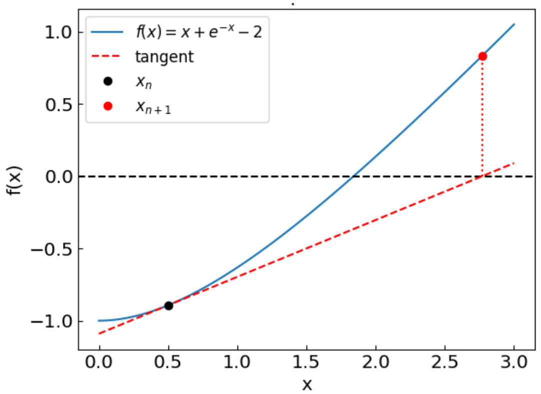
# Computational Physics (PHYS6350)

*Lecture 6: Non-linear equations and root-finding*

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**Course materials:** https://github.com/vlvovch/PHYS6350-ComputationalPhysics/tree/spring2025

# Non-linear equations

Suppose we have an equation $f(x) = 0$

We can evaluate $f(x)$, but we do not know how to solve it for $x$

**Examples:**

- Roots of high-order polynomials (physics example: Lagrange $L_1$ point)
- Transcendental equations
  - e.g. magnetization equation

$$M = \mu \tanh \frac{JM}{k_B T}$$

*References:* Chapter 6 of *Computational Physics* by Mark Newman

Chapter 9 of *Numerical Recipes Third Edition* by W.H. Press et al.

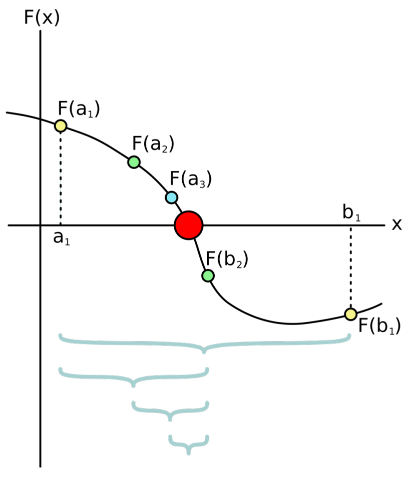
# Root-finding techniques

**Numerical root-finding method:** iterative process to determine the root(s) of non-linear equation(s) to desired accuracy

**Types:**

- Two-point (bracketing)
  - Bisection method
  - False position method

involves branching

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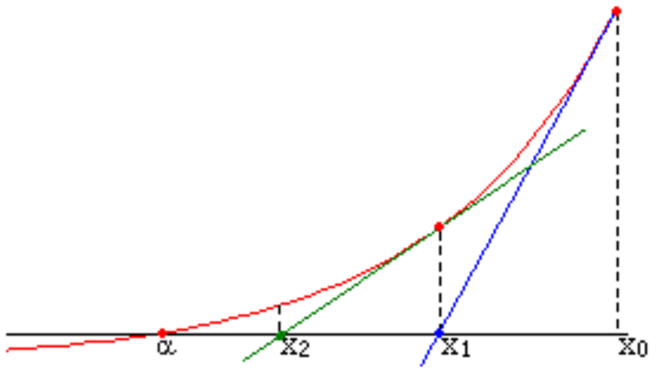
- Local
  - Secant method
  - Newton-Raphson method (using the derivative)
  - Relaxation method

no branching

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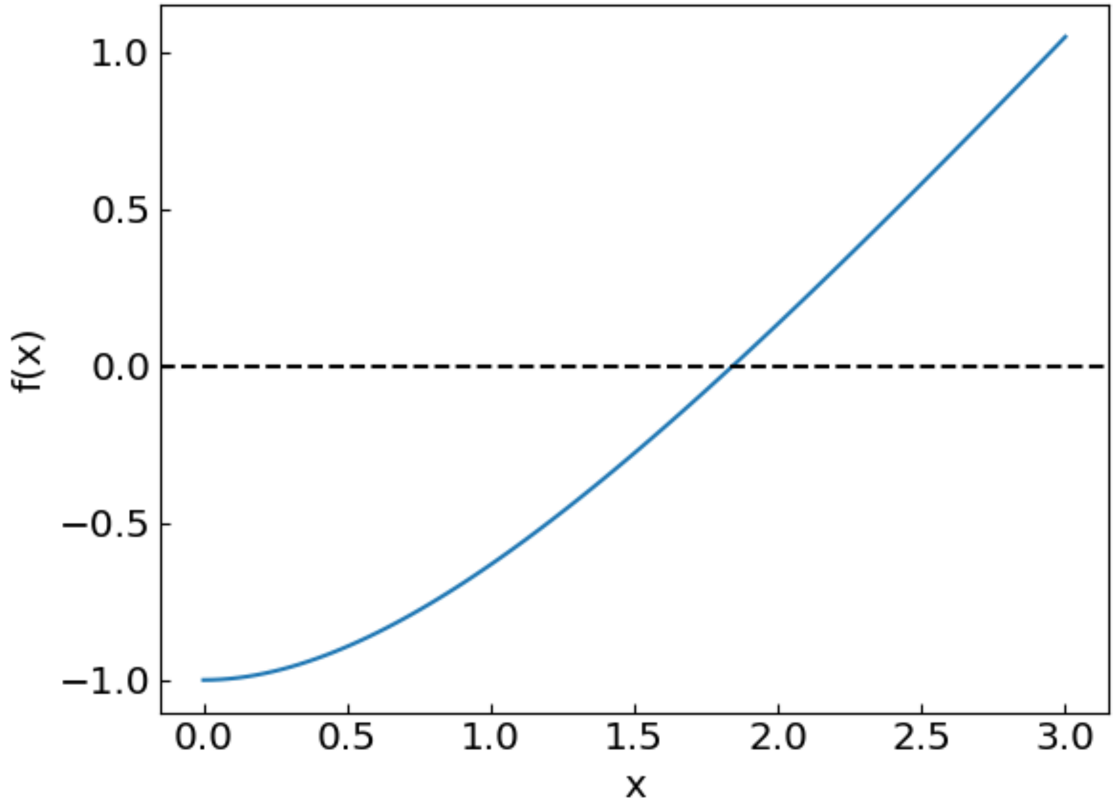
- Multi-dimensional
  - Newton method
  - Broyden method

# Non-linear equations

Consider an equation

$$x + e^{-x} - 2 = 0$$



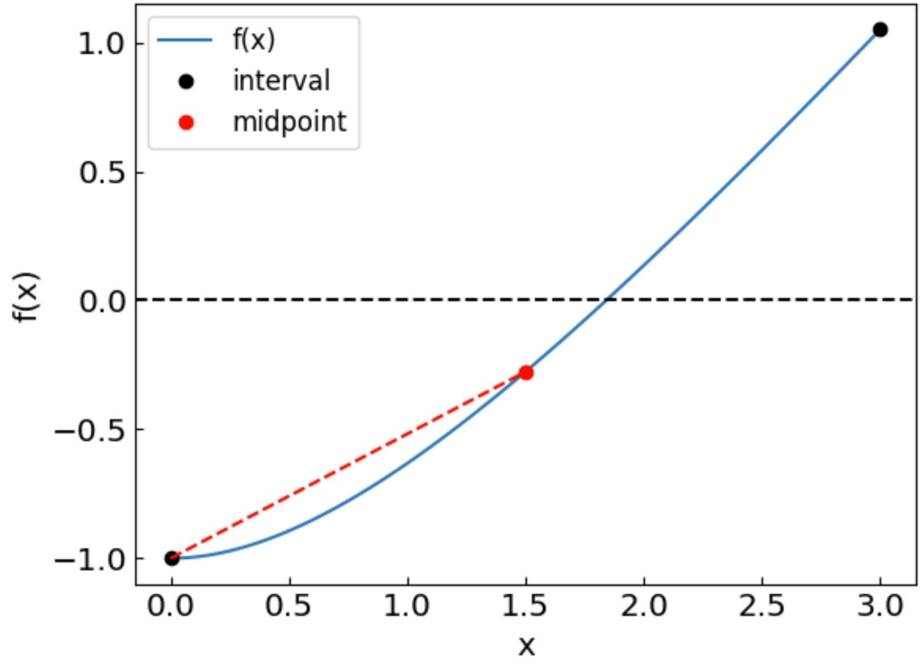
# Bisection method

**Bisection method:**

1. Find an interval $(a, b)$ which brackets the root $x^*$
   - $x^* \in (a, b)$
   - $f(a)$ & $f(b)$ have opposite signs

2. Take the midpoint $c = (a + b)/2$ and halve the interval bracketing the root

3. Repeat the process until the desired precision is achieved



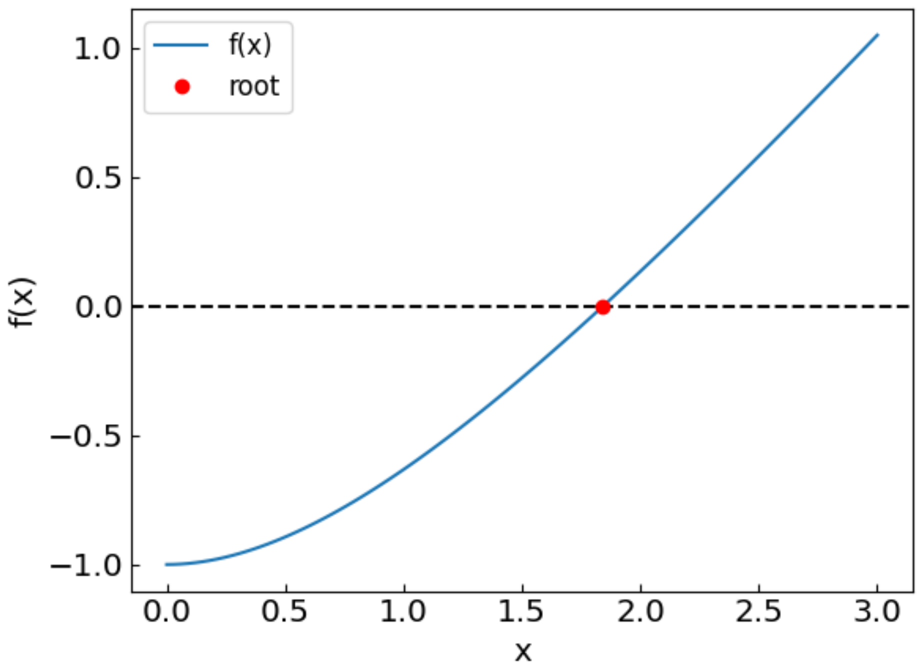

**Error:** $\varepsilon_{n+1} = \frac{\varepsilon_n}{2}$ (linear)

Method is guaranteed to converge to the root
The error is halved at each step ("linear" convergence)

