THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 04: Interpolation, Integration and Root Finding

Sergei V. Kalinin

This and that

- Any questions re 2nd homework?
- Remember: when interpolating, integrating, and finding roots we always have to think about whether these operations are well-defined
- Good news: R^1 and R^n

Interpolation

Sometimes we know the value of some function f(x) at a discrete set of points x_0, x_1, …, x_N, but we do not know how to (easily) calculate its value at arbitrary x

Examples:

- Physical measurements
- Long numerical calculations

Interpolation is a method to generate new data points from existing data points consisting of two steps:

1. Fitting the interpolating function to data points
2. Evaluating the interpolating function at a target point x

References: Chapter 3 of *Numerical Recipes Third Edition* by W.H. Press et al.

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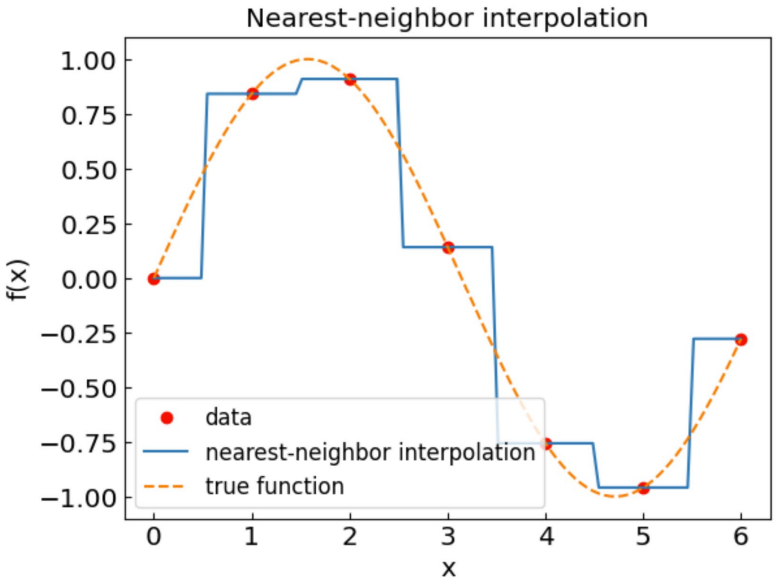
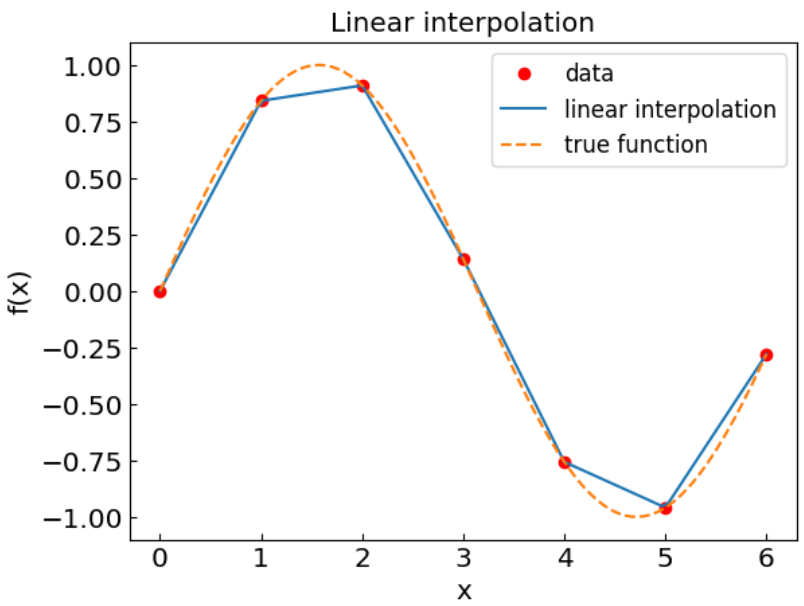
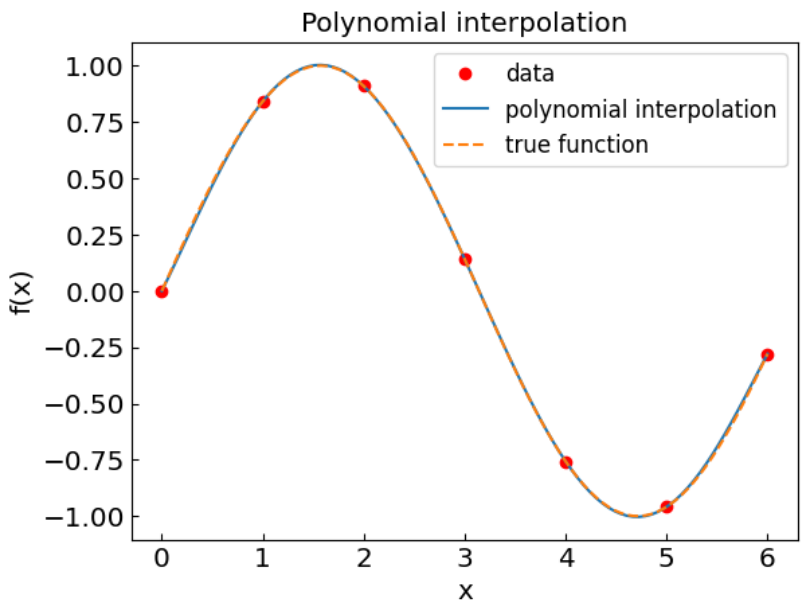
https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Interpolation methods







