01.05 rootfinding: without derivatives

what if $f(x)$ has no (or unknown) $f'(x)$?

1 secant method, variants

secant method

replace the derivative with a difference quotient. ie, replace tangent line with secant line through previous two guesses. ie, approximation for derivative at x_i is difference quotient

$$\frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}.$$

secant method

$$x_0, x_1 = \text{initial guesses}$$

$$x_{i+1} = x_i - f(x_i) \cdot \underbrace{\frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}}_{\sim \frac{1}{f'(x_i)}}, \quad i = 1, 2, 3, \ldots$$

algorithm

```
icount = 0

fx_old = f(x_old)
if abs(fx_old) < epsilon # epsilon ~ eta
  return x_old
fx_older = f(x_older)
if abs(fx_older) < epsilon # epsilon ~ eta
  return x_older

dq = (fx_old - fx_older)/(x_old - x_older)
x_new = x_old - fx_old/dq
fx = f(x_new)
icount = icount + 1
```

```
# while (abs(fx) > epsilon) and (icount <= imax): # epsilon ~ eta
while (abs(x_new - x_old) > epsilon) and (icount <= imax):
  x_older = x_old
  fx_older = fx_old
  x_old = x_new
  fx_old = fx
  dq = (fx_old - fx_older)/(x_old - x_older)
  x_new = x_old - fx_old/dq
  fx = f(x_new)
  icount = icount + 1

return x_new
```

convergence

assume that method converges to r and $f'(r) \neq 0$, then the approximate error relationship

$$e_{i+1} \approx \left| \frac{f''(r)}{2f'(r)} \right| e_i e_{i-1}$$

holds and implies

$$e_{i+1} \approx \left| \frac{f''(r)}{2f'(r)} \right|^{\alpha - 1} e_i^{\alpha},$$

where $\alpha = \frac{1+\sqrt{5}}{2} \approx 1.62$. secant method convergence to simple roots is called **superlinear**, meaning that it lies between linearly and quadratically convergent methods.

example 16

example 01, revisted. apply secant method with $x_0 = 0, x_1 = 1$ to find root of $f(x) = x^3 + x - 1$.

$$x_{i+1} = x_i = \frac{(x_i^3 + x_i - 1)(x_i - x_{i-1})}{x_i^3 + x_i - (x_{i-1}^3 + x_{i-1})}$$

