Lecture 3

Rootfinding

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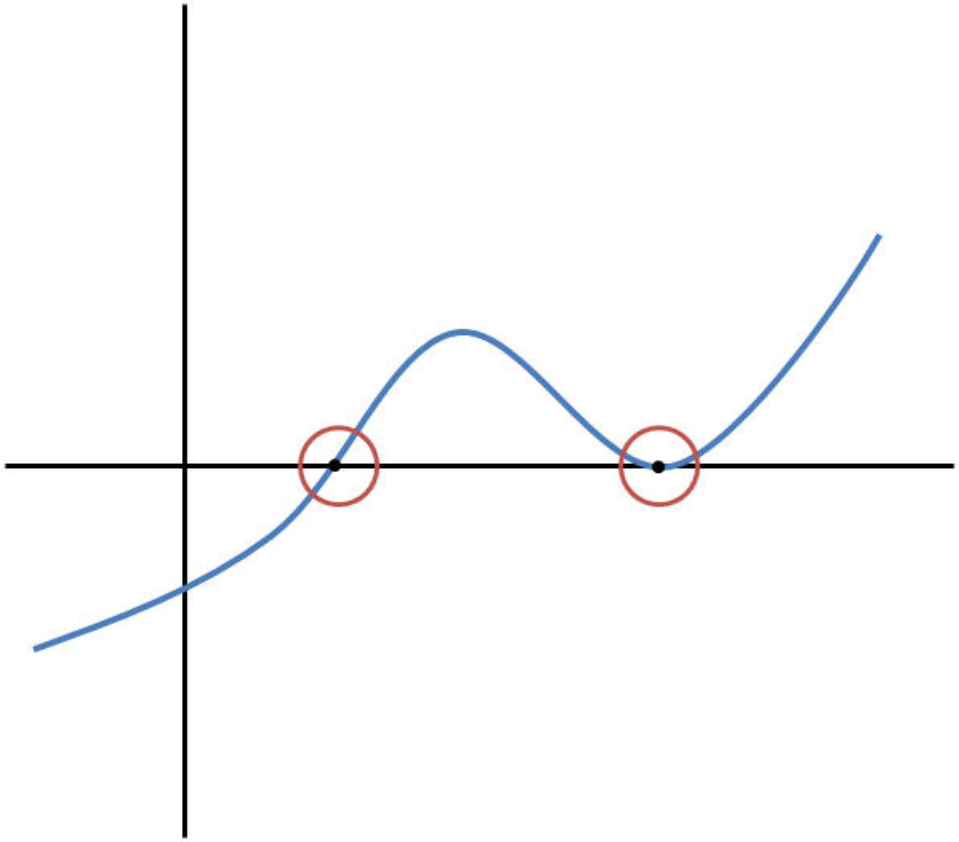
February 14, 2012

Root Finding

Given a function $f(x)$, find x so that $f(x) = 0$



Rootfinding

Goals:

- Find roots to equations
- Compare usability of different methods
- Compare convergence properties of different methods

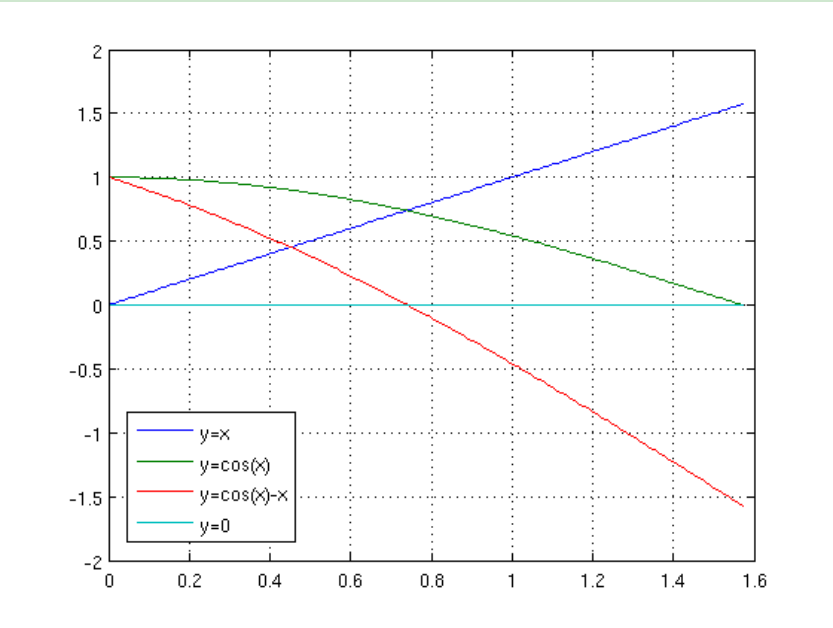
1. bracketing methods
2. Bisection Method
3. Newton's Method
4. Secant Method
5. (opt) fixed point iterations
6. (opt) special Case: Roots of Polynomials