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Polynomial interpolation (Lagrange form)

Theorem: There exists a *unique* polynomial of order *n* that interpolates through n+1 data points (x_0,y_0), (x_1,y_1), …, (x_n,y_n)

How to build such a polynomial?

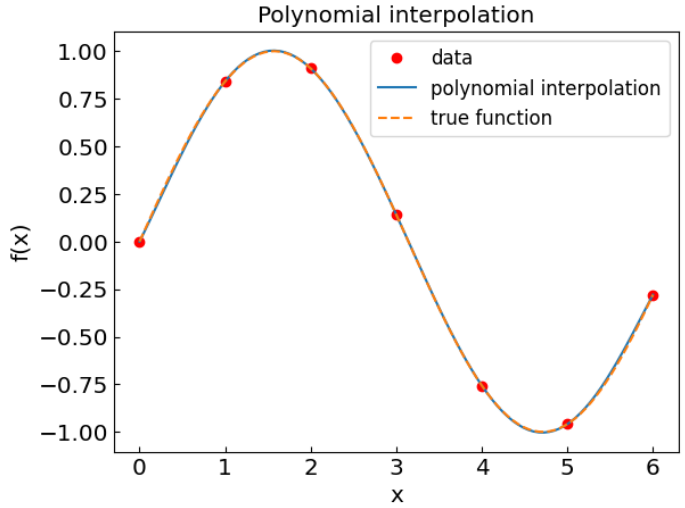
Consider *Lagrange basis functions*:

$$L_{n,j}(x) = \prod_{k \neq j} \frac{x - x_k}{x_j - x_k}.$$

Easy to see that for $x=x_k$ one has $L_{n,j}(x_k) = \delta_{kj}.$

Therefore:

$$f(x) \approx p(x) = \sum_{j=0}^{n} y_j L_{n,j}(x)$$



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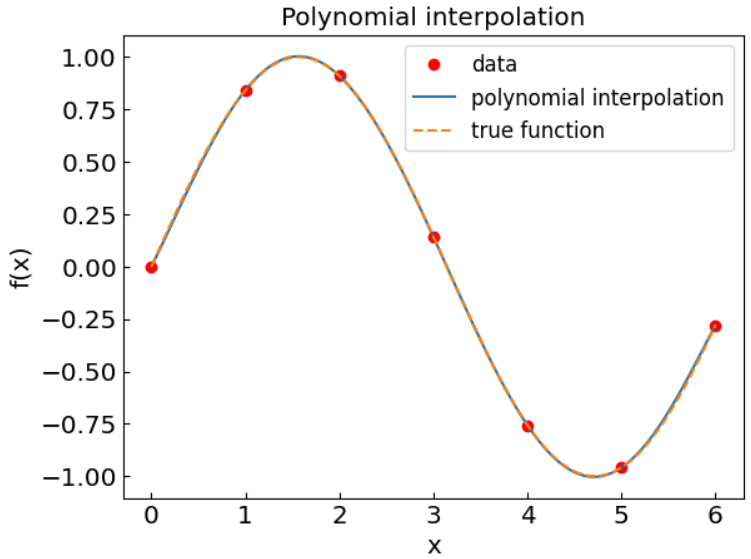
Polynomial interpolation

For our example f(x) = sin(x)

x	sin(x)
0	0.
1	0.841471
2	0.9092974
3	0.14112
4	-0.7568025
5	-0.9589243
6	-0.2794155



one obtains

$$p(x) = -0.0001521x^6 - 0.003130x^5 + 0.07321x^4 - 0.3577x^3 + 0.2255x^2 + 0.9038x.$$