$$\Downarrow \quad x_0 = 0, x_1 = 1$$

$$x_2 = 1 - \frac{(1)(1-0)}{(1+1-0} = \frac{1}{2}$$

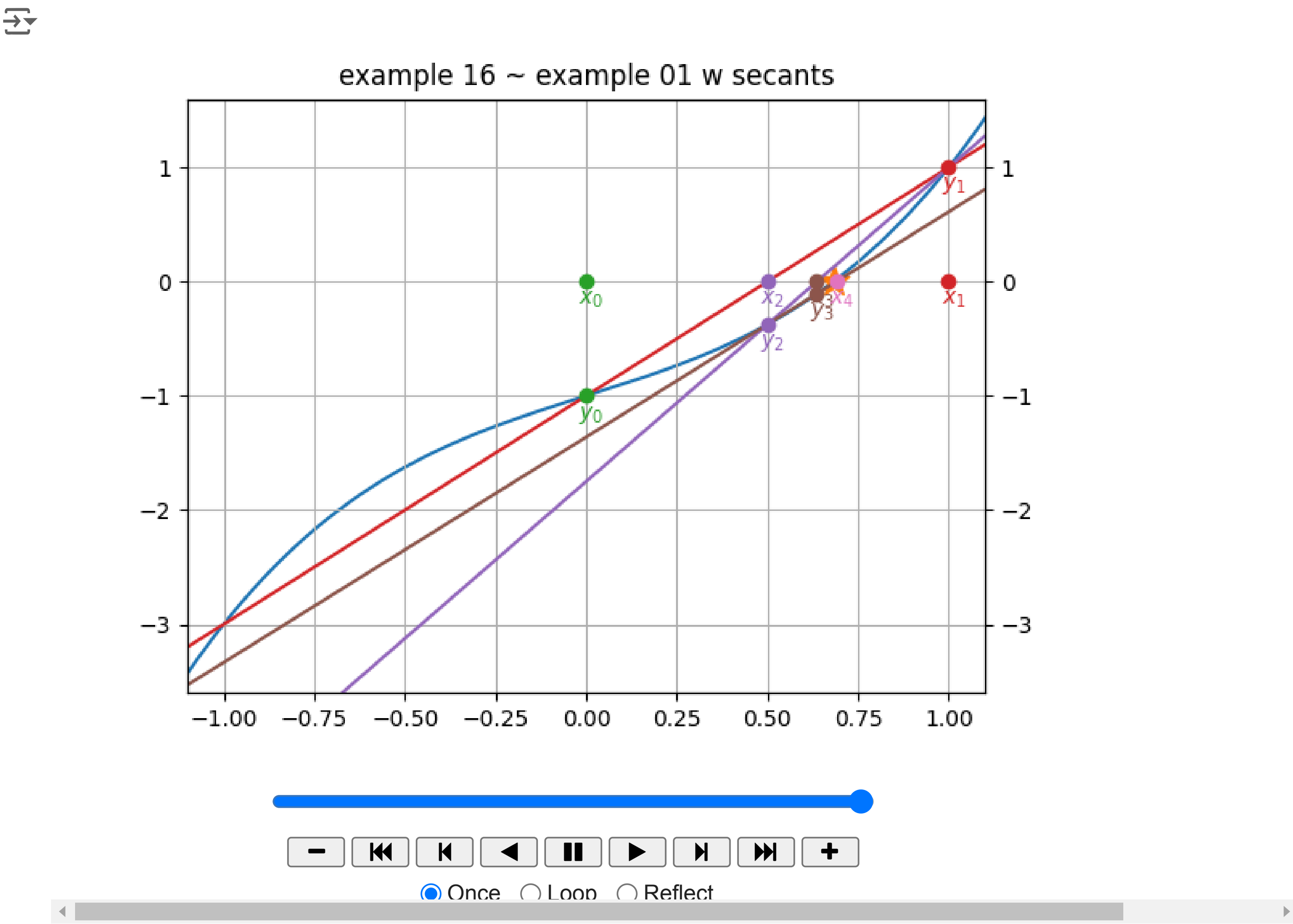
$$x_3 = \frac{1}{2} - \frac{-\frac{3}{8}(\frac{1}{2} - 1)}{\frac{3}{8} - 1} = \frac{7}{11}.$$

code, example 16

```
# example 16, secant method for example 01 # mod example 14

if __name__ == "__main__":

```

```
expected convergence: [0.8068743]


example 16 ~ example 01 w secants. x0 = [0, 1].

|   i |             x[i] |             e[i] |               "/e[i-1]^α |
|-----|------------------|------------------|--------------------------|
| 000 | 0.00000000000000 | 0.68232780382802 |                          |
| 001 | 1.00000000000000 | 0.31767219617198 |         0.58963609730649 |
| 002 | 0.50000000000000 | 0.18232780382802 |         1.16591656728344 |
| 003 | 0.63636363636364 | 0.04596416746438 |         0.72174623555971 |
| 004 | 0.69005235602094 | 0.00772455219292 |         1.12751982884733 |
| 005 | 0.68202041964819 | 0.00030738417983 |         0.80384864065885 |
| 006 | 0.68232578140989 | 0.00000202241813 |         0.97481374069426 |
| 007 | 0.68232780435903 | 0.00000000053101 |         0.86774886684321 |
| 008 | 0.68232780382802 | 0.00000000000000 |         1.01567939794005 |
| 009 | 0.68232780382802 | 0.00000000000000 | 207243987.96379616856575 |
```

```
ani
```



generalizations of secant method

regula falsi

aka "method of false position". regula falsi is similar to bisection but midpoint replaced by secant-like approximation. ie, given bracketing interval $[a, b]$,

