2072U Computational Science I
Winter 2022

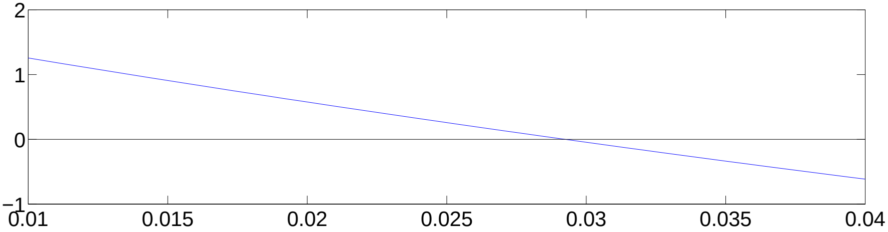
Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. First method: bisection
2. Bisection
3. Newton iteration
4. Comparing the two
5. Secant method
6. Recursion

The problem

Suppose we have a continuous function f on some domain $[a, b]$. Find $x^* \in [a, b]$ such that

$$f(x^*) = 0.$$

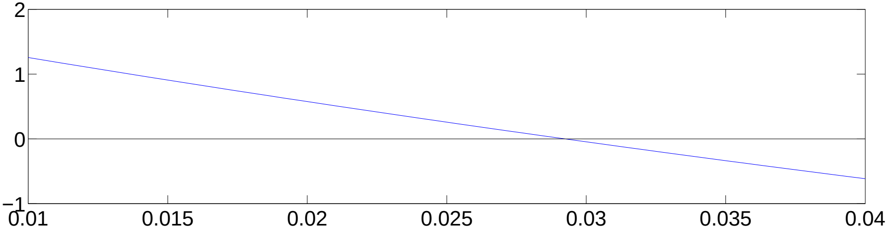


Intermediate Value Theorem

Suppose we have a continuous function f on some domain $[a, b]$. Then if k is some number between $f(a)$ and $f(b)$ then there exists at least one number c in the interval $[a, b]$ such that $f(c) = k$. That is,

$$f(a) < k < f(b) \quad \text{or} \quad f(a) > k > f(b),$$

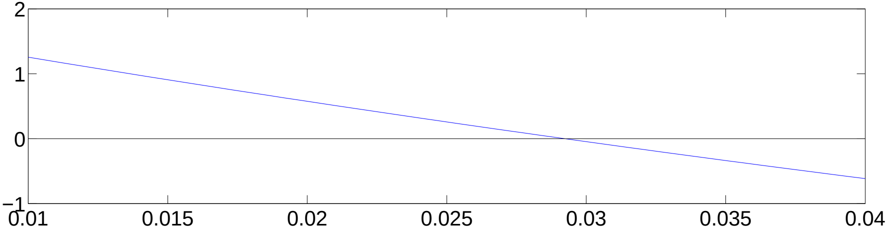
$$\rightarrow \quad \exists\, c \in [a, b] \quad \text{s.t.} \quad f(c) = k$$



Intermediate Value Theorem for $k = 0$

Suppose we have a continuous function f on some domain $[a, b]$. Then if $f(a)f(b) < 0$ then there exists at least one number c in the interval $[a, b]$ such that $f(c) = 0$. That is,

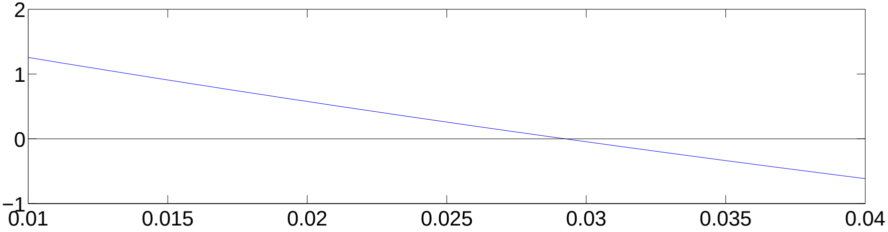
$$f(a)f(b) < 0 \quad \rightarrow \quad \exists\ c \in [a, b] \quad \text{s.t.} \quad f(c) = 0$$