In practice, the Lagrange form is more stable with respect to round-off errors

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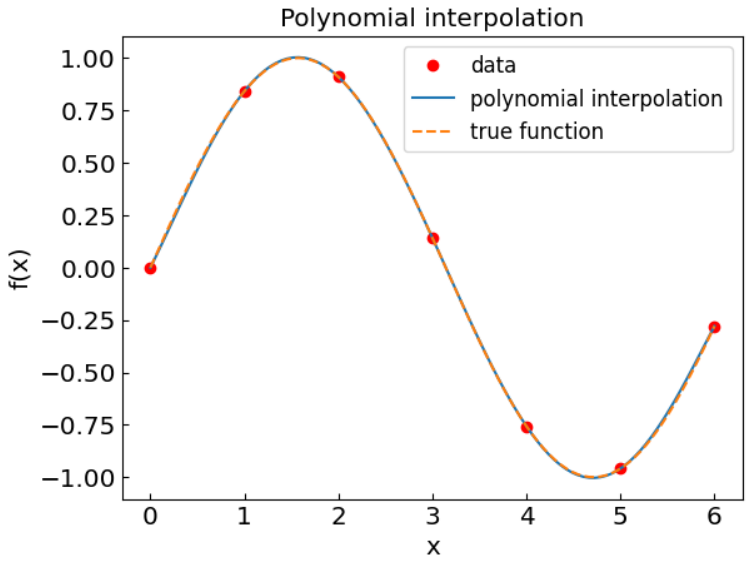
Polynomial interpolation

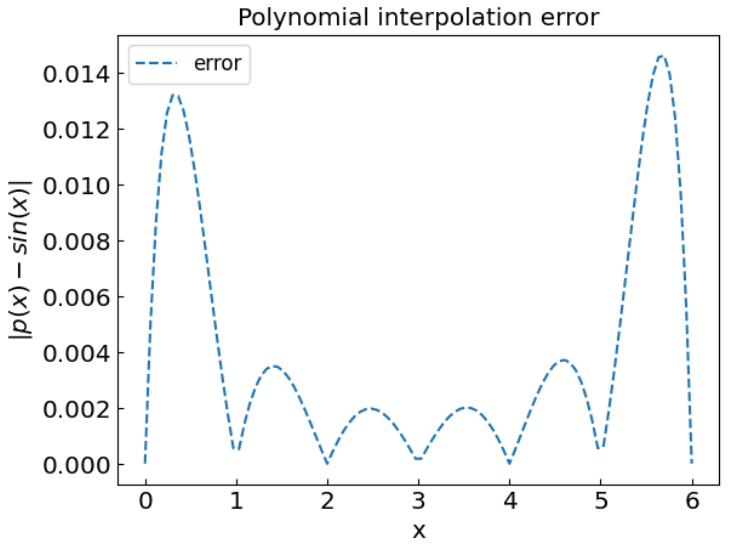
In Python:

```
def Lnj(x,n,j,xdata):
    """Lagrange basis function."""
    ret = 1.
    for k in range(0, len(xdata)):
        if (k != j):
            ret *= (x - xdata[k]) / (xdata[j] - xdata[k])
    return ret


def f_poly_int(x, xdata, fdata):
    """Returns the polynomial interpolation of a function at point x.
    xdata and ydata are the data points used in interpolation."""
    ret = 0.
    n = len(xdata) - 1
    for j in range(0, n+1):
        ret += fdata[j] * Lnj(x,n,j,xdata)
    return ret

xpoly = np.linspace(0,6,100)
fpoly = [f_poly_int(xin,xdat,fdat) for xin in xpoly]
```





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Polynomial interpolation: Errors and artefacts

- Truncation errors

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{n+1} \prod_{i=0}^{n} (x - x_i)$$

- Round-off errors
  - Especially for high-order polynomials

Truncation errors can be a problem if

- High-order derivatives $f^{(n+1)}(x)$ of the function are significant
- The choice of nodes leads to a large value of the product factor

Runge phenomenon: Oscillation at the edges of the interval which gets *worse* as the interpolation order is increased

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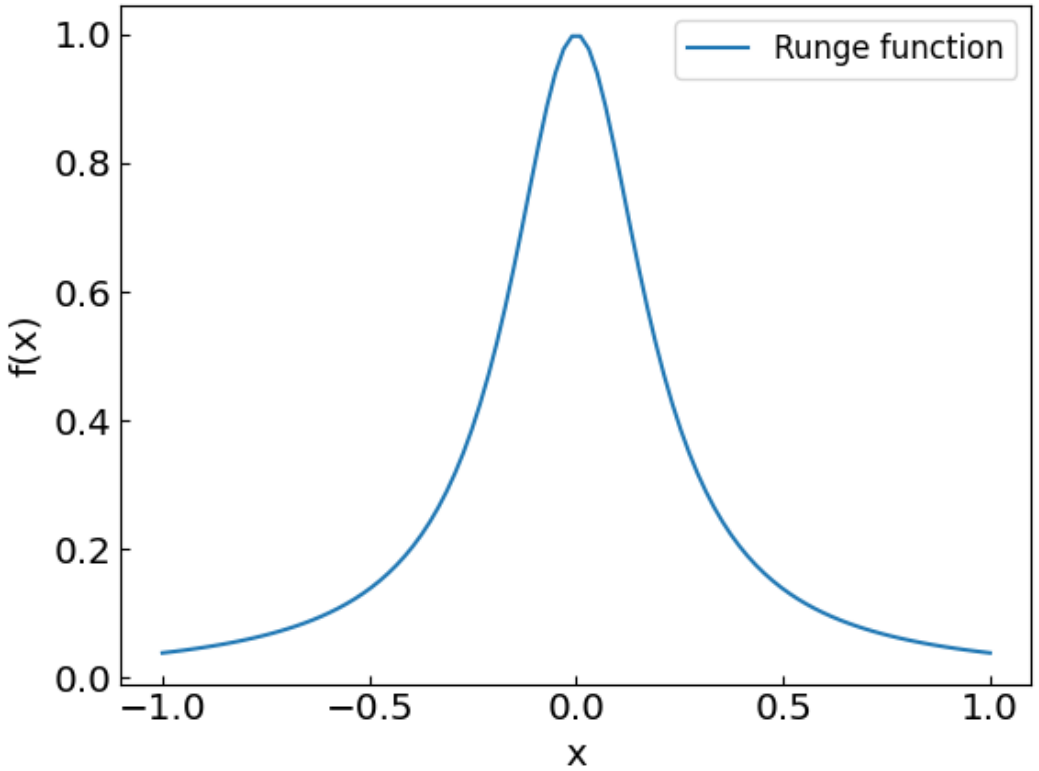
Polynomial interpolation: Runge phenomenon