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

where $c \in [a, b]$ and next subinterval chosen to bracket root.

algorithm, regula falsi

```
# given [a,b] st f(a)·f(b) < 0

for i = 1,2,3,...
```

```
  c = [b·f(a) - a·f(b)] / [f(a) - f(b)]
  if f(c) == 0 stop
  if f(a)·f(c) < 0
    b = c
  else
    a = c
  end
next
```

code, regula falsi

```
# algorithm, basic

def secant_rf(f,ab,tol=1e-8):

```

```
# algorithm, basic # modified bisect_expanded from lecture 01_01

def secant_rf_expanded(f,ab,tol=1e-8,all=False,workspace=False):

```

example 17

apply regula falsi on interal $[-1,1]$ to find root $r=0$ of $f(x)=x^3-2\,x^2+\frac{3}{2}\,x$.

$$x_0=-1,\,x_1=1$$

$$x_2=\frac{x_1\cdot f(x_0)-x_0\cdot f(x_1)}{f(x_0)-f(x_1)}=\frac{1(-\frac{9}{2})-(-1)(\frac{1}{2})}{-\frac{9}{2}-\frac{1}{2}}=\frac{4}{5}.$$

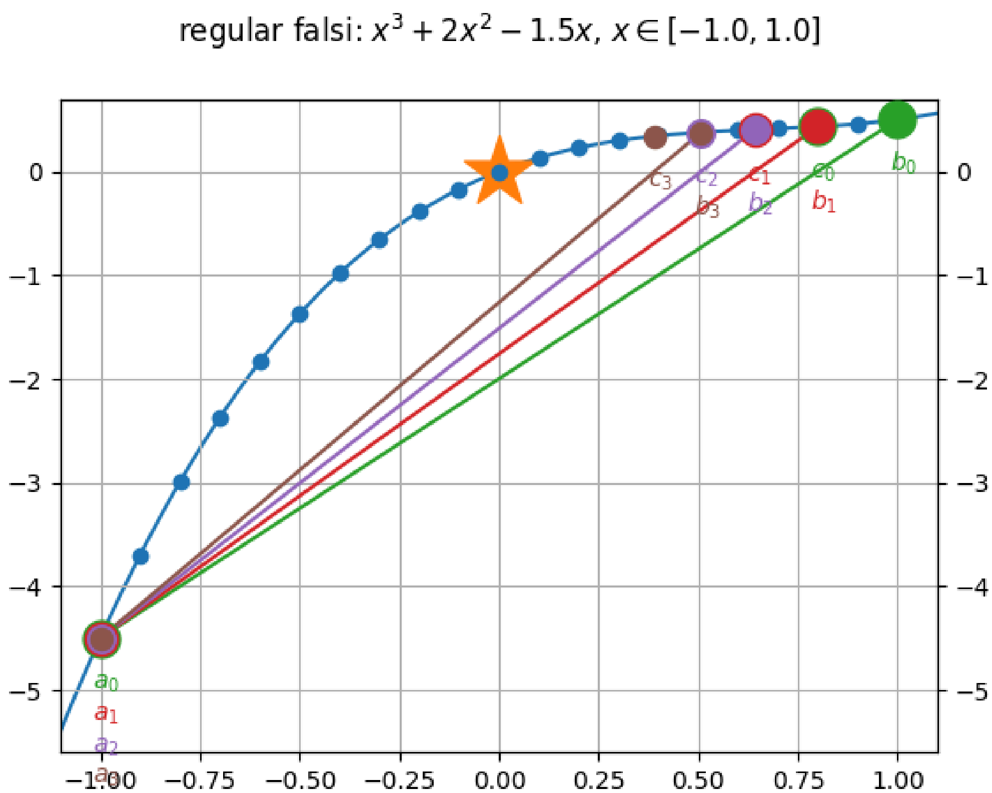
$f(-1)\cdot f(\frac{4}{5})<0 \implies [x_0,x_2]=[-1,\frac{4}{5}]\sim$ better than $\frac{1}{2}$ of bisection; however, sometimes its not your birthday.