Bisection

Suppose we have a continuous function f on some domain $[a, b]$. Find a, b such that $f(a)f(b) < 0$, then by the Intermediate Value Theorem, there exists at least one solution $x^* \in [a, b]$ to the equation

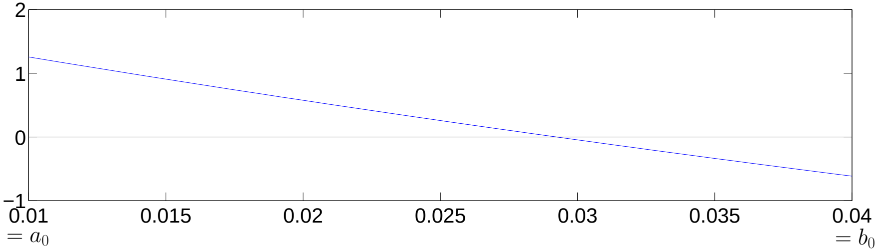
$$f(x^*) = 0.$$



Bisection in *pseudo-code*:

Input: f, a, b, $k_{\max}$, ϵ_x, ϵ_f.

1. Set $a_0 = a$, $b_0 = b$.
2. Do for $k = 1, \ldots, k_{\max}$
    - Let $c_k = (a_{k-1} + b_{k-1})/2$ and $f_k = f(c_k)$.
    - If $f_k f(a_{k-1}) > 0$ then let $a_k = c_k$ and $b_k = b_{k-1}$ else let $a_k = a_{k-1}$ and $b_k = c_k$.
    - If $|b_k - a_k| < \epsilon_x$ or $|f(c_k)| < \epsilon_f$ break.
3. Return $x^* = c_k$ and $|b_k - a_k|$.



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   - If $|b_k - a_k| < \epsilon_x$ or $|f(c_k)| < \epsilon_f$ break.
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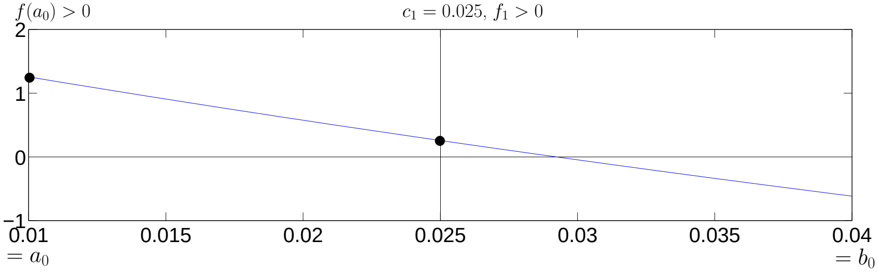
For $\epsilon_x = \epsilon_f = 0.001$, $x^* \approx 0.0296875$ with error 9.375×10^{-4}.



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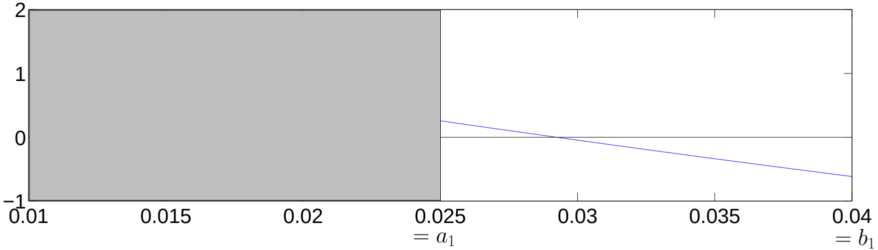

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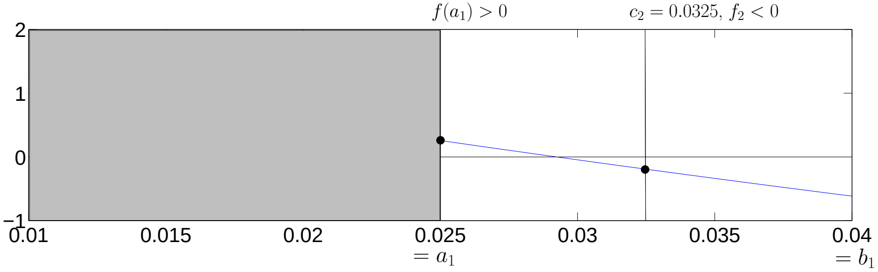