Consider the Runge function: $$f(x) = \frac{1}{1 + 25x^2}$$



Let us do polynomial interpolation using equidistant nodes

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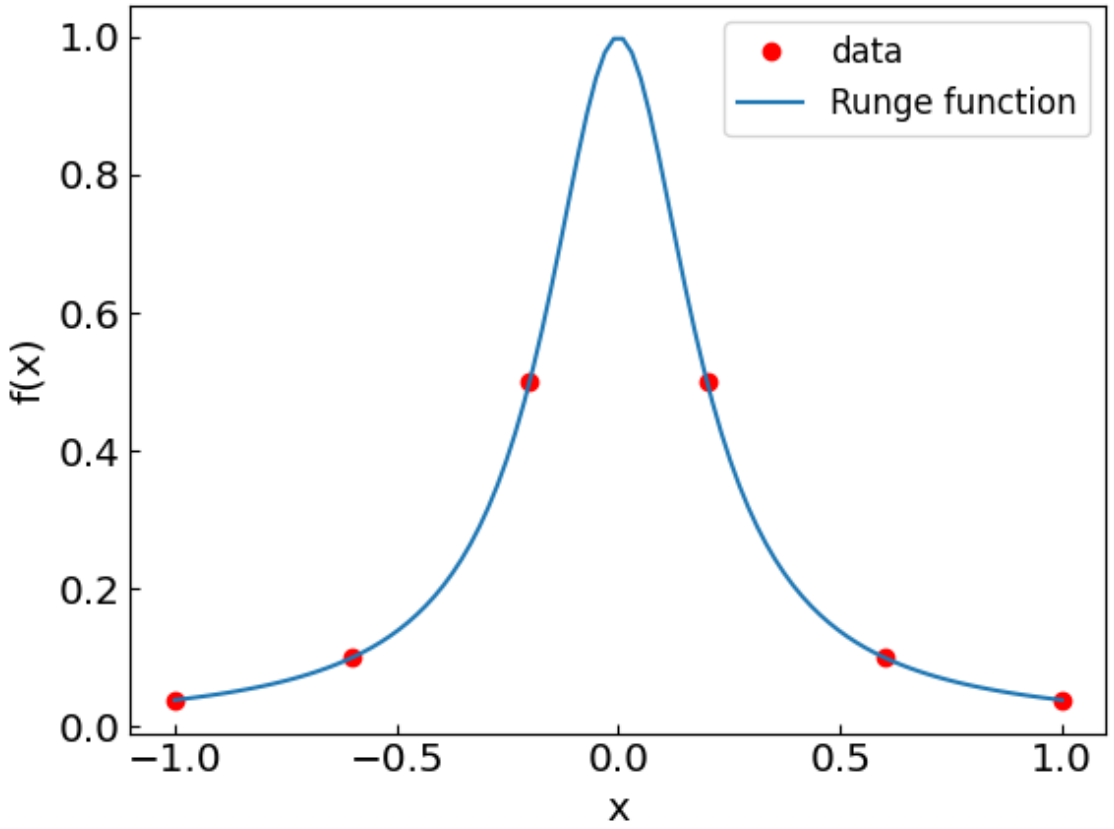
Polynomial interpolation: Runge phenomenon