code, example 17, regula falsi

```
# requires prior execution of secant_rf_expanded() # mod lecture 01_01 first code

if __name__ == "__main__":

```

```
regular falsi: $x^3 + 2x^2 - 1.5x$, $x \in[-1.0,1.0]$

|   i |           a |        f(a) |          b |       f(b) |          c |       f(c) |   ±
|-----|-------------|-------------|------------|------------|------------|------------|-----
| 000 | -1.00000000 | -4.50000000 | 1.00000000 | 0.50000000 | 0.80000000 | 0.43200000 | 001
| 001 | -1.00000000 | -4.50000000 | 0.80000000 | 0.43200000 | 0.64233577 | 0.40333785 | 001
| 002 | -1.00000000 | -4.50000000 | 0.64233577 | 0.40333785 | 0.50724082 | 0.37678437 | 001
| 003 | -1.00000000 | -4.50000000 | 0.50724082 | 0.37678437 | 0.39079015 | 0.34043162 | 001
```

```
ani
```



Once Loop Reflect

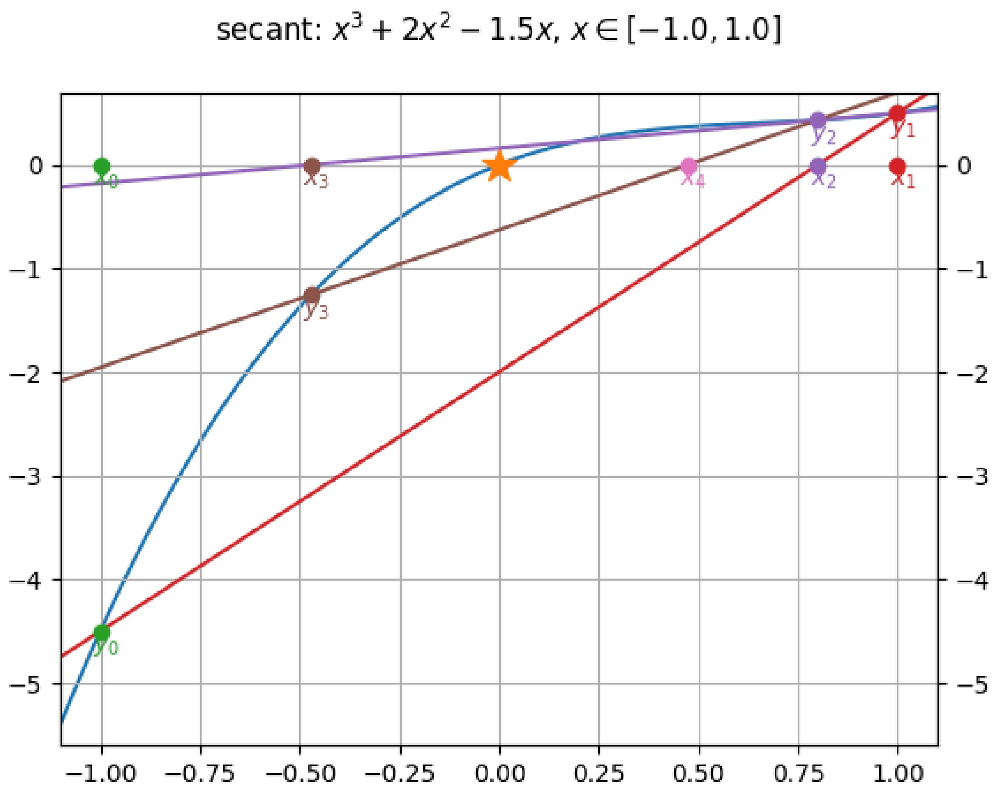
code, example 17, secant

```
# example 17, secant method # mod example 16

if __name__ == "__main__":⋯
```

```
expected convergence: [1.19458315]

secant: $x^3 + 2x^2 - 1.5x$, $x \in[-1.0,1.0]$

|   i |              x[i] |             e[i] |       "/e[i-1]^α |
|-----|-------------------|------------------|------------------|
| 000 | -1.00000000000000 | 1.00000000000000 |                  |
| 001 |  1.00000000000000 | 1.00000000000000 | 1.00000000000000 |
| 002 |  0.80000000000000 | 0.80000000000000 | 0.80000000000000 |
| 003 | -0.47058823529412 | 0.47058823529412 | 0.67521916496024 |
| 004 |  0.47424724729948 | 0.47424724729948 | 1.60576763820552 |
| 005 |  0.25965464146786 | 0.25965464146786 | 0.86822303833010 |
|-----|-------------------|------------------|------------------|
| 008 |  0.03994345289533 | 0.03994345289533 | 1.49983922882677 |
| 009 | -0.00643218295752 | 0.00643218295752 | 1.17833000297553 |
| 010 |  0.00035223951983 | 0.00035223951983 | 1.23876434915084 |
| 011 |  0.00000300563144 | 0.00000300563144 | 1.16216844505921 |
```

