be factorized into

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

if we can estimate z_1 of the above cubic then

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

where

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

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Root Counting

- Consider a polynomial of degree n:

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

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

Sturm - example

- Consider the polynomial

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

The Sturm functions are then

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

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)

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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

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

as r is a root $b_0 = 0$ so

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

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Newton's Method

- Remember we can do root search/refinement

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

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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6. **Müller's Method**
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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