# Bisection method

```python
def bisection_method(
    f,                      # The function whose root we are trying to find
    a,                      # The left boundary
    b,                      # The right boundary
    tolerance = 1.e-10,     # The desired accuracy of the solution
    ):
    fa = f(a)                           # The value of the function at the left boundary
    fb = f(b)                           # The value of the function at the right boundary
    if (fa * fb > 0.):
        return None                     # Bisection method is not applicable

    global last_bisection_iterations
    last_bisection_iterations = 0


    while ((b-a) > tolerance):
        last_bisection_iterations += 1
        c = (a + b) / 2.                # Take the midpoint
        fc = f(c)                       # Calculate the function at midpoint


        if (fc * fa < 0.):
            b = c                       # The midpoint is the new right boundary
            fb = fc
        else:
            a = c                       # The midpoint is the new left boundary
            fa = fc

    return (a+b) / 2.
```

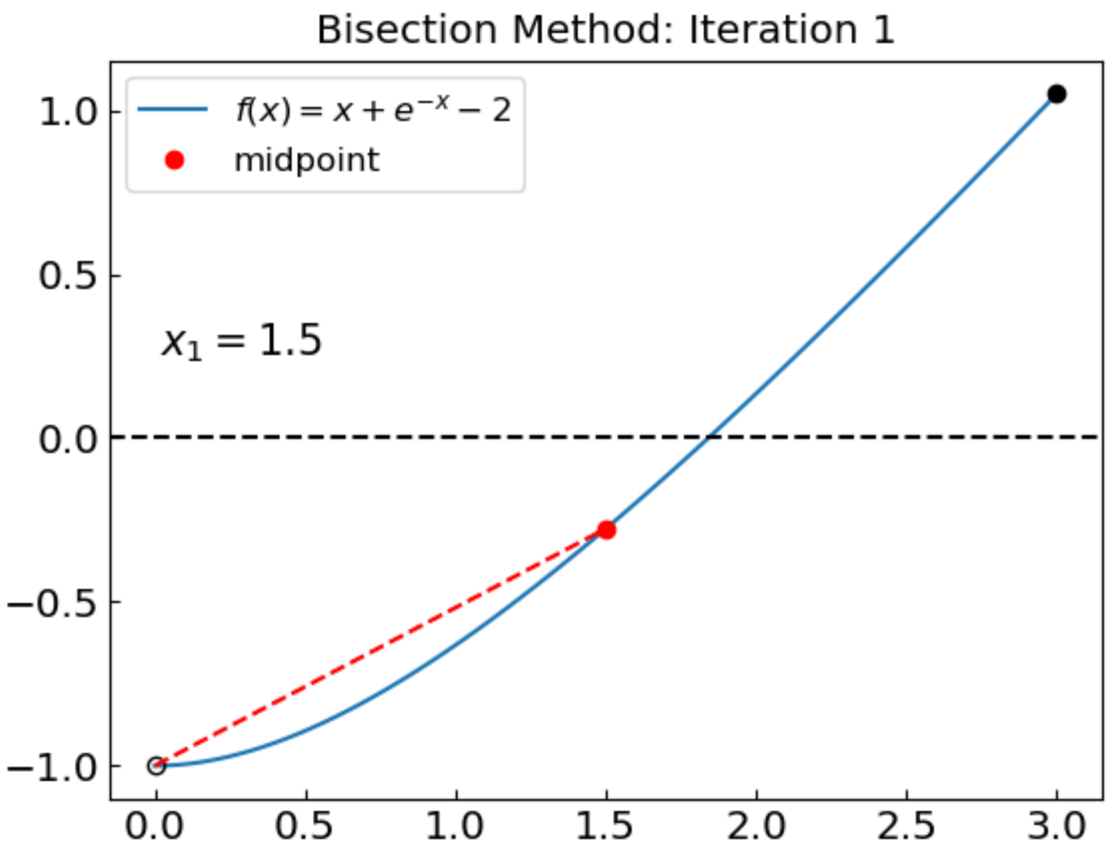
$$x + e^{-x} - 2 = 0$$




```
Solving the equation x + e^-x - 2 = 0 on an interval ( 0.0 , 3.0 ) using bisection method
The solution is x =  1.8414056604233338  obtained with  35  iterations
```

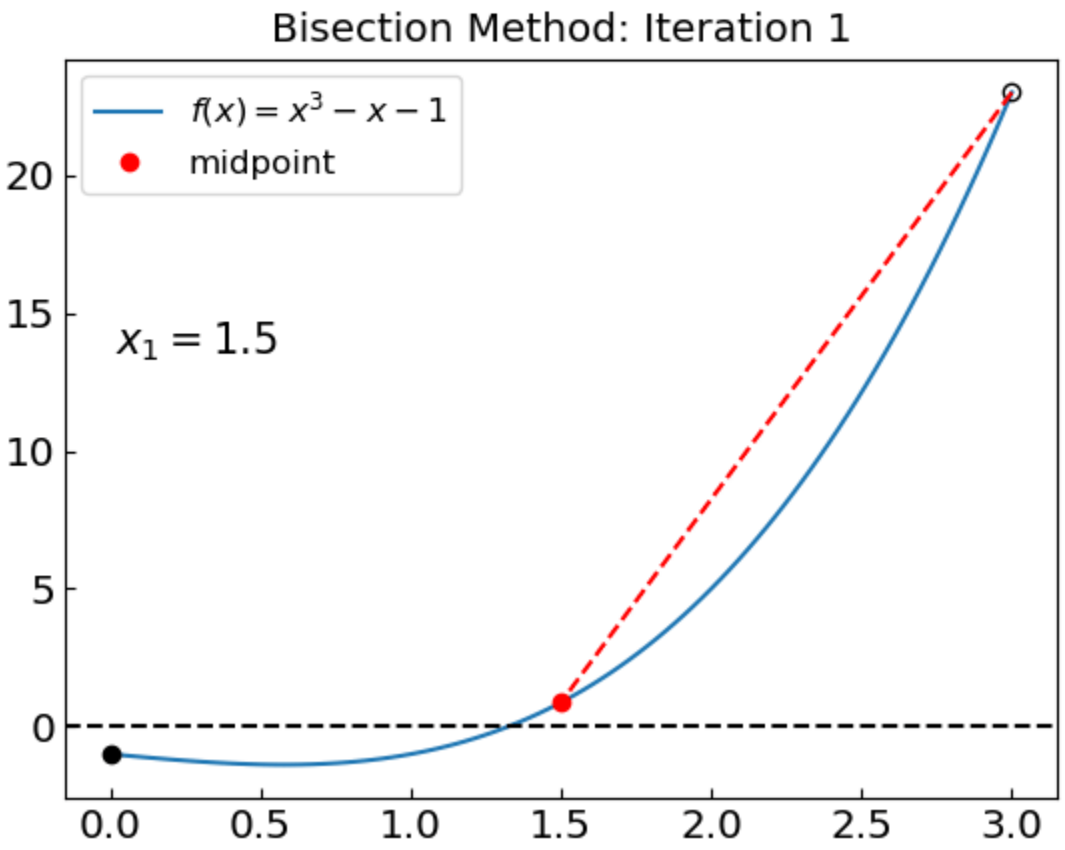
# Bisection method: how the iterations look like

$$x + e^{-x} - 2 = 0$$



# Bisection method: another example

Let us consider another equation: $x^3 - x - 1 = 0$




35 iterations in both cases

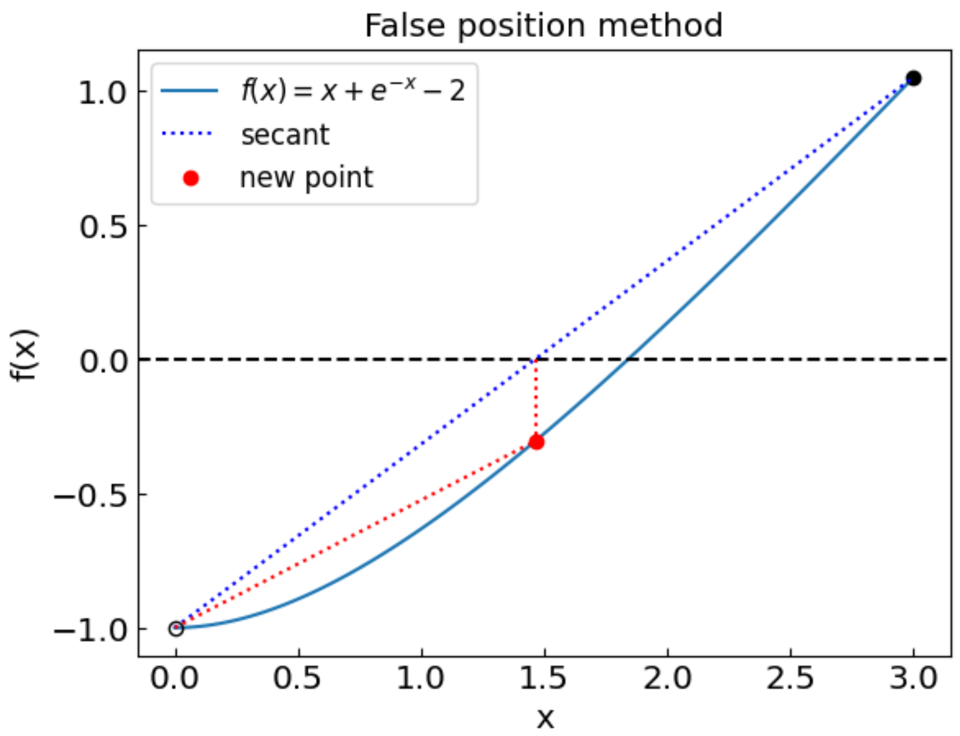
# False position method

**False position method:**

1. Find an interval $(a, b)$ which brackets the root $x^*$ (same as in bisection method)

2. Instead of midpoint take a point where the straight line between the endpoints crosses the $y = 0$ axis
$$c = a - f(a)\frac{b-a}{f(b)-f(a)}$$