| 012 | -0.00000000141202 | 0.00000000141202 | 1.21542677765262 |

```
ani
```



Once Loop Reflect

mullers method

draw parabola $y = p(x)$ through three previous points (vs line through two previous points) and its intersection with x-axis closest to x_i is next iteration x_{i+1}.

- for multiple intersections, select the one closest to previous iteration;
- if parabola misses x-axis then it gets complex and costs extra tuition. 👀

oscar velize [@youtube]

code, mullers method

```
# https://en.wikipedia.org/wiki/Muller%27s_method # mod

import cmath as cm
import numpy as np

```

```
# newtons divided difference
def dd(f,xx):
  if len(xx) == 2:
    a,b = xx
```

```
# instead of complex number hack, use future methods

import numpy as np

def mullers_lol(f,xs,max_iter=100,tol=1e-8,method=0):
  """
```

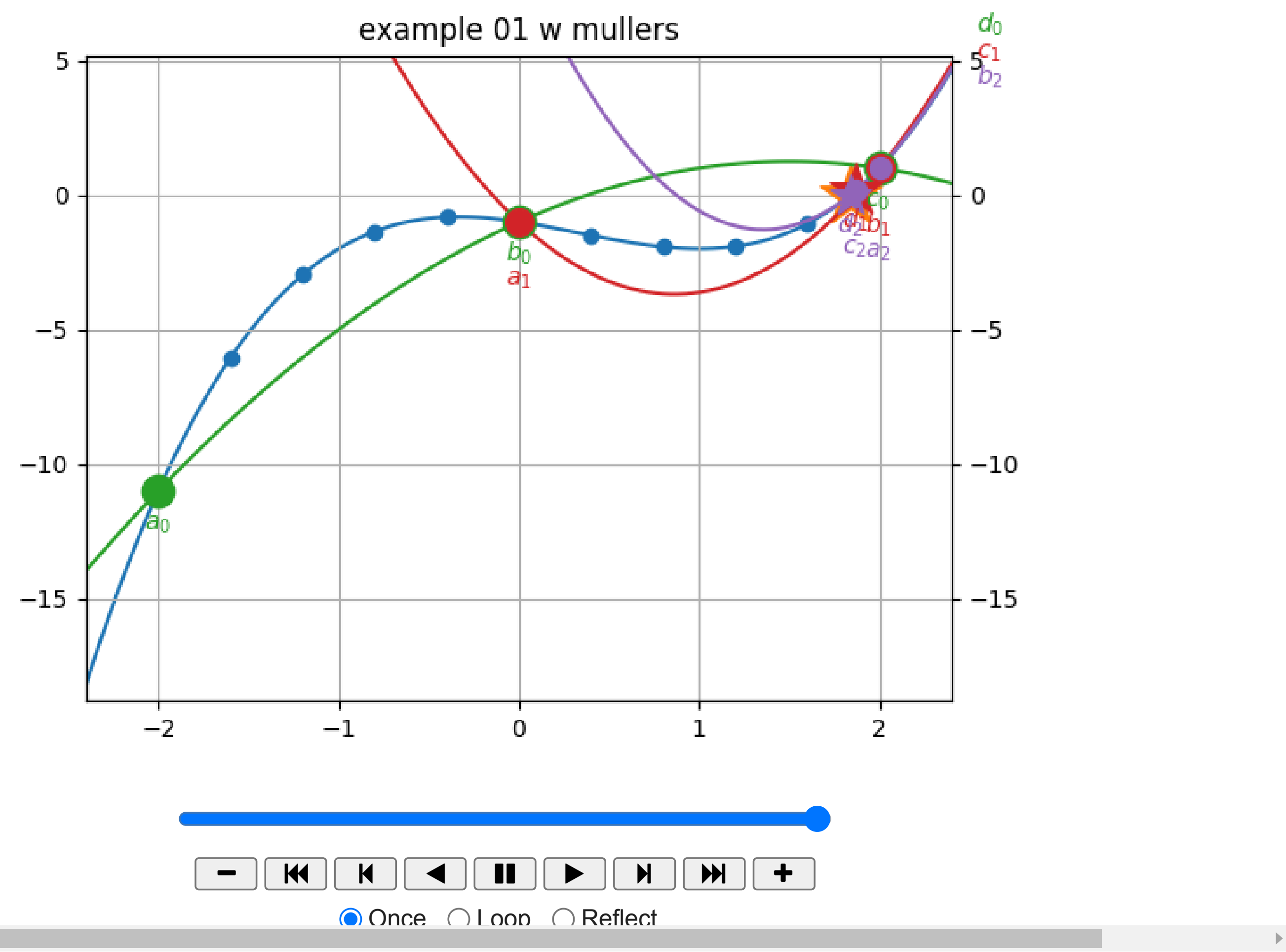
```
# example 01 with mullers # mod secant example

if __name__ == "__main__":

  import scipy as sp
```

```
step 0, parabola: -1.0 + 3.0·x - 1.0·x²
           roots: [2.6180339887498976,0.38196601125010493]


step 1, parabola: -1.0 - 6.23606798·x + 3.61803399·x²