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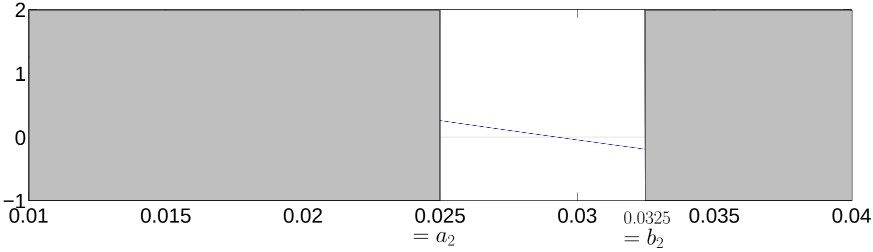

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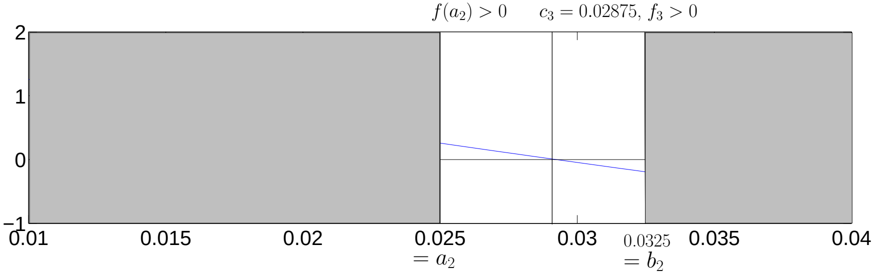

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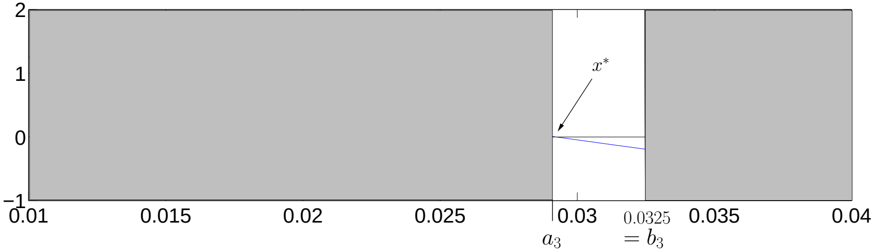

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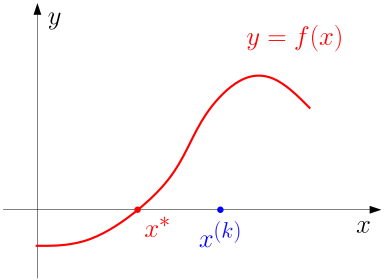
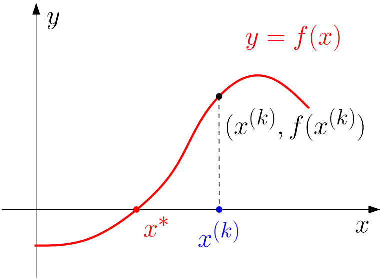
Newton's method: derivation

- Start with $x^{(k)}$ (intended to approximate x^* such that $f(x^*) = 0$)



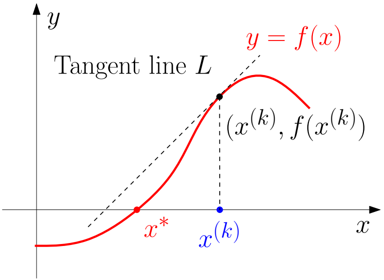
Newton's method: derivation

- Start with $x^{(k)}$ (intended to approximate x^* such that $f(x^*) = 0$)
- Evaluate f at $x^{(k)}$