3. Repeat the process until the desired precision is achieved



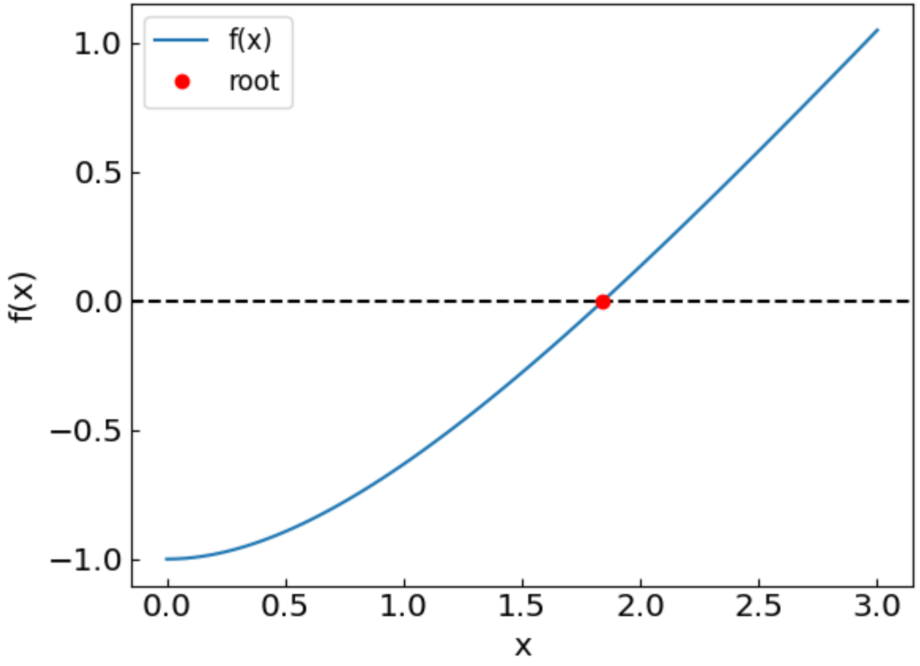

**Error:** $\varepsilon_{n+1} \approx C\varepsilon_n$ (linear)

Method is guaranteed to converge to the root
"Linear" convergence; typically faster than bisection, but not always (see example further)

# False position method

```python
def falseposition_method(
    f,                      # The function whose root we are trying to find
    a,                      # The left boundary
    b,                      # The right boundary
    tolerance = 1.e-10,     # The desired accuracy of the solution
    max_iterations = 100    # Maximum number of iterations
    ):
    fa = f(a)                           # The value of the function at the left boundary
    fb = f(b)                           # The value of the function at the right boundary
    if (fa * fb > 0.):
        return None                     # False position method is not applicable

    xprev = xnew = (a+b) / 2.                  # Estimate of the solution from the previous step

    global last_falseposition_iterations
    last_falseposition_iterations = 0

    for i in range(max_iterations):
        last_falseposition_iterations += 1

        xprev = xnew
        xnew = a - fa * (b - a) / (fb - fa) # Take the point where straight line between a and b crosses y = 0
        fnew = f(xnew)                      # Calculate the function at midpoint

        if (fnew * fa < 0.):
            b = xnew                        # The intersection is the new right boundary
            fb = fnew
        else:
            a = xnew                        # The midpoint is the new left boundary
            fa = fnew

        if (abs(xnew-xprev) < tolerance):
            return xnew

    print("False position method failed to converge to a required precision in " + str(max_iterations) + " iterations")
    print("The error estimate is ", abs(xnew - xprev))

    return xnew
```

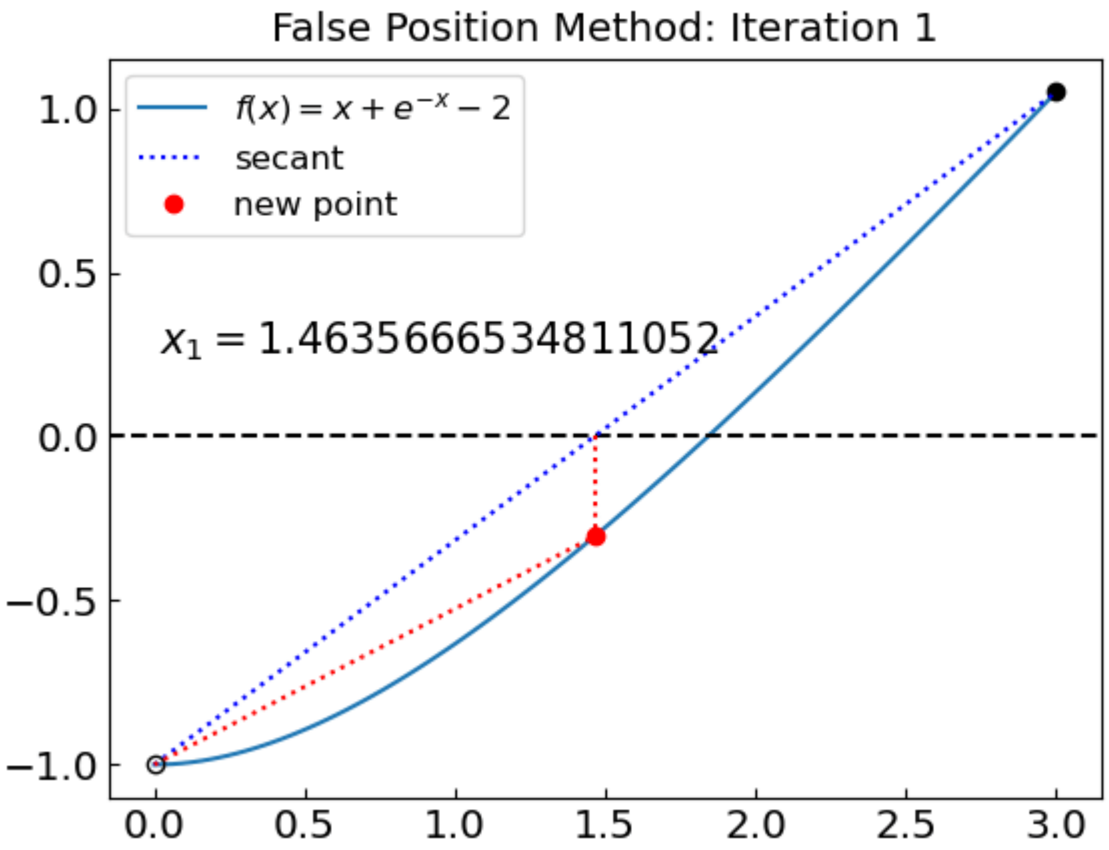
$$x + e^{-x} - 2 = 0$$




```
Solving the equation x + e^-x - 2 = 0 on an interval ( 0.0 , 3.0 ) using the false position method
The solution is x =  1.8414056604354012 obtained after  11  iterations
```

# False position method

$$x + e^{-x} - 2 = 0$$



# False position vs bisection (to 10 decimal digits)

$$x + e^{-x} - 2 = 0$$

**Bisection method:**

```
Iteration:     1, c =    1.500000000000000
Iteration:     2, c =    2.250000000000000
Iteration:     3, c =    1.875000000000000
Iteration:     4, c =    1.687500000000000
Iteration:     5, c =    1.781250000000000
Iteration:     6, c =    1.828125000000000
Iteration:     7, c =    1.851562500000000
Iteration:     8, c =    1.839843750000000
Iteration:     9, c =    1.845703125000000
Iteration:    10, c =    1.842773437500000
Iteration:    11, c =    1.841308593750000
Iteration:    12, c =    1.842041015625000
Iteration:    13, c =    1.841674804687500
Iteration:    14, c =    1.841491699218750
Iteration:    15, c =    1.841400146484375
Iteration:    16, c =    1.841445922851562
Iteration:    17, c =    1.841423034667969
Iteration:    18, c =    1.841411590576172
Iteration:    19, c =    1.841405868530273
Iteration:    20, c =    1.841403007507324
                  ...
Iteration:    35, c =    1.841405660466990
```

**False position method:**

```
Iteration:     1, x =    1.463566653481105
Iteration:     2, x =    1.809481253839539
Iteration:     3, x =    1.839095511827520
Iteration:     4, x =    1.841240588240115
Iteration:     5, x =    1.841393875903701
Iteration:     6, x =    1.841404819191791
Iteration:     7, x =    1.841405600384506
Iteration:     8, x =    1.841405656150106
Iteration:     9, x =    1.841405660130943
Iteration:    10, x =    1.841405660415115
Iteration:    11, x =    1.841405660435401
```

# False position vs bisection: not always clear who wins

$$x^3 - x - 1 = 0$$

**Bisection method:**

```
Iteration:     1, c =    1.500000000000000
Iteration:     2, c =    0.750000000000000
Iteration:     3, c =    1.125000000000000
Iteration:     4, c =    1.312500000000000
Iteration:     5, c =    1.406250000000000
Iteration:     6, c =    1.359375000000000
Iteration:     7, c =    1.335937500000000
Iteration:     8, c =    1.324218750000000
Iteration:     9, c =    1.330078125000000
Iteration:    10, c =    1.327148437500000
Iteration:    11, c =    1.325683593750000
Iteration:    12, c =    1.324951171875000
Iteration:    13, c =    1.324584960937500
Iteration:    14, c =    1.324768066406250
Iteration:    15, c =    1.324676513671875
Iteration:    16, c =    1.324722290039062
Iteration:    17, c =    1.324699401855469
Iteration:    18, c =    1.324710845947266
Iteration:    19, c =    1.324716567993164
Iteration:    20, c =    1.324719429016113
                  ...
Iteration:    35, c =    1.324717957206303
```