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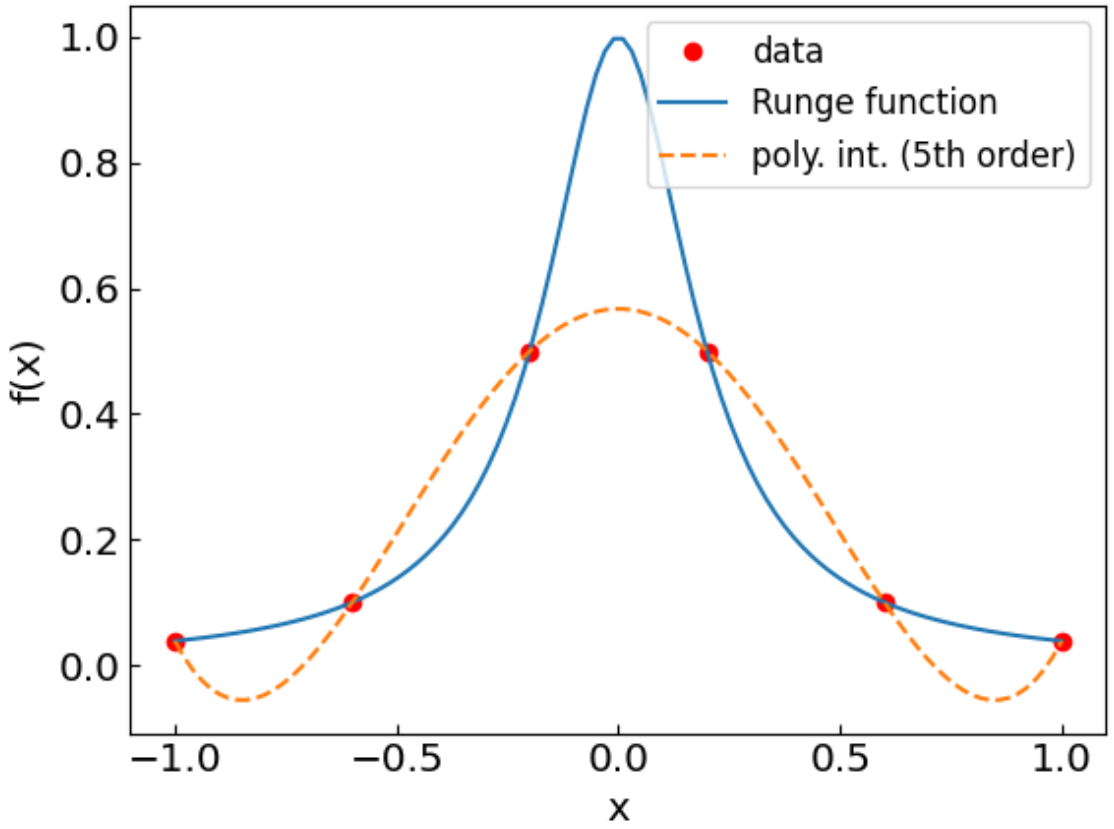
Polynomial interpolation: Runge phenomenon



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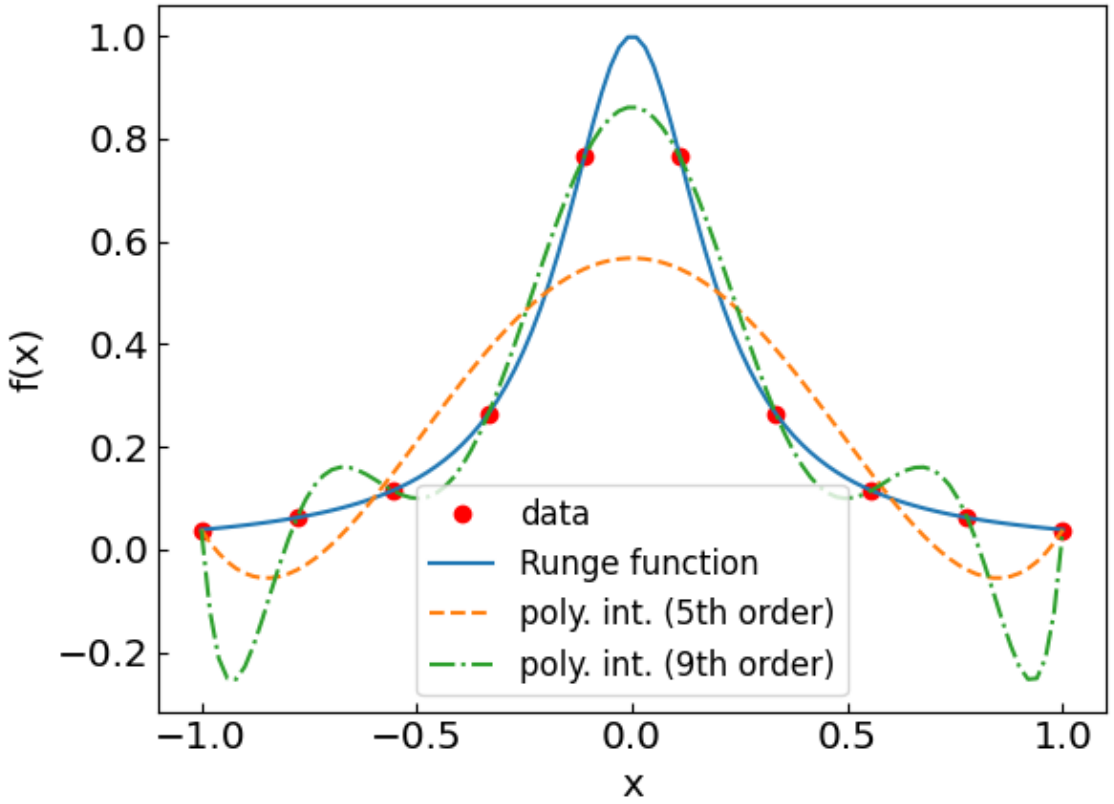
Polynomial interpolation: Runge phenomenon