           roots: [1.871307386268059,-0.14770058851807896]


step 2, parabola: 8.79829268 - 14.87782909·x + 5.48934138·x²
           roots: [1.8385321777112726,0.8717800572671759]


step 3, parabola: 8.00723819 - 14.15294492·x + 5.32787355·x²
           roots: [1.8392902102200412,0.8171063380988388]


step 4, parabola: 5.32800227 - 11.26393044·x + 4.54912977·x²
           roots: [1.8392867552294225,0.6367759193327744]
```

example 01 w mullers: $x^3 - x^2 - x - 1$

i	a	b	c	gap	e[i]	"/e[i-1]
000	-2.00000000	0.00000000	2.00000000	2.00000000	0.16071324	
001	0.00000000	2.00000000	2.61803399	0.61803399	0.77874723	4.84556973
002	2.00000000	2.61803399	1.87130739	-0.74672660	0.03202063	0.04111813
003	2.61803399	1.87130739	1.83853218	-0.03277521	0.00075458	0.02356535
004	1.87130739	1.83853218	1.83929021	0.00075803	0.00000346	0.00457873
005	1.83853218	1.83929021	1.83928676	-0.00000345	0.00000000	0.00000442

```
ani
```



inverse quadratic interpolation (IQI)

similar to mullers but with parabola $x = p(y)$, which is handy for limiting the x-axis intesection to a single point.

consider second-degree polynomial $x = P(y)$ through points $(a, A), (b, B), (c, C)$.