Roots of $f(x)$

- Any single valued equation $g(x) = h(x)$ can be written as $f(x) = g(x) - h(x) = 0$

Example

- Find x so that $\cos(x) = x$
- That is, find where $f(x) = \cos(x) - x = 0$



Analyze your Application

- Is the function complicated to evaluate?
  - lots of expresions?
  - singularities?
  - simplify? polynomial?
- How accurate does our root need to be?
- How fast/robust should our method be?

!

From this, you can pick the right method...

Basic Root Finding Strategy

1. Plot the function
   - Get an initial guess
   - Identify problematic parts
2. Start with the initial guess and iterate

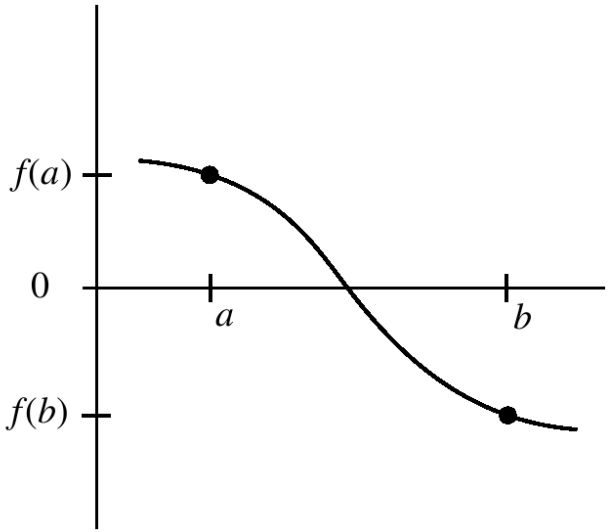
Iteration

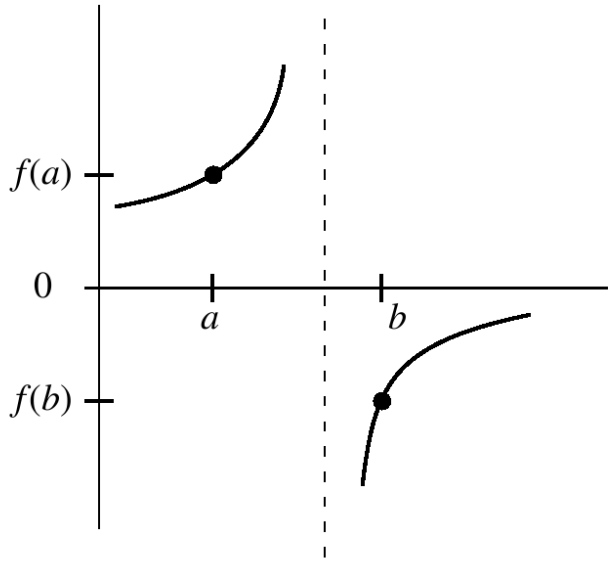
We need to study some iterations.

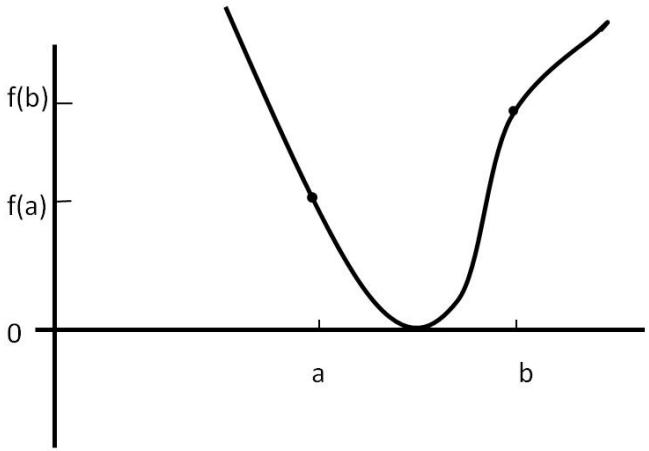
- iteratively finding a root to an equation
- iteratively finding the solution to an algebraic system
- iteratively finding solutions to Ordinary Differential Equations (ODEs)
- ...