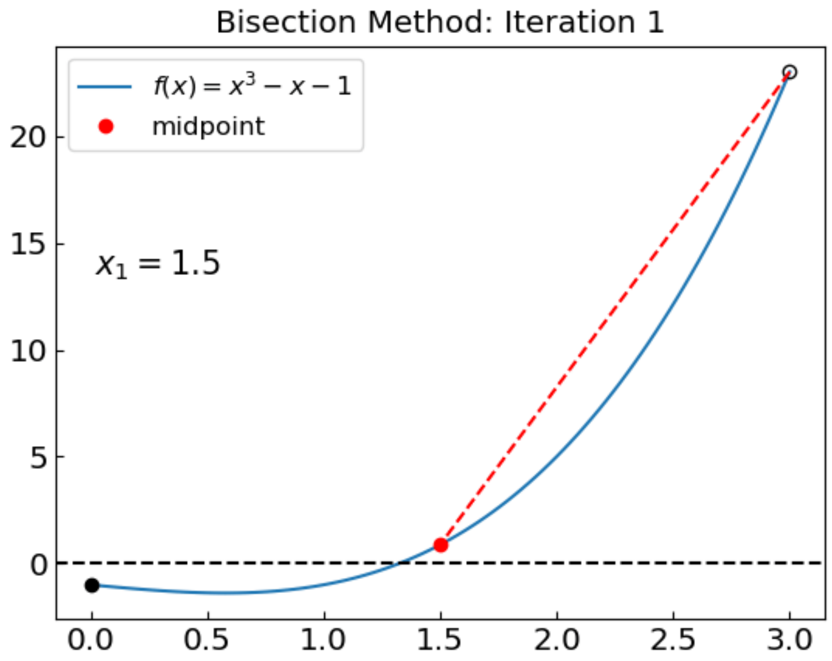
**False position method:**

```
Iteration:     1, x =    0.125000000000000
Iteration:     2, x =    0.258845437616387
Iteration:     3, x =    0.399230727605107
Iteration:     4, x =    0.541967526475374
Iteration:     5, x =    0.681365453934702
Iteration:     6, x =    0.811265467641601
Iteration:     7, x =    0.926423756077868
Iteration:     8, x =    1.023635980751716
Iteration:     9, x =    1.102112700940041
Iteration:    10, x =    1.163084623011103
Iteration:    11, x =    1.209004461867383
Iteration:    12, x =    1.242759715838447
Iteration:    13, x =    1.267123755869329
Iteration:    14, x =    1.284474915416815
Iteration:    15, x =    1.296712725379603
Iteration:    16, x =    1.305284823099690
Iteration:    17, x =    1.311260149895704
Iteration:    18, x =    1.315411216706803
Iteration:    19, x =    1.318288144277179
Iteration:    20, x =    1.320278742279728
                  ...
Iteration:    66, x =    1.324717957079699
```

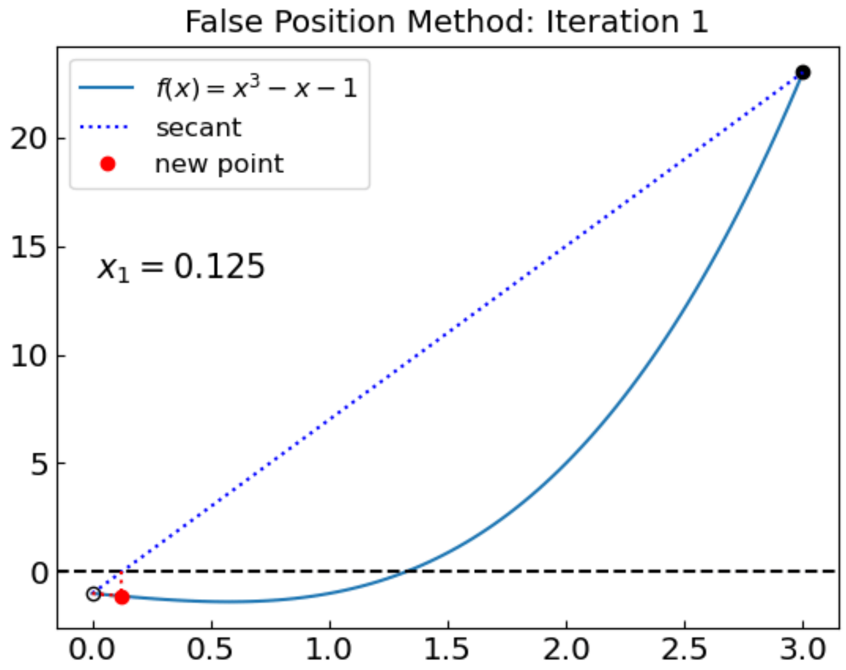
# False position vs bisection: not always clear who wins

$$x^3 - x - 1 = 0$$

**Bisection method:**




**False position method:**




More advanced methods combine the two and add other refinements*

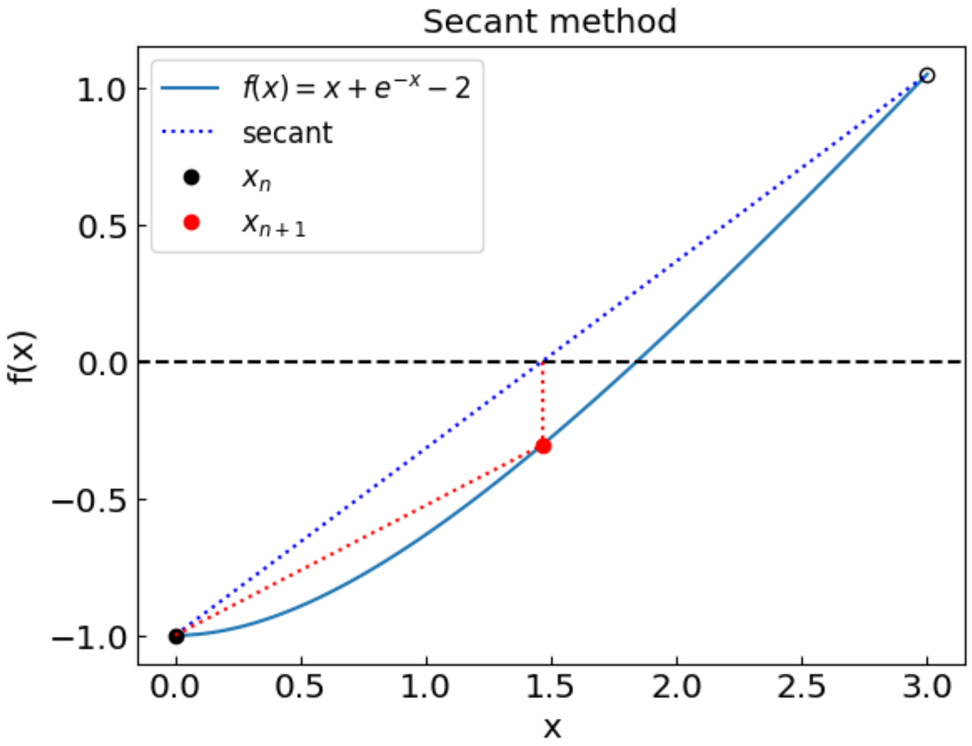
- Ridders' method
- Brent method

*final project idea(?)*

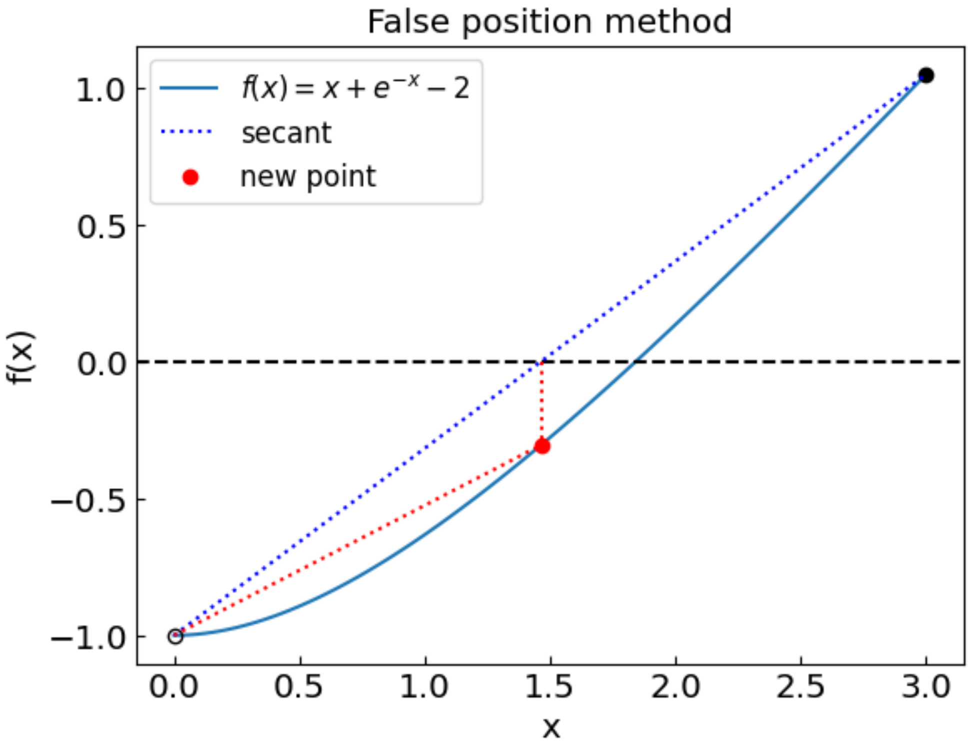
see chapters 9.2, 9.3 of *Numerical Recipes Third Edition* by W.H. Press et al.