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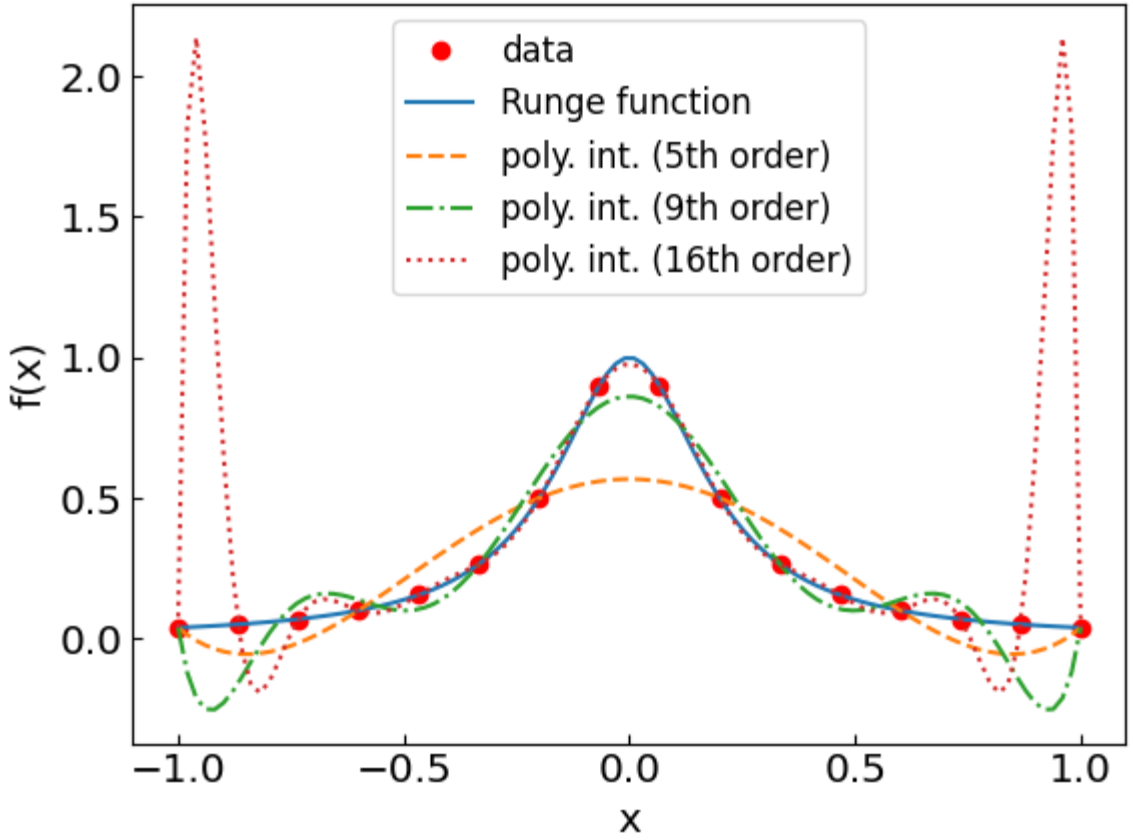
Polynomial interpolation: Runge phenomenon



We have a real problem at the edges!

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Polynomial interpolation: Chebyshev nodes

Recall the truncation error

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{n+1} \prod_{i=0}^{n} (x - x_i)$$

So far, we used the equidistant nodes:

$$x_k = a + hk, \qquad k = 0, \dots, n, \qquad h = (b-a)/n$$

Can we choose the nodes x_i differently to minimize the product factor? *Yes!*

Chebyshev nodes:

$$x_k = \frac{a+b}{2} + \frac{b-a}{2} \cos\left(\frac{2k+1}{2n+2}\pi\right), \qquad k = 0, \dots, n,$$