Bracket Basics

- A root x is *bracketed* on $[a, b]$ if $f(a)$ and $f(b)$ have opposite sign.
- Changing signs does not guarantee bracketed, however: singularity







Bracket Algorithm

Listing 1: Bracket Algorithm

```
given: f(x), x_min, x_max, n

dx = (x_max − x_min)/n
x_left = x_min
i = 0

while i < n
   i = i + 1
   x_right = x_left + dx
   if f(x) changes sign in [x_left, x_right]
      save [x_left, x_right] as an interval with a root
   end
   x_left = x_right
end
```

Testing Sign

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

Should we use?

```
fa = myfunc(a);
fb = myfunc(b);

if(fa*fb<0)
  (save)
end
```

Better Sign Test

!

Nope. Underflow...

sign()

Use matlab's sign

```
fa = myfunc(a);
fb = myfunc(b);

if(sign(fa) ~= sign(fb))
  (save)
end
```

Moving forward...

Bracketing is fine. But we need to find the actual root:

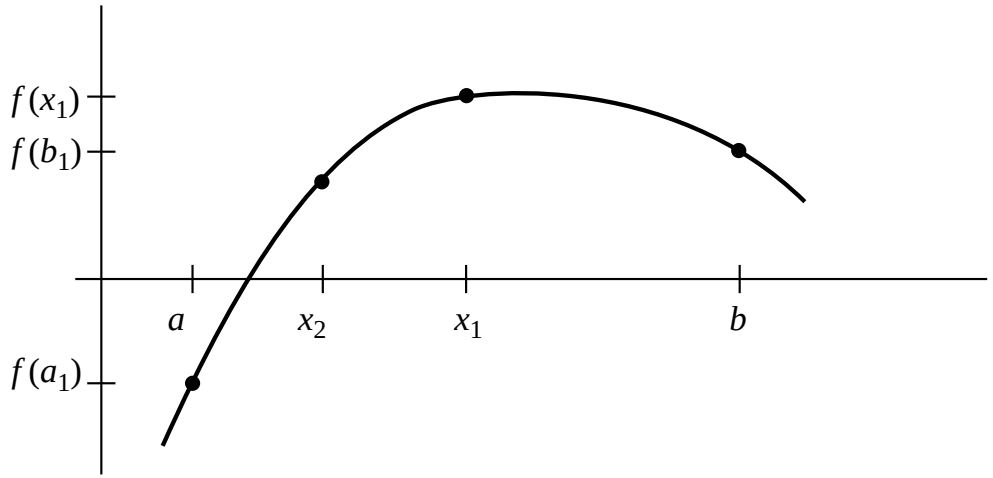
- Bisection
- Newton's Method
- Secant Method
- Fixed Point Iteration

Process:

1. Implement the bracket algorithm to get a visual and brackets
2. search brackets with these methods

Bisection

Given $f : \mathbb{R} \to \mathbb{R}$ and $f \in C([a, b])$ and $sign(f(a)) \neq sign(f(b))$ by the Intermediate Value Theorem we know we have a bracketed root on the interval $[a, b]$. Bisection Method: halve the interval while continuing to bracket the root.