# Secant method

**Secant method:** same as false position, except the interval *need not bracket the root*
Always uses the last two points, no branching (if-statement) involved in the procedure




vs



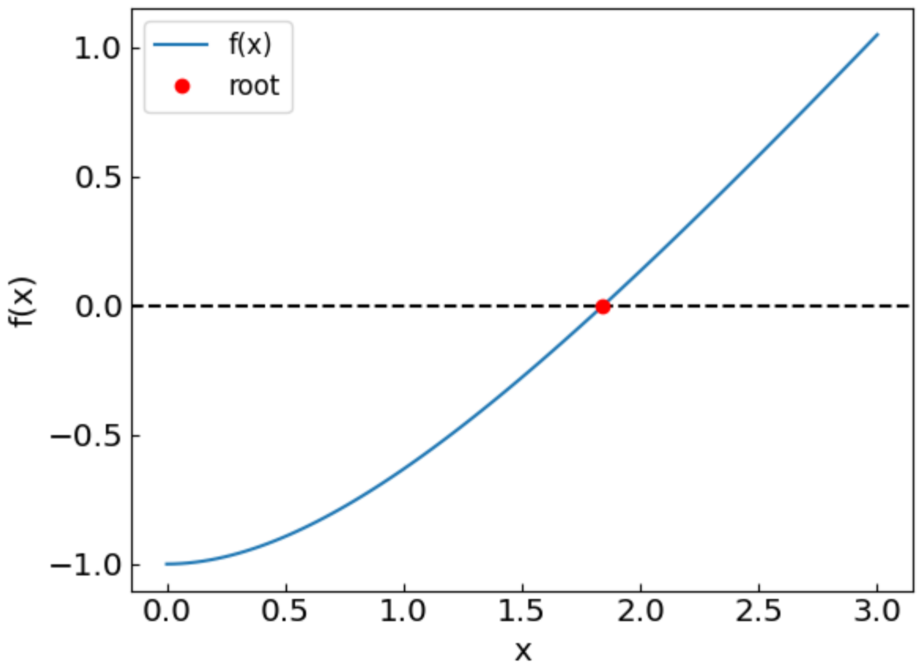

Typically, "superlinear" convergence occurs when the algorithm is effective.
However, it can still be slower than bisection or may not converge at all (e.g., the secant method may be parallel to the y-axis).

# Secant method

```python
def secant_method(
    f,                      # The function whose root we are trying to find
    a,                      # The left boundary
    b,                      # The right boundary
    tolerance = 1.e-10,     # The desired accuracy of the solution
    max_iterations = 100    # Maximum number of iterations
    ):
    fa = f(a)                              # The value of the function at the left boundary
    fb = f(b)                              # The value of the function at the right boundary

    xprev = xnew = a                              # Estimate of the solution from the previous step

    global last_secant_iterations
    last_secant_iterations = 0

    for i in range(max_iterations):
        last_secant_iterations += 1

        xprev = xnew
        xnew = a - fa * (b - a) / (fb - fa) # Take the point where straight line between a and b crosses y = 0
        fnew = f(xnew)                      # Calculate the function at midpoint

        b = a
        fb = fa
        a = xnew
        fa = fnew

        if (abs(xnew-xprev) < tolerance):
            return xnew

    print("Secant method failed to converge to a required precision in " + str(max_iterations) + " iterations")
    print("The error estimate is ", abs(xnew - xprev))

    return xnew
```

```
Solving the equation x + e^-x - 2 = 0 on an interval ( 0.0 , 3.0 ) using the secant method
The solution is x =  1.8414056604369606 obtained after  7  iterations
```

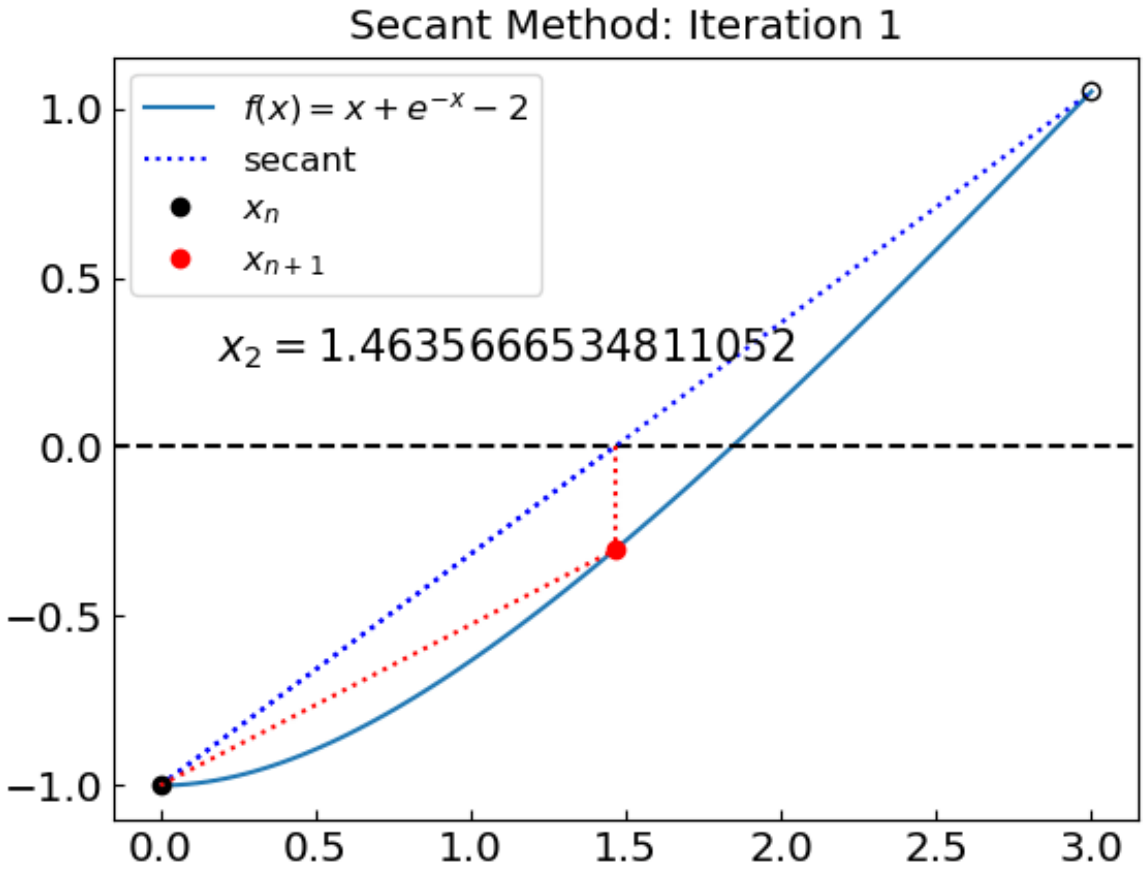
$$x + e^{-x} - 2 = 0$$




**Error:** $\varepsilon_{n+1} \approx C\varepsilon_n^{1+\alpha}$ (superlinear)

# Secant method

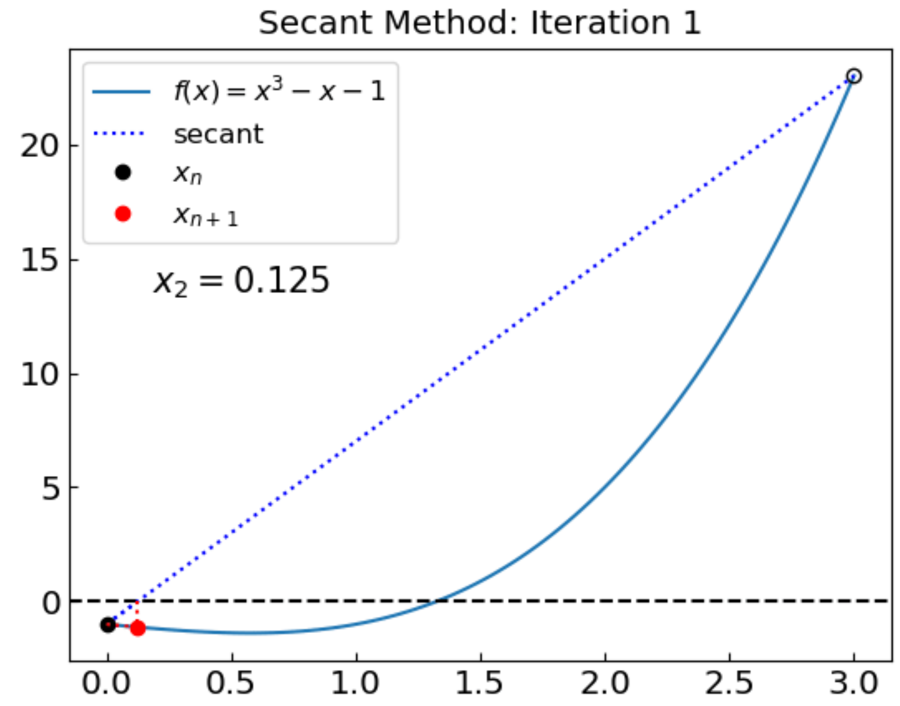
$$x + e^{-x} - 2 = 0$$



# Secant method

$$x^3 - x - 1 = 0$$

```
Iteration:    1, x =    0.125000000000000    Iteration:    17, x =   -1.058303471905222
Iteration:    2, x =   -1.015873015873016    Iteration:    18, x =   -0.643978481189561
Iteration:    3, x =  -14.026092564115256    Iteration:    19, x =   -0.131674045244213
Iteration:    4, x =   -1.010979901305751    Iteration:    20, x =   -1.933586024088406
Iteration:    5, x =   -1.006133240911884    Iteration:    21, x =    0.157497929951306
Iteration:    6, x =   -0.512666258317272    Iteration:    22, x =    0.626623389695762
Iteration:    7, x =    0.273834681149844    Iteration:    23, x =   -2.226715128003442
Iteration:    8, x =   -1.287767830907429    Iteration:    24, x =    1.093727500240917
Iteration:    9, x =    3.565966235528240    Iteration:    25, x =    1.382563036703896
Iteration:   10, x =   -1.077368321415013    Iteration:    26, x =    1.310687668369503
Iteration:   11, x =   -0.947522156044583    Iteration:    27, x =    1.323983763313963
Iteration:   12, x =   -0.513174359589628    Iteration:    28, x =    1.324727653842468
Iteration:   13, x =    0.447558454314033    Iteration:    29, x =    1.324717950607204
Iteration:   14, x =   -1.325124217388110    Iteration:    30, x =    1.324717957244686
Iteration:   15, x =    4.186373891812861    Iteration:    31, x =    1.324717957244746
Iteration:   16, x =   -1.167930924631363
```