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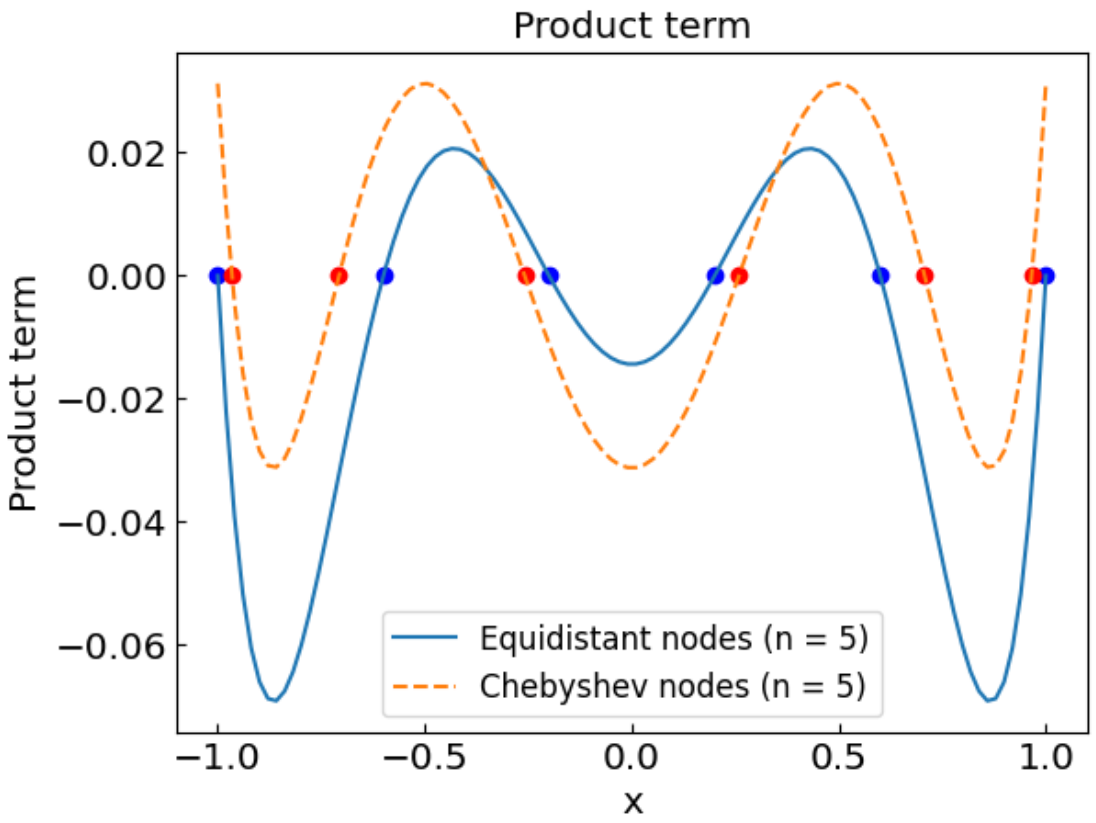
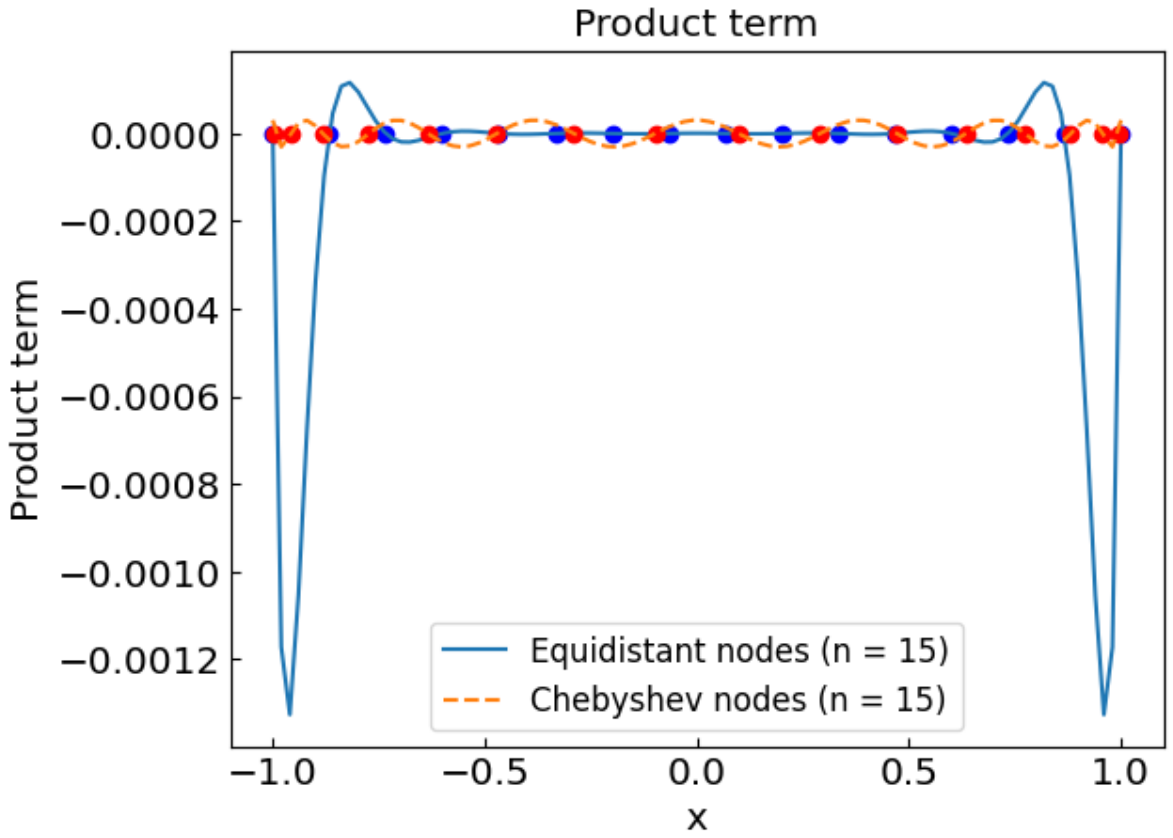
Equidistant vs Chebyshev nodes