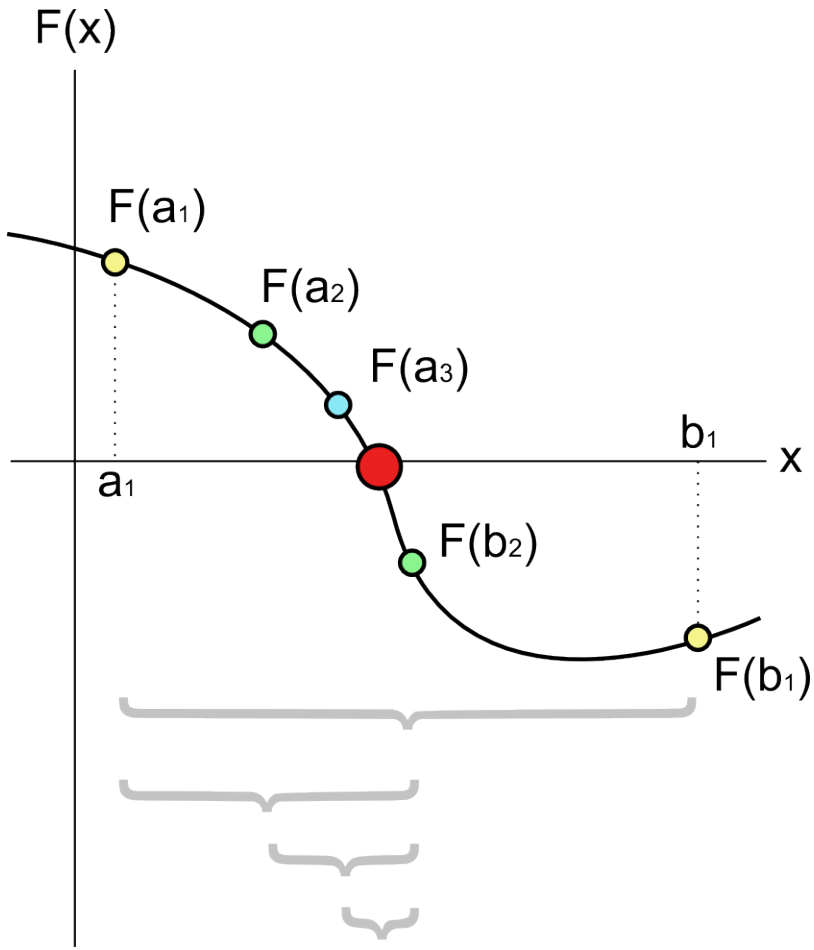
Bisection (2)

For the bracket interval $[a, b]$ the midpoint is

$$x_m = \frac{1}{2}(a + b)$$

idea:

1. split bracket in half
2. select the bracket that has the root
3. goto step 1



Bisection Algorithm

```
function [a,b]=bisection(f,a1,b1,tol)
a=a1; b=b1; sfb=sign(feval(f,b));
k=1;
disp('    k     a         b          x_mid       f(x_mid) width')
while b-a > tol
    x = (a+b)/2; y= feval(f,x); sfx=sign(y); w = abs(b-a);

    fprintf('%5i %10.6f %10.8f %10.8f %11.8f %11.8f\n',[k a b x y w])
    if sfx == 0
         a = x; b =x; break;
    elseif sfx == sfb
        b=x;
    else
        a=x;
    end
    k=k+1;
end
```

Bisection Example

Solve with bisection:

$$x - x^{1/3} - 2 = 0$$ solution from Matlab:3.521379706804568

```
>> [a,b] = bisection(@(x) x-x^(1/3)-2,3,4,1.e-3)
    k      a          b           x_mid        f(x_mid)
    1   3.000000 4.00000000 3.50000000 -0.01829449
    2   3.500000 4.00000000 3.75000000  0.19638375
    3   3.500000 3.75000000 3.62500000  0.08884159
    4   3.500000 3.62500000 3.56250000  0.03522131
    5   3.500000 3.56250000 3.53125000  0.00845016
    6   3.500000 3.53125000 3.51562500 -0.00492550
    7   3.515625 3.53125000 3.52343750  0.00176150
    8   3.515625 3.52343750 3.51953125 -0.00158221
    9   3.519531 3.52343750 3.52148438  0.00008959
   10   3.519531 3.52148438 3.52050781 -0.00074632
```