$$P(y) = a\frac{(y-B)(y-C)}{(A-B)(A-C)} + b\frac{(y-A)(y-C)}{(B-A)(B-C)} + c\frac{(y-A)(y-B)}{(C-A)(C-B)}$$

$$\Downarrow \quad P(A) = a, P(B) = b, P(C) = c, y = 0$$

$$P(0) = c - \frac{r(r-q)(c-b) + (1-r)s(c-a)}{(q-1)(r-1)(s-1)}, \qquad q = \frac{f(a)}{f(b)}, r = \frac{f(c)}{f(b)}, s = \frac{f(c)}{f(a)}$$

$$\Downarrow \quad a = x_i, b = x_{i+1}, c = x_{i+2}, A = f(x_i), B = f(x_{i+1}), C = f(x_{i+2})$$

$$x_{i+3} = x_{i+2} - \frac{r(r-q)(x_{i+2}-x_{i+1}) + (1-r)s(x_{i+2}-x_i)}{(q-1)(r-1)(s-1)}, \qquad q = \frac{f(x_i)}{f(x_{i+1})}, r = \frac{f(x_{i+2})}{f(x_{i+1})}, s = \frac{f(x_{i+2})}{f(x_i)}.$$

here x_{i+3} replaces x_i but an alternative implementation replaces the largest source of backward error.

lemonfully @youtube @wiki

- lemonfully points out that while this method is asymptotically faster than secants, it only is if initial points chosen well.
- oscar veliz (in the lead up to brents method) also points out this unreliability.

oh, why not

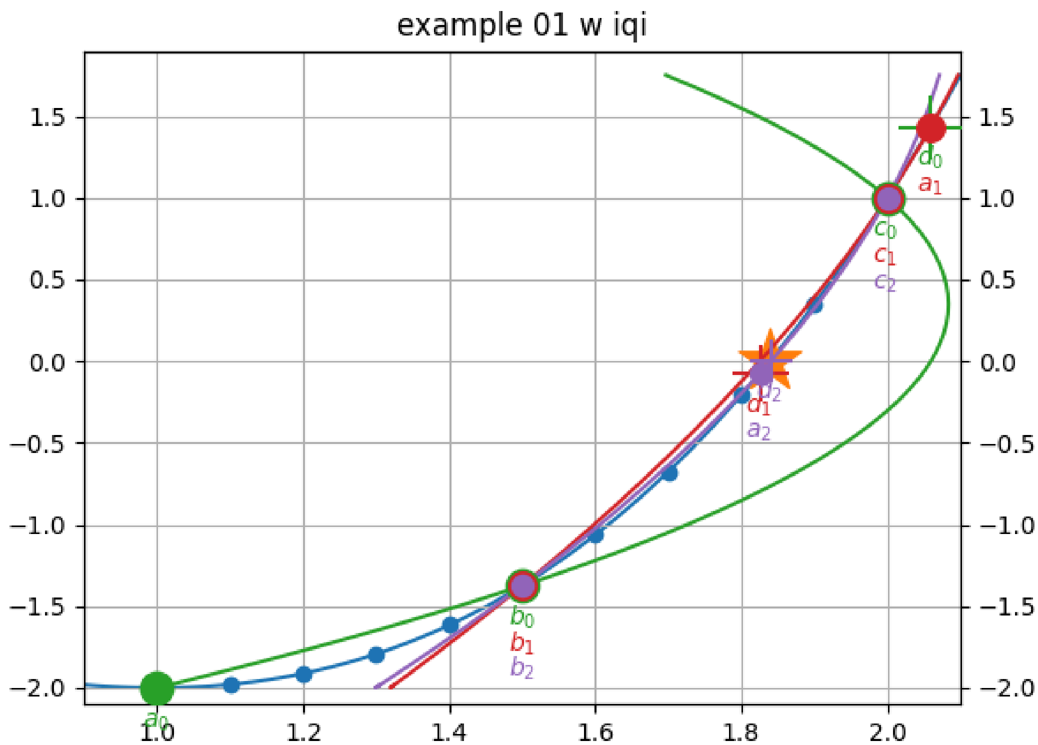
```
# a few reasons come to mind

import numpy as np
import statistics as st

def iqi(f,xs,max_iter=100,tol=1e-8,doyourworst=False,workspace=False):