Newton's method: derivation

- Start with $x^{(k)}$ (intended to approximate x^* such that $f(x^*) = 0$)
- Evaluate f at $x^{(k)}$
- Extend tangent line L from $(x^{(k)}, f(x^{(k)}))$ (using $f'(x^{(k)})$)



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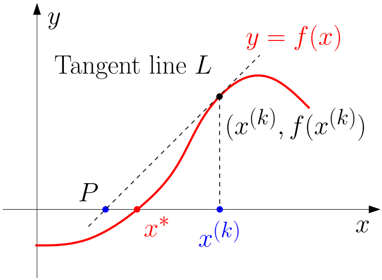
- Follow L to P (where it cuts x-axis)



Newton's method: derivation

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- Evaluate f at $x^{(k)}$
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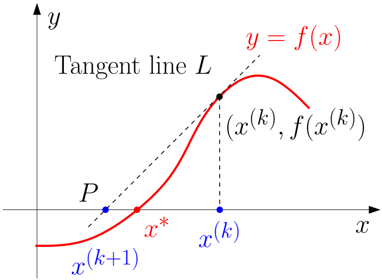
- Follow L to P (where it cuts x-axis)
- $x^{(k+1)}$ defined as x-coordinate of point P



Newton's method: derivation

- Slope of L is $f'(x^{(k)})$ & x-intercept is $x^{(k+1)}$, so

$$f'(x^{(k)}) = \frac{f(x^{(k)}) - 0}{x^{(k)} - x^{(k+1)}}.$$

- Solving for $x^{(k+1)}$ gives the formula for Newton's method.

$$\boxed{x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}} \qquad (k \geq 0)$$

- Hopefully, $x^{(k+1)}$ closer to true zero x^* than $x^{(k)}$.

Newton's method

Given an iterate $x^{(k)}$ approximating a zero of f, the next iterate is

$$\boxed{x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}} \qquad (k \geq 0)$$

- Iterative procedure to locate zeros of f.
- Requires initial iterate $x^{(0)}$ to start.
- Near true zero x^* of f, iteration converges quickly.

Algorithm for Newton's method

Input: $f, f', x^{(0)}$
for $k = 0, 1, 2, \ldots$ **until** convergence

$r^{(k)} \leftarrow f\left(x^{(k)}\right)$	(evaluate nonlinear residual)
$\delta x^{(k)} \leftarrow -\left[f'\left(x^{(k)}\right)\right]^{-1} r^{(k)}$	(compute Newton step)
$x^{(k+1)} \leftarrow x^{(k)} + \delta x^{(k)}$	(compute next iterate)
Test for convergence	(break if necessary)

end for
Output: $x^{(k)}$

- Terminology: $r^{(k)} := f(x^{(k)}) = \text{residual}$
- Terminology: $\delta x^{(k)} := -\left[f'\left(x^{(k)}\right)\right]^{-1} r^{(k)} = \text{Newton step}$

Example:
Carry out Newton's method starting from $x^{(0)} = 0.75$ to find $x^{(3)}$ that approximates the real solution of $x = \cos x$.

- Define $f(x) = x - \cos x$, so $f'(x) = 1 + \sin x$

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- Define $f(x) = x - \cos x$, so $f'(x) = 1 + \sin x$
- Then, Newton's method is $x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$, or, in steps,

$$
\begin{aligned}
r^{(k)} &= f(x^{(k)}) = x^{(k)} - \cos(x^{(k)}), \\
\delta x^{(k)} &= \frac{-r^{(k)}}{f'(x^{(k)})} = \frac{-r^{(k)}}{1 + \sin(x^{(k)})}, \\
x^{(k+1)} &= x^{(k)} + \delta x^{(k)}
\end{aligned}
$$

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\end{aligned}
$$

- Use formulas above 3 times starting from $k = 0$, $x^{(0)} = 0.75$ to obtain sequence $x^{(1)}$,$x^{(2)}$,$x^{(3)}$ (see following table)