Analysis of Bisection

Let $\delta_n = x_{b_n} - x_{a_n}$ be the size of the bracketing interval $[x_{a_n}, x_{b_n}]$ with x_n the middle of the n^{th} stage of bisection. If r is the bracketed root then

$$|x_n - r| \leqslant \frac{1}{2}\delta_n \text{ where}$$

$$\begin{aligned}
\delta_1 &= b - a = \text{initial bracketing interval} \\
\delta_2 &= \frac{1}{2}\delta_1 \\
\delta_3 &= \frac{1}{2}\delta_2 = \frac{1}{4}\delta_1 \\
&\vdots \\
\delta_{n+1} &= \left(\frac{1}{2}\right)^n \delta_1 \qquad \text{thus}
\end{aligned}$$

$$|x_n - r| \leqslant \left(\frac{1}{2}\right)^n \delta_1$$

Analysis of Bisection

$$\frac{\delta_{n+1}}{\delta_1} = \left(\frac{1}{2}\right)^n = 2^{-n} \qquad \text{or} \qquad n = \log_2\left(\frac{\delta_1}{\delta_{n+1}}\right)$$

n	$\frac{\delta_{n+1}}{\delta_1}$	function evaluations
5	3.1×10^{-2}	7
10	9.8×10^{-4}	12
20	9.5×10^{-7}	22
30	9.3×10^{-10}	32
40	9.1×10^{-13}	42
50	8.9×10^{-16}	52

Remember the game Twenty questions?

Convergence Criteria

An automatic root-finding procedure needs to monitor progress toward the root and stop when current guess is close enough to the desired root.

- Convergence checking will avoid searching to unnecessary accuracy.
- Check how closeness of successive approximations

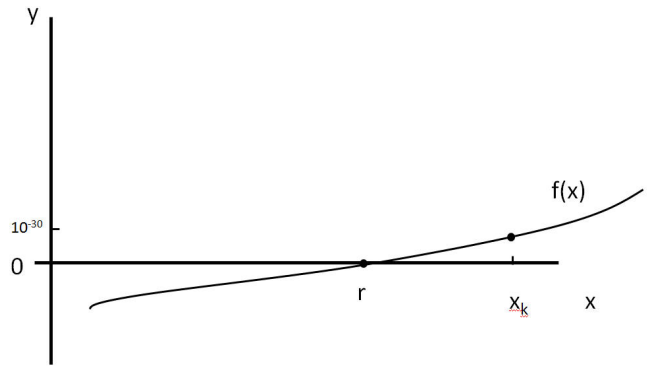
$$|x_k - x_{k-1}| < \delta_x$$

- Check how close $f(x)$ is to zero at the current guess.

$$|f(x_k)| < \delta_f$$

- Which one you use depends on the problem being solved

Convergence Criteria on x versus $f(x)$



Is x_k a sufficient approximation of a root at r? What if $r = 1$ and $x_k = 100$?

Alternative view

We have two views for finding roots

- Find r such that $f(r) = 0$
- Compute $r = f^{-1}(0)$

The two views give us two ways to determine errors. We denote $y_k = f(x_k)$.

Alternative view

- absolute error $= |f(x_k) - 0|$
- absolute error $= |x_k - r| = |f^{-1}(y_k) - r|$

  relative error $= |\frac{x_k - r}{r}| = |\frac{f^{-1}(y_k) - r}{r}|$ when $r \neq 0$

Condition Number of Problem

Given a function $G : \mathbb{R} \to \mathbb{R}$,suppose we wish to compute $y = G(x)$. How sensitive is the solution to changes in x? We can measure this sensitivity in two ways:

- Absolute Condition Number = $\lim_{h \to 0} \frac{|G(x+h) - G(x)|}{|h|}$
- Relative Condition Number = $\lim_{h \to 0} \frac{\frac{|G(x+h) - G(x)|}{|G(x)|}}{\frac{|h|}{|x|}}$

Condition numbers much greater than one mean that the problem is inherently sensitive.

Condition Number Example

Given the problem of finding a root of a function $f : \mathbb{R} \to \mathbb{R}$,consider the absolute condition number applied to the problem of computing $f^{-1}(0)$.

$$\begin{aligned}
\text{Absolute Condition Number} &= \lim_{h \to 0} \frac{|f^{-1}(0+h) - f^{-1}(0)|}{|h|} \\
&= \left. \frac{df^{-1}(y)}{dy} \right|_{y=0} \quad \text{and from Calculus} \\
&= \frac{1}{\left. \frac{df(x)}{dx} \right|_{x=r}}
\end{aligned}$$

We conclude that the root finding problem is inherently sensitive to change if $\left| \frac{df(r)}{dx} \right| \approx 0$.