```

```
if __name__ == "__main__":

```

```
root: [1.83928676]

example 01 w iqi: $x^3 - x^2 - x - 1$
```

i	a	b	c	bwe (Δy)	e[i]	"/e[i-1]
000	1.00000000	1.50000000	2.00000000	0.50000000	0.83928676	
001	2.05964912	1.50000000	2.00000000	0.43554618	0.22036237	0.26255909
002	1.82546813	1.50000000	2.00000000	1.07473271	0.01381863	0.06270865
003	1.82546813	1.84037070	2.00000000	0.08066758	0.00108394	0.07844079
004	1.82546813	1.84037070	1.83928426	0.00594852	0.00000250	0.00230327
005	1.83928676	1.84037070	1.83928426	0.00001366	0.00000000	0.00001790
006	1.83928676	1.83928676	1.83928426	0.00000000	0.00000000	0.00000497

```
  ani

```



Once Loop Reflect

```
# briefly

if __name__ == "__main__":

  f = lambda x: pow(x,3) + x - 1

  if True:
    x = iqi(f,[0.,0.5,1.])
    print(f"iqi, std: {x}\n")

    x = iqi(f,[0.,0.5,1.],doyourworst=True)
    print(f"iqi, bwe: {x}\n")

```

```
iqi, std: 0.6823278038280194

iqi, bwe: 0.6823278038280194
```

2 brents method

this hybrid method uses concepts of secant method, its generalizations and bisection. it expands dekkers method which uses secant backed up by bisection.

for continuous function f over bounded interval $[a, b]$ where $f(a) \cdot f(b) < 0$, brents method keeps track of current x_i that is best in sense of backward error and bracket $[a_i, b_i]$ of root. roughly speaking brents uses IQI to replace one of x_i, a_i, b_i if (1) the backward error improves and (2) the bracketing interval is cut at least in half. if that fails, the secant method is attempted. if that fails, bisection occurs which guarantees that uncertainty is lat least halved.

code, dekker

```
# https://blogs.mathworks.com/cleve/2015/10/12/zeroin-part-1-dekkers-algorithm/

import numpy as np
import scipy as sp

def dekker(f,a,b,display=0):

  fa = f(a)
  fb = f(b)
  if fa*fb > 0:
    raise Exception("interval does not bracket root.")

  print(f"{1:5.0f} initial {a:19.15f} {fa:23.15e}")
  print(f"{2:5.0f} initial {b:19.15f} {fb:23.15e}")
  k = 2
  c = a; fc = fa
```

Show hidden output

code, brent

```
# extends dekkers

import scipy as sp

f = lambda x: pow(x,3) - pow(x,2) - x - 1

def brent(f,a,b,tol=1e-8,max_iter=10):
  c = a
  fc = f(c)
  fb = f(b)

  i = 0
  while (abs(c-b)>tol) and (i<max_iter): # fwe
```

```
scipy : 1.8392867552141612
dekker: 1.8392867464516185
```

code, brent @scipy

```
import scipy as sp

f = lambda x: pow(x,3) - pow(x,2) - x - 1
ab = (0.,2.)

root,soln = sp.optimize.brentq(f,ab[0],ab[1],full_output=True)
print(f"root: {root}\n")
print(soln)
#print(soln.method) # sigh = n/a

```

```
root: 1.8392867552141612

      converged: True
           flag: converged
 function_calls: 10
     iterations: 9
           root: 1.8392867552141612
```

- oscar veliz @youtube (multiple methods including brents method)

- brents method
- richard brent
- theodorus dekker with a bonus

- library function documentation @scipy @matlab
- matlab @online