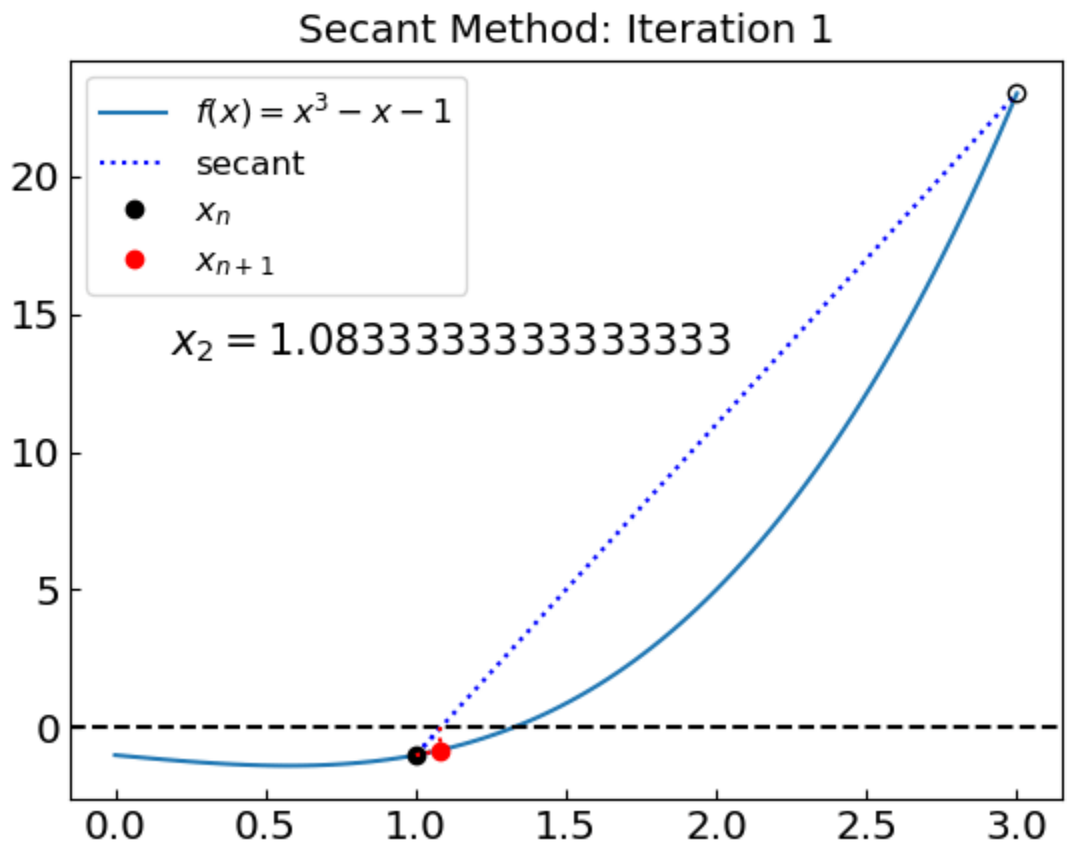



The secant method is not assured to converge since it does not bracket the root.
In this particular example, it eventually succeeded after initially diverging.

# Secant method: Choice of interval

$$x^3 - x - 1 = 0$$

Choose the initial interval as (1,3) instead of (0,3)




If possible, select the initial interval as close as possible to the root

# Newton-Raphson method

**Newton-Raphson method:**

- Local method (uses only the current estimate to get the next one)
- Requires the evaluation of the derivative (tangent)
  - Not always available or easy to compute

**Idea:** Assume that a given point x is close to the root $x^*$ [$f(x^*) = 0$]

Then (Taylor theorem)

$$f(x^*) \approx f(x) + f'(x)(x^* - x)$$

and since $f(x^*) = 0$ we have

$$x^* \approx x - \frac{f(x)}{f'(x)}$$

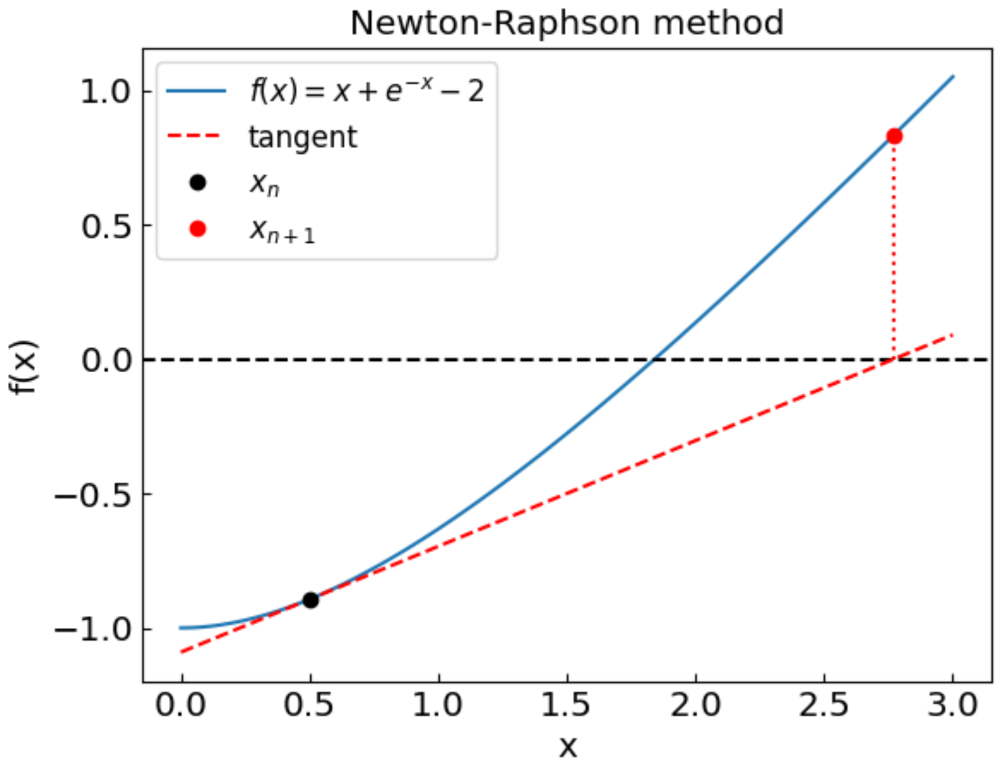
**Iterative procedure:**

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

starting from an initial guess $x_0$

# Newton-Raphson method

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




"Quadratic" convergence when works

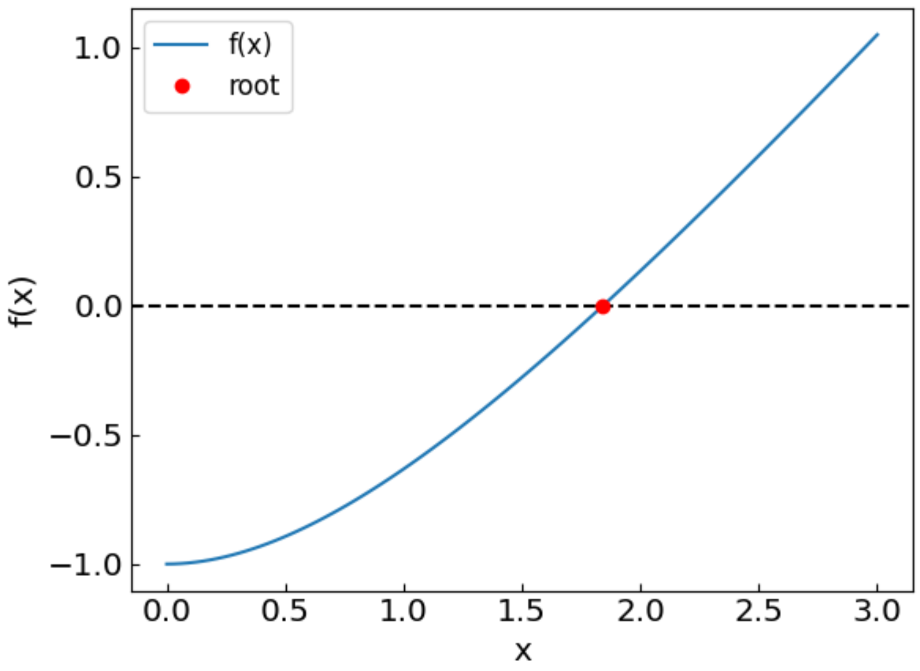
However, when we are close to $f' = 0$, we have a problem

**Error:** $\varepsilon_{n+1} \approx C\varepsilon_n^2$ (quadratic)

# Newton-Raphson method

```python
def newton_method(
    f,                      # The function whose root we are trying to find
    df,                     # The derivative of the function
    x0,                     # The initial guess
    tolerance = 1.e-10,     # The desired accuracy of the solution
    max_iterations = 100    # Maximum number of iterations
    ):

    xprev = xnew = x0

    global last_newton_iterations
    last_newton_iterations = 0
    diff = 0.

    for i in range(max_iterations):
        last_newton_iterations += 1

        xprev = xnew
        fval  = f(xprev)                        # The current function value
        dfval = df(xprev)                       # The current function derivative value

        xnew = xprev - fval / dfval             # The next iteration

        if (abs(xnew-xprev) < tolerance):
            return xnew


    print("Newton-Raphson method failed to converge to a required precision in " + str(max_iterations) + " iterations")
    print("The error estimate is ", abs(xnew-xprev))

    return xnew
```