Condition Number Example

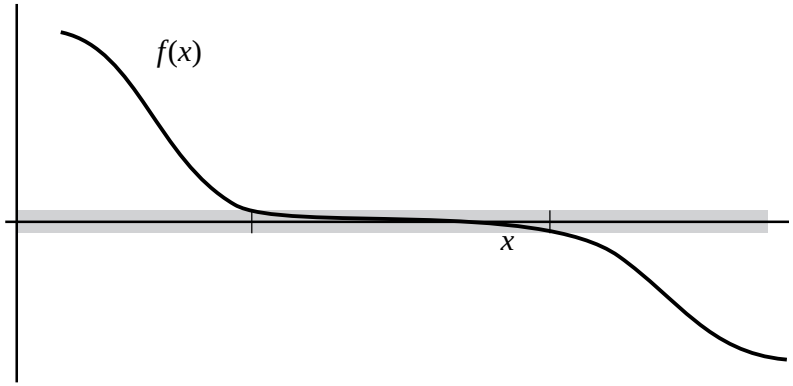
Given the problem of finding a root of a function $f : \mathbb{R} \to \mathbb{R}$,consider the absolute condition number applied to the problem of computing $f(r)$ where r is a root of f.

$$\begin{aligned} \text{Absolute Condition Number} &= \lim_{h \to 0} \frac{|f(r+h) - f(r)|}{|h|} \\ &= \left. \frac{df(x)}{dx} \right|_{x=r} \end{aligned}$$

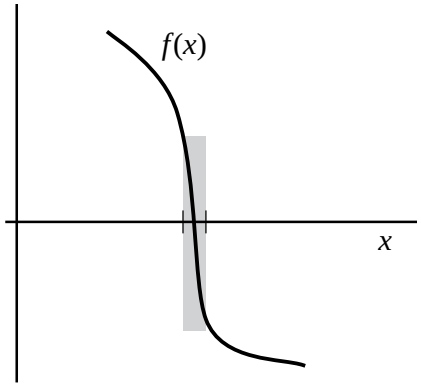
We conclude that the root finding problem is inherently sensitive to change if $\left| \frac{df(r)}{dx} \right| >> 1$.

Convergence Criteria Compared

If $f'(x)$ is small near the root, it is easy to satisfy tolerance on $f(x)$ for a large range of Δx.



If $f'(x)$ is large near the root, it is possible to satisfy the tolerance on Δx when $|f(x)|$ is still large.



Convergence rate of a root finding iteration

- Let $e_n = x^* - x_n$ be the error.
- In general, a sequence is said to converge with rate if r is the largest real for which the limit below is finite.

$$\lim_{n \to \infty} \frac{|e_{n+1}|}{|e_n|^r} = C$$

Special Cases:

- If $r = 1$ and $C = 1$, then the rate is *sublinear*
- If $r = 1$ and $C < 1$, then the rate is *linear*
- If $r > 1$ (i.e. $r = 1$ and $C = 0$), then the rate is *superlinear*
- If $r = 2$ and $C > 0$, then the rate is *quadratic*

Convergence rate of the bisection method

When the bisection method ”converges” it can be shown that,

Bisection Method

The bisection method converges with rate $r = 1$ and $C = 0.5$.

Example

Convergence Rate

1. $10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}...$
2. $10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}...$
3. $10^{-2}, 10^{-3}, 10^{-5}, 10^{-8}...$
4. $10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}...$
5. $10^{-2}, 10^{-6}, 10^{-18}, ...$

Example

Convergence Rate

1. $10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$... (linear with $C = 10^{-1}$)
2. $10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}$... (linear with $C = 10^{-2}$)
3. $10^{-2}, 10^{-3}, 10^{-5}, 10^{-8}$... (superlinear, not quadratic)
4. $10^{-2}, 10^{-4}, 10^{-8}, 10^{-16}$...(quadratic)
5. $10^{-2}, 10^{-6}, 10^{-18}$, ... (cubic)