Example 1:
Carry out Newton's method starting from $x^{(0)} = 0.75$ to find $x^{(3)}$ that approximates the real solution of $x = \cos x$.

$$f(x) = x - \cos x \qquad f'(x) = 1 + \sin x$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.75		

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.75	1.83111×10^{-2}	

$x^{(0)} = 0.75,$

$r^{(0)} = f(x^{(0)}) = x^{(0)} - \cos(x^{(0)}) = 0.75 - \cos(0.75) = 1.83111 \times 10^{-2},$

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}

$$x^{(0)} = 0.75,$$

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}
1	0.739111138752579		

$$x^{(0)} = 0.75,$$

$$r^{(0)} = f(x^{(0)}) = x^{(0)} - \cos(x^{(0)}) = 0.75 - \cos(0.75) = 1.83111 \times 10^{-2},$$

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$$x^{(1)} = x^{(0)} + \delta x^{(0)} = 0.75 + (-1.08889 \times 10^{-2}) = 0.739111138752579$$

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0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}
1	0.739111138752579	4.35234×10^{-5}	

$$x^{(1)} = 0.739111138752579,$$

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0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}
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$$x^{(1)} = 0.739111138752579,$$

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0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}
1	0.739111138752579	4.35234×10^{-5}	-2.60055×10^{-5}
2	0.739085133364485		

$$x^{(1)} = 0.739111138752579,$$

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$$x^{(2)} = x^{(1)} + \delta x^{(1)} = 0.739111 + (-2.60055 \times 10^{-5}) = 0.73908513336448$$

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0	0.75	1.83111×10^{-2}	-1.08889×10^{-2}
1	0.739111138752579	4.35234×10^{-5}	-2.60055×10^{-5}
2	0.739085133364485	2.49910×10^{-10}	

$$x^{(2)} = 0.739085133364485,$$

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2	0.739085133364485	2.49910×10^{-10}	-1.49324×10^{-10}

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2	0.739085133364485	2.49910×10^{-10}	-1.49324×10^{-10}
3	0.739085133215161	$< 10^{-14}$	$< 10^{-14}$

$$x^{(2)} = 0.739085133364485,$$

$$r^{(2)} = f(x^{(2)}) = 0.739085 - \cos(0.739085) = 2.49910 \times 10^{-10},$$

$$\delta x^{(2)} = -\frac{r^{(2)}}{f'(x^{(2)})} = -\frac{2.49910 \times 10^{-10}}{1 + \sin(0.739085)} = -1.49324 \times 10^{-10},$$

$$x^{(3)} = x^{(2)} + \delta x^{(2)} = 0.739085 + (-1.49324 \times 10^{-10}) = 0.73908513321516$$

Example 2:
Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^{x} = 2$.

- Define $g(x) = x\exp(x) - 2$, so $g'(x) = (x+1)\exp(x)$

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- Then, Newton's method is $x^{(k+1)} = x^{(k)} - \frac{g(x^{(k)})}{g'(x^{(k)})}$, or, in steps,

$$
\begin{aligned}
r^{(k)} &= g(x^{(k)}) = x^{(k)}\exp(x^{(k)}) - 2,\\
\delta x^{(k)} &= \frac{-r^{(k)}}{g'(x^{(k)})} = \frac{-r^{(k)}}{(x^{(k)}+1)\exp(x^{(k)})},\\
x^{(k+1)} &= x^{(k)} + \delta x^{(k)}
\end{aligned}
$$

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x^{(k+1)} &= x^{(k)} + \delta x^{(k)}
\end{aligned}$$

- Use formulas above 3 times starting from $k = 0$, $x^{(0)} = 0.5$ to obtain sequence $x^{(1)}$,$x^{(2)}$,$x^{(3)}$ (see following table)

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$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5		

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	

$$x^{(0)} = 0.5,$$

$$r^{(0)} = g(x^{(0)}) = x^{(0)}\exp(x^{(0)}) - 2 = 0.5\exp(0.5) - 2 = -1.17564,$$

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Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^x = 2$.