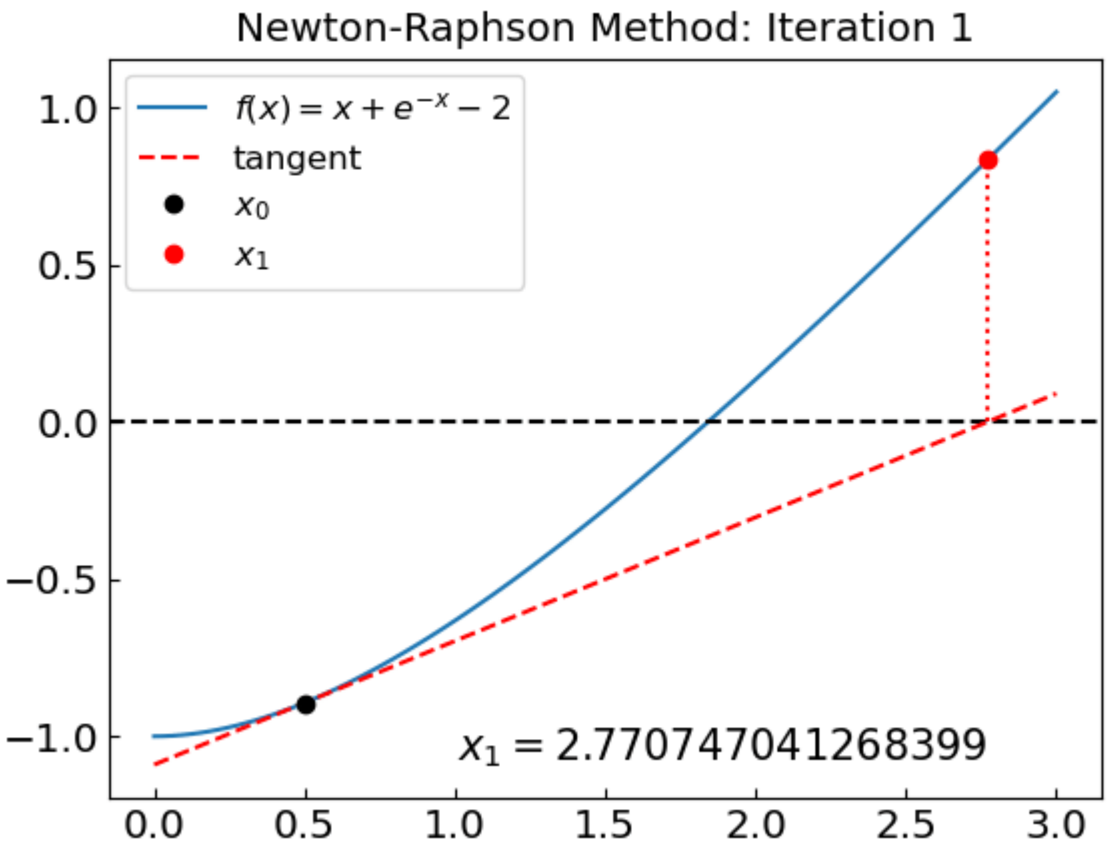
$$x + e^{-x} - 2 = 0$$




```
Solving the equation x + e^-x - 2 = 0 with an initial guess of x0 =  0.5
The solution is x =  1.8414056604369606 obtained after  6  iterations
```

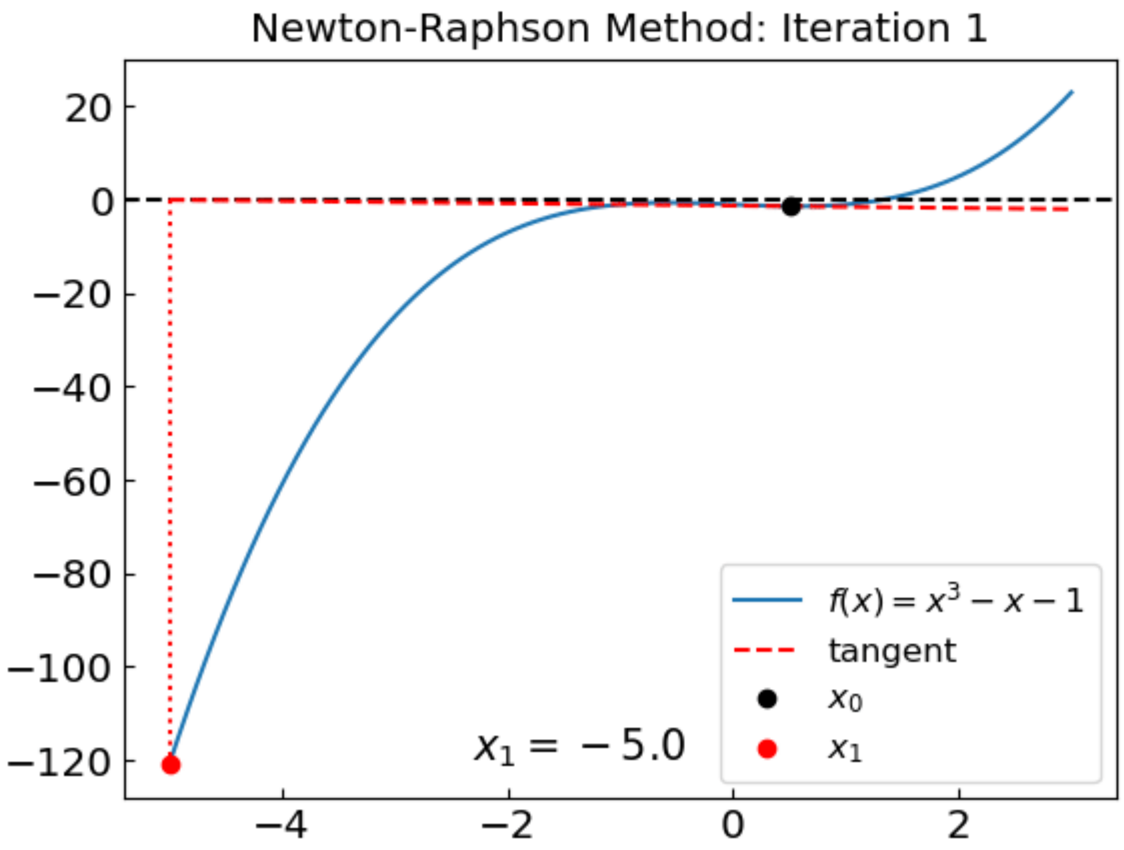
# Newton-Raphson method

$$x + e^{-x} - 2 = 0$$



# Newton-Raphson method: issues

$$x^3 - x - 1 = 0$$




Similar issue as with the secant method; the reason: $f' = 0$ at $x = 0.577...$

# Newton-Raphson method: issues

Try finding the root of $f(x) = x^3 - 2x + 2$ with an initial guess of $\underline{x_0 = 0}$

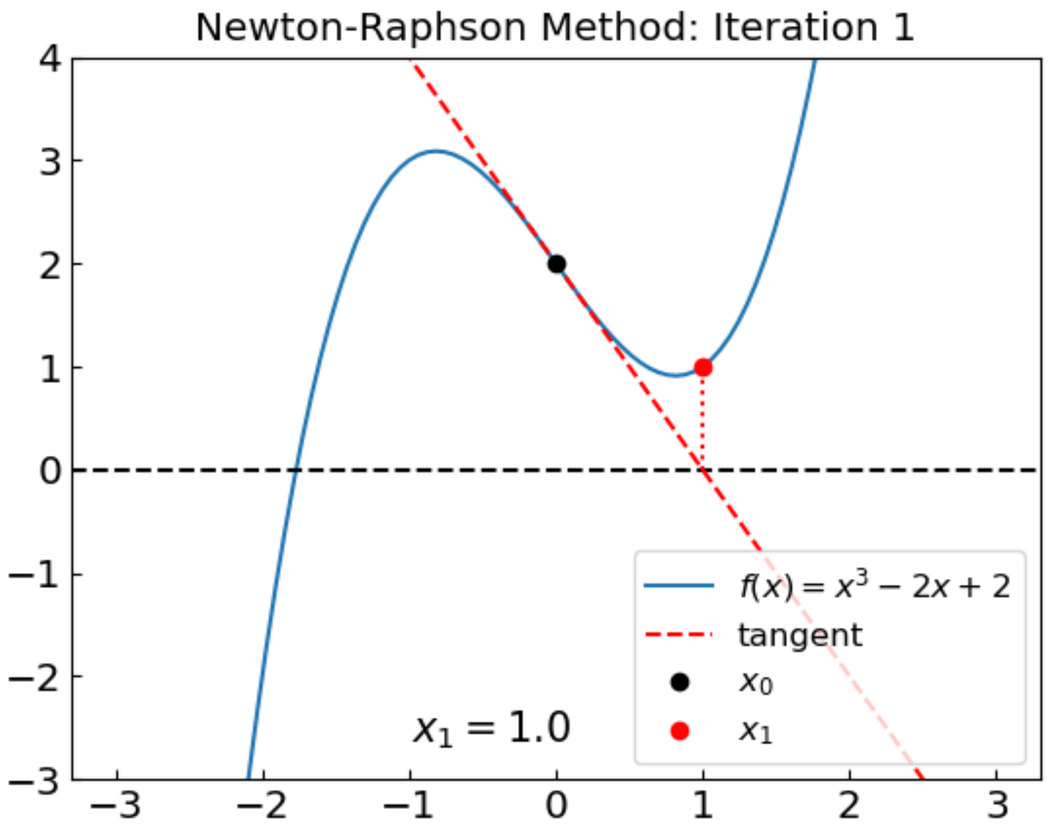
**Iteration 1:** $f(x_0) = 2, \quad f'(x_0) = -2$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 1$$

**Iteration 2:** $f(x_1) = 1 \quad f'(x_1) = 1$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 0$$

We are back to $x_0$!