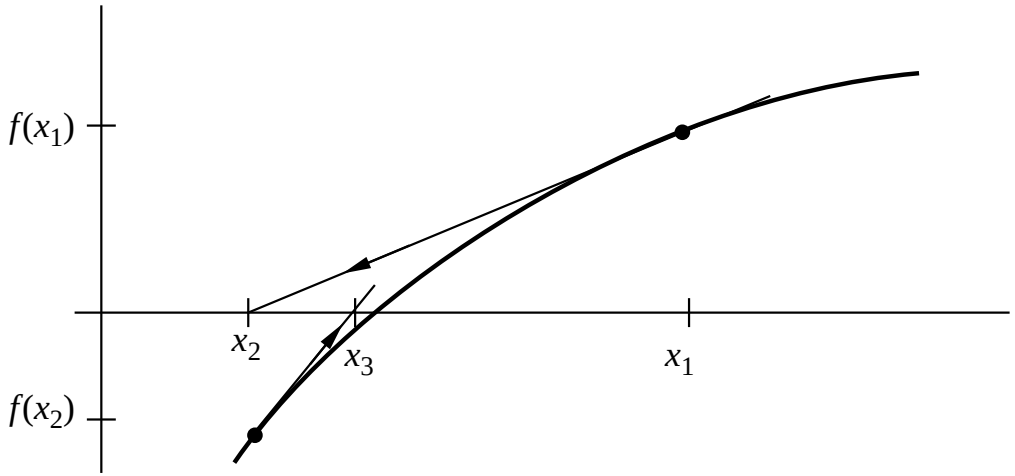
- Linear: Adds equal number of digits of accuracy at each step
- Quadratic: Doubles the number of digits at each step

Performing Division

- Ever wondered how a computer process performs division?
- “Long” division requires lookup, subtraction, shifts
- Generates one digit and a time. Can we do better?

To answer this, we need to look at faster methods than bisection

Newton's Method



For a current guess x_k, use $f(x_k)$ and the slope $f'(x_k)$ to predict where $f(x)$ crosses the x axis.

Newton's Method

Expand $f(x)$ in Taylor Series around x_k

$$f(x_k + \Delta x) = f(x_k) + \Delta x \left.\frac{df}{dx}\right|_{x_k} + \frac{(\Delta x)^2}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_k} + \cdots$$

Substitute $\Delta x = x_{k+1} - x_k$
and neglect 2^{nd} order terms to get

$$f(x_{k+1}) \approx f(x_k) + (x_{k+1} - x_k) f'(x_k)$$

where

$$f'(x_k) = \left.\frac{df}{dx}\right|_{x_k}$$

Newton's Method

Goal is to find x such that $f(x) = 0$.
Set $f(x_{k+1}) = 0$ and solve for x_{k+1}

$$0 = f(x_k) + (x_{k+1} - x_k) f'(x_k)$$

or, solving for x_{k+1}

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

Newton's Method Algorithm

```
initialize:  x_1 = ...
for k = 2, 3, ...
    x_k = x_{k-1} - f(x_{k-1}) / f'(x_{k-1})
    if converged, stop
end
```

Newton's Method Example

Solve:

$$x - x^{1/3} - 2 = 0$$

First derivative is

$$f'(x) = 1 - \frac{1}{3}x^{-2/3}$$

The iteration formula is

$$x_{k+1} = x_k - \frac{x_k - x_k^{1/3} - 2}{1 - \frac{1}{3}x_k^{-2/3}}$$

Newton's Method Example

$$x_{k+1} = x_k - \frac{x_k - x_k^{1/3} - 2}{1 - \frac{1}{3}x_k^{-2/3}}$$

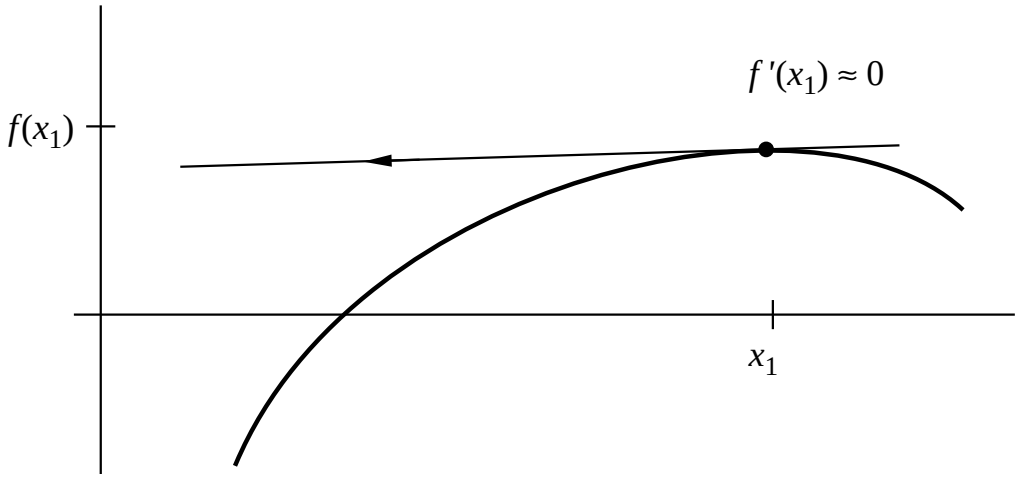
Matlab solution root = 3.52137970680456 8e+00