$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374

$$x^{(0)} = 0.5,$$
$$r^{(0)} = g(x^{(0)}) = x^{(0)}\exp(x^{(0)}) - 2 = 0.5\exp(0.5) - 2 = -1.17564,$$
$$\delta x^{(0)} = -\frac{r^{(0)}}{g'(x^{(0)})} = -\frac{(-1.17564)}{(0.5+1)\exp(0.5)} = 0.475374,$$

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Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^x = 2$.

$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178		

$$
\begin{aligned}
x^{(0)} &= 0.5, \\
r^{(0)} &= g(x^{(0)}) = x^{(0)}\exp(x^{(0)}) - 2 = 0.5\exp(0.5) - 2 = -1.17564, \\
\delta x^{(0)} &= -\frac{r^{(0)}}{g'(x^{(0)})} = -\frac{(-1.17564)}{(0.5+1)\exp(0.5)} = 0.475374, \\
x^{(1)} &= x^{(0)} + \delta x^{(0)} = 0.5 + (0.475374) = 0.975374212950178
\end{aligned}
$$

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Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^x = 2$.

$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	

$$x^{(1)} = 0.975374212950178,$$
$$r^{(1)} = g(x^{(1)}) = 0.975374\exp(0.975374) - 2 = 0.586848,$$

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Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^x = 2$.

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	-0.112015

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k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	-0.112015
2	0.863359106097814		

$$x^{(1)} = 0.975374212950178,$$

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$$x^{(2)} = x^{(1)} + \delta x^{(1)} = 0.975374212950178 + -0.112015 = 0.86335910609$$

Example 2:
Carry out Newton's method starting from $x^{(0)} = 0.5$ to find $x^{(3)}$ that approximates a zero of the equation $xe^x = 2$.

$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	-0.112015
2	0.863359106097814	4.71213×10^{-2}	

$$x^{(2)} = 0.863359106097814,$$

$$r^{(2)} = g(x^{(2)}) = 0.863359\exp(0.863359) - 2 = 4.71213 \times 10^{-2},$$

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$$g(x) = x\exp(x) - 2 \qquad g'(x) = (x+1)\exp(x)$$

k	$x^{(k)}$	$r^{(k)}$	$\delta x^{(k)}$
0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	-0.112015
2	0.863359106097814	4.71213×10^{-2}	-1.06652×10^{-2}

$$x^{(2)} = 0.863359106097814,$$

$$r^{(2)} = g(x^{(2)}) = 0.863359\exp(0.863359) - 2 = 4.71213 \times 10^{-2},$$

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0	0.5	-1.17564	0.475374
1	0.975374212950178	0.586848	-0.112015
2	0.863359106097814	4.71213×10^{-2}	-1.06652×10^{-2}
3	0.852693923733206	3.84285×10^{-4}	—

$$x^{(2)} = 0.863359106097814,$$
$$r^{(2)} = g(x^{(2)}) = 0.863359\exp(0.863359) - 2 = 4.71213 \times 10^{-2},$$
$$\delta x^{(2)} = -\frac{r^{(2)}}{g'(x^{(2)})} = -\frac{4.71213 \times 10^{-2}}{(0.863359 + 1)\exp(0.863359)} = -1.06652 \times 10^{-2},$$
$$x^{(3)} = x^{(2)} + \delta x^{(2)} = 0.863359106097814 + (-1.06652 \times 10^{-2}) = 0.85269$$

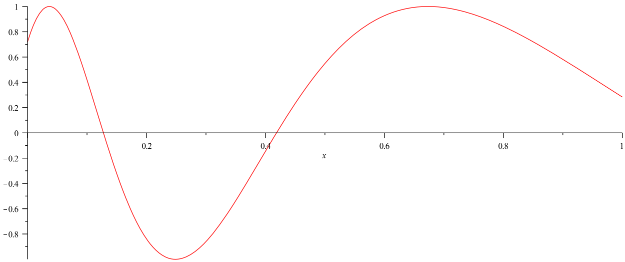
Now we have to answer the three essential questions:

1. Under what conditions does the algorithm converge?
2. How accurate will the result be?
3. How fast does it converge?

Since bisection and Newton iterations serve the same pupose (find x^* such that $f(x^*) = 0$) we can compare them...