The main issue is, again, we have points with $f' = 0$ in the neighborhood

# Relaxation method

- Cast the equation $f(x) = 0$ in a form

$$x = \varphi(x)$$

- For example $\varphi(x) = f(x) + x$ but this choice is not unique

- The root is approximated by an iterative procedure

$$x_{n+1} = \varphi(x_n)$$

**Convergence criterion:**

$$|\varphi'(x_n)| < 1, \qquad \text{for all } x_n$$

# Relaxation method

```python
def relaxation_method(
    phi,                      # The function from the equation x = phi(x)
    x0,                       # The initial guess
    tolerance = 1.e-10,       # The desired accuracy of the solution
    max_iterations = 100      # Maximum number of iterations
    ):

    xprev = xnew = x0

    global last_relaxation_iterations
    last_relaxation_iterations = 0

    for i in range(max_iterations):
        last_relaxation_iterations += 1

        xprev = xnew
        xnew = phi(xprev) # The next iteration

        if (abs(xnew-xprev) < tolerance):
            return xnew


    print("The relaxation method failed to converge to a required precision in " + str(max_iterations) + " iterations")
    print("The error estimate is ", abs(xnew - xprev))

    return xnew
```

# Relaxation method

$x + e^{-x} - 2 = 0$ as $x = 2 - e^{-x}$ i.e. $\phi(x) = 2 - e^{-x}$

Starting with $x_0$=0.5 we have

```
Solving the equation x = 2 - e^-x with relaxation method an initial guess of x0 =  0.5
Iteration:     0, x =    0.500000000000000, phi(x) = 1.393469340287367
Iteration:     1, x =    1.393469340287367, phi(x) = 1.751787325113973
Iteration:     2, x =    1.751787325113973, phi(x) = 1.826536369684999
Iteration:     3, x =    1.826536369684999, phi(x) = 1.839029855597129
Iteration:     4, x =    1.839029855597129, phi(x) = 1.841028423293983
Iteration:     5, x =    1.841028423293983, phi(x) = 1.841345821475382
Iteration:     6, x =    1.841345821475382, phi(x) = 1.841396170032424
Iteration:     7, x =    1.841396170032424, phi(x) = 1.841404155305379
Iteration:     8, x =    1.841404155305379, phi(x) = 1.841405421731432
Iteration:     9, x =    1.841405421731432, phi(x) = 1.841405622579610
Iteration:    10, x =    1.841405622579610, phi(x) = 1.841405654432999
Iteration:    11, x =    1.841405654432999, phi(x) = 1.841405659484766
Iteration:    12, x =    1.841405659484766, phi(x) = 1.841405660285948
Iteration:    13, x =    1.841405660285948, phi(x) = 1.841405660413011
Iteration:    14, x =    1.841405660413011, phi(x) = 1.841405660433162
Iteration:    15, x =    1.841405660433162, phi(x) = 1.841405660436358
The solution is x =  1.8414056604331623 obtained after  15  iterations
```

Not as fast as Newton-Raphson but does not require evaluation of the derivative

# Relaxation method

$x^3 - x - 1 = 0$ as $x = x^3 - 1$ i.e. $\varphi(x) = x^3 - 1$

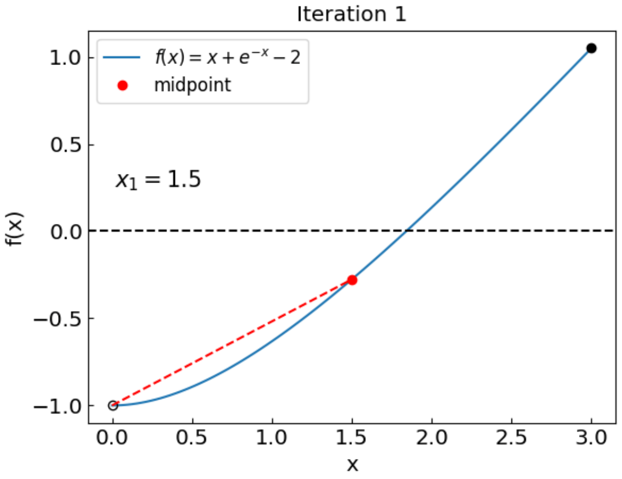
Starting with $x_0$=0.5 we have

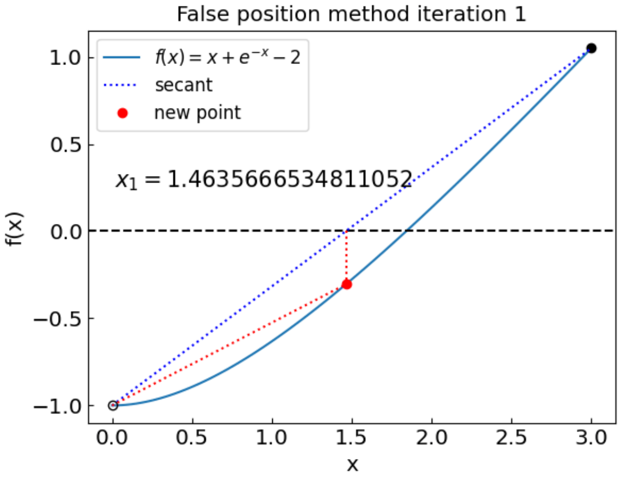
```
Solving the equation x = x^3 - 1 with relaxation method an initial guess of x0 =  0.0
Iteration:     0, x =    0.000000000000000, phi(x) = -1.000000000000000
Iteration:     1, x =   -1.000000000000000, phi(x) = -2.000000000000000
Iteration:     2, x =   -2.000000000000000, phi(x) = -9.000000000000000
Iteration:     3, x =   -9.000000000000000, phi(x) = -730.000000000000000
Iteration:     4, x = -730.000000000000000, phi(x) = -389017001.000000000000000
Iteration:     5, x = -389017001.000000000000000, phi(x) = -58871587162270591457689600.000000000000000
Iteration:     6, x = -58871587162270591457689600.000000000000000, phi(x) = -204040901322752646989478259680513109526757826056202557355691431285390611316736.000000000000000
Iteration:     7, x = -204040901322752646989478259680513109526757826056202557355691431285390611316736.000000000000000, phi
(x) = -8494771472237387691242611538599472199333045034070888643295870583150028612258583145101302119543367284932616097722814131127104275290993706669943943557518825041720139256751756296514363510463501782805696167407096791414943273033163341824.000000000000000
```

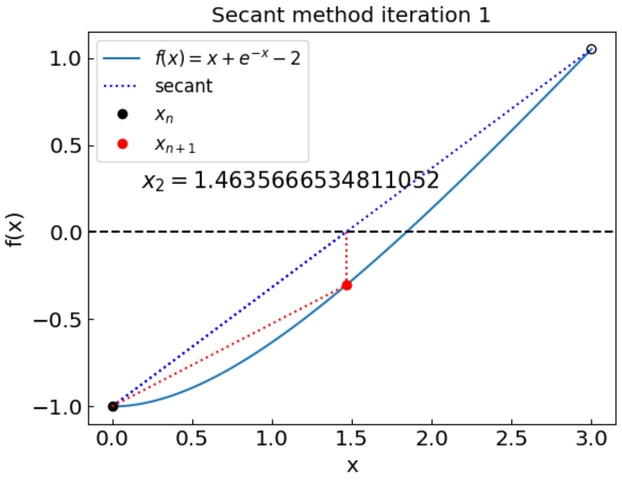
Divergent!

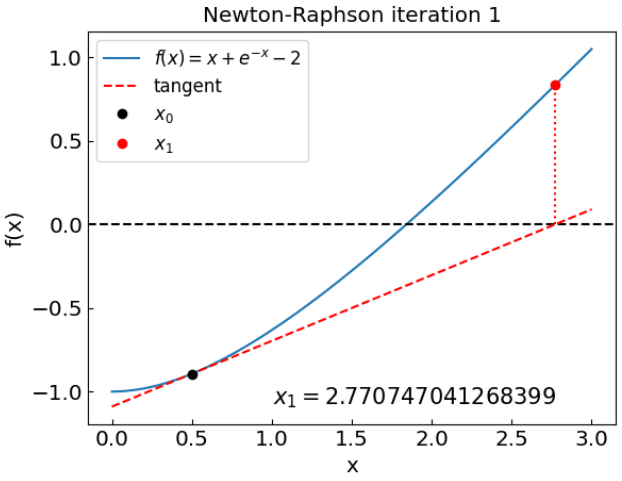
Reason: $|\varphi'(x_n)| < 1$ violated [try to come up with a better choice of $\varphi(x)$?]

# Summary


Iteration 1
$f(x) = x + e^{-x} - 2$
midpoint
$x_1 = 1.5$
f(x)
x


False position method iteration 1
$f(x) = x + e^{-x} - 2$
secant
new point
$x_1 = 1.4635666534811052$
f(x)
x


Secant method iteration 1
$f(x) = x + e^{-x} - 2$
secant
$x_n$
$x_{n+1}$
$x_2 = 1.4635666534811052$
f(x)
x


Newton-Raphson iteration 1
$f(x) = x + e^{-x} - 2$
tangent
$x_0$
$x_1$
$x_1 = 2.770747041268399$
f(x)
x

# Summary

## Bracketing methods

**Bisection method:**

- Guaranteed to converge with a fixed rate
- Need to bracket the root

**False position method:**

- Guaranteed to converge
- Can be faster than bisection but not always
- Need to bracket the root

## Local method

**Secant method:**

- Typically faster than bisection/false position
- May not always converge
- Does not need derivative

**Newton-Raphson method:**

- Very fast when converges
- Can be sensitive to initial guess
- May not converge if $f'(x) = 0$
- Requires evaluation of the derivative at each step

**Relaxation method:**

- Simple to implement
- Does not require derivative
- Often does not converge

# Summary

| **Method** | **Convergence Rate** | **Requires Derivative?** | **Guaranteed to Converge?** |
|---|---|---|---|
| Bisection | Linear $O(1/2^n)$ | ❌ | ✅ |
| False Position | Linear (but variable) | ❌ | ✅ |
| Secant | Superlinear $O(e^{-(1+\alpha)n})$ | ❌ | ❌ |
| Newton-Raphson | Quadratic $\mathrm{O}(e^{-2n})$ | ✅ | ❌ |
| Relaxation | Variable | ❌ | ❌ |