k	x_k	$f'(x_k)$	$f(x)$
1	3	0.83975005	-0.44224957
2	3.52664429	0.85612976	0.00450679
3	3.52138015	0.85598641	3.771×10^{-7}
4	3.52137971	0.85598640	2.664×10^{-15}
5	3.52137971	0.85598640	0.0

Conclusion

- Newton's method converges *much* more quickly than bisection
- Newton's method requires an analytical formula for $f'(x)$
- The algorithm is simple as long as $f'(x)$ is available.
- Iterations are not guaranteed to stay inside an ordinal bracket.

Divergence of Newton's Method



Since

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

the new guess, x_{k+1}, will be far from the old guess whenever $f'(x_k) \approx 0$

Newton's Method: Convergence

Recall

Convergence of a method is said to be of order r if there is a constant C such that

$$\lim_{k\to\infty} \frac{|e_{k+1}|}{|e_k|^r} = C$$

If Newton's method converges then it is of order 2 (quadratic) when $f'(x_*) \neq 0$. (assuming f'' is continuous. For ξ_k between x_k and x_*

$$f(x_*) = f(x_k) + (x_* - x_k)f'(x_k) + \frac{1}{2}(x_* - x_k)^2 f''(\xi_k) = 0$$

So

$$\frac{f(x_k)}{f'(x_k)} + x_* - x_k + \frac{1}{2}(x_* - x_k)^2 \frac{f''(\xi_k)}{f'(x_k)} = 0$$

Then

$$x_* - x_{k+1} + \frac{1}{2}(x_* - x_k)^2 \frac{f''(\xi_k)}{f'(x_k)} = 0$$

Thus

$$\frac{|x_* - x_{k+1}|}{|x_* - x_k|^2} = \frac{1}{2}\left|\frac{f''(\xi_k)}{f'(x_k)}\right| \to \frac{1}{2}\left|\frac{f''(x_*)}{f'(x_*)}\right| \text{ as } x_k \to x_*$$

Reciprocal Approximation

- Consider the task of computing $1/q$ for some q without using division.
- We can write this as: find the root x of $f(x) = 1/(xq) - 1 = 0$.
- What is Newton's Method for this?
- $f'(x) = -1/(x^2 q)$. Thus

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

or

$$x_{n+1} = x_n - \frac{1/(x_n q) - 1}{-1/(x_n^2 q)}$$

Reciprocal Approximation

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or

$$x_{n+1} = x_n - \frac{1/(x_n q) - 1}{-1/(x_n^2 q)} \frac{x_n^2 q}{x_n^2 q}$$

$$x_{n+1} = x_n + x_n - x_n^2 q = 2x_n - x_n^2 q = 2x_n - x_n^2 q$$

Example: Compute 1/3 = 0.01010101... binary

- Find the bracket:
- $1/2 > 1/3 > 1/4$

1. $x_1 = 1/4$
2. $x_2 = 2x_1 - x_1^2 q = 1/2 - 3/16 = 5/16 = 0.0101 \quad (binary)$
3. $x_3 = 2 \times 5/2^4 - 3 \times 25/2^8 = (160 - 75)/2^8 = 85/2^8 = 0.01010101 \quad (binary)$
4. $x_4 = 2 \times 85/2^8 - 3 \times 85^2/2^{16} = 21845/2^{16} = 0.0101010101010101 \quad (binary)$

In 3 steps, computed 16 bits in $1/3$

How many binary digits are computed in the next step?

Instructor Notes

- Modification of Newton's Method for root finding when $\frac{df}{dx}(root) = 0$. Use the formula,

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

  where m is the multiplicity of the root.
- or solve $0 = g(x) = \frac{f(x)}{f'(x)}$