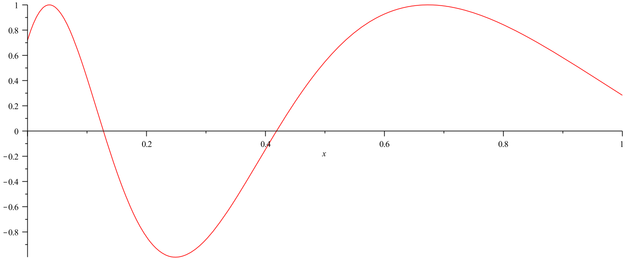
1. Under what conditions does the algorithm converge?

Bisection converges to some x^* such that $f(x^*) = 0$ in $[a, b]$, if f is continuous and $f(a)f(b) < 0$.
If there are two or more solutions, we don't know to which one it will converge.



1. Under what conditions does the algorithm converge?

Newton iteration converges if x_0 is *sufficiently close* to x^*. Usually, we do not know a priori how close is close enough and we must resort to trial and error....



2. How accurate will the result be?

Both methods can give us x^* up to machine precision.

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Both methods can give us x^* up to machine precision.

3. How fast does it converge?

In bisection, the error $|x^* - x^{(k)}|$ decreases by a factor of 1/2 in each iteration.
In Newton iterations, the error is approximately squared in each iteration (provided it is small enough!).

$$\epsilon_0, \frac{\epsilon_0}{2}, \frac{\epsilon_0}{4}, \frac{\epsilon_0}{8}, \dots \qquad \text{vs.} \qquad \epsilon_0, \epsilon_0^2, \epsilon_0^4, \epsilon_0^8, \dots$$

Newton's method converges very quickly, but requires the computation of $f'(x)$.
Sometimes, we cannot compute it, for instance if f is shorthand for some complicated procedure:

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In that case, we have two options:

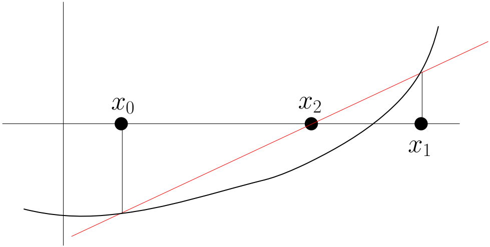
1. bisection, or
2. the secant method.

Suppose we have *two* intial points, x_0 and x_1.
Then we can *estimate* the derivative of f at x_1 as

$$f'(x_1) \approx \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

and substitute this in the Newton iteration:

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \approx x_1 - \frac{f(x_1)(x_1 - x_0)}{f(x_1) - f(x_0)}$$



Then we iterate to find:

Secant method

Given iterates $x^{(k)}$ and $x^{(k-1)}$ approximating a zero of f, compute

$$\boxed{x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})\left[x^{(k)} - x^{(k-1)}\right]}{f(x^{(k)}) - f(x^{(k-1)})}} \quad (k \geq 1)$$

Secant methods needs *two* initial guesses: $x^{(0)}$ and $x^{(1)}$

Some remarks:

- This method uses a *finite difference* approximation to f'.
- Asymptotically (meaning if $|x_k - x^*|$ is small enough) the secant method converges as fast as Newton's method does.
- The secant method has extensions to problems with more than 1 unknown, but in this case Newton's method tends to be less cumbersome.
- The secant method is a *second order recurrence relation*. It relates the next approximation to the *two* previous approximations.
- If we can find an a and b such that $x^* \in [a, b]$, then $x_0 = a$ and $x_1 = b$ is a good starting point.

Recurrence and *iteration* really mean procedures in which we repeat the same action over and over.
One way to program this is by using `for` and `while` loops.
We can also make the recurrent nature of the computation explicit by *making the function call itself.*
This is called *recursive* programming.
Simple example:

```
def fact(k):
    if k == 1:
        return 1
    else:
        return fact(k-1) * k
```