Plot $\prod_{i=0}^{n}(x - x_i)$ as a function of x for different number of nodes n on a (-1,1) interval





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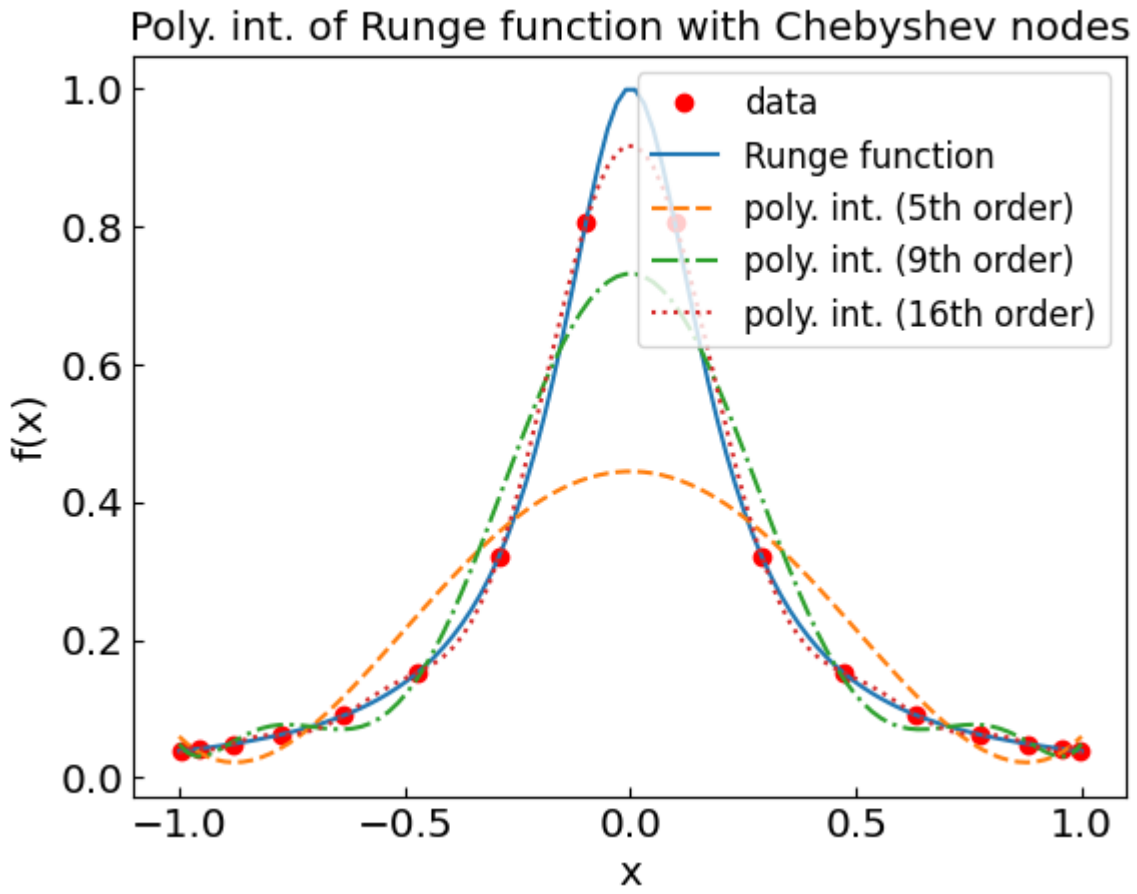
Back to the Runge function: Chebyshev nodes



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Polynomial interpolation: Summary

Advantages:

- Generally more accurate than the linear interpolation
- Derivatives are continuous
- Can be used for numerical integration and differential equations

Disadvantages:

- Implementation not so simple
- Artefacts possible (such as large oscillations between nodes)
- Polynomials of large order susceptible to round-off errors
- Not easily generalized to multiple dimensions

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Spline interpolation

Connect each pair of nodes by a cubic polynomial

$$q_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i, \qquad x \in (x_i, x_{i+1})$$

4n coefficients a_i, b_i, c_i, d_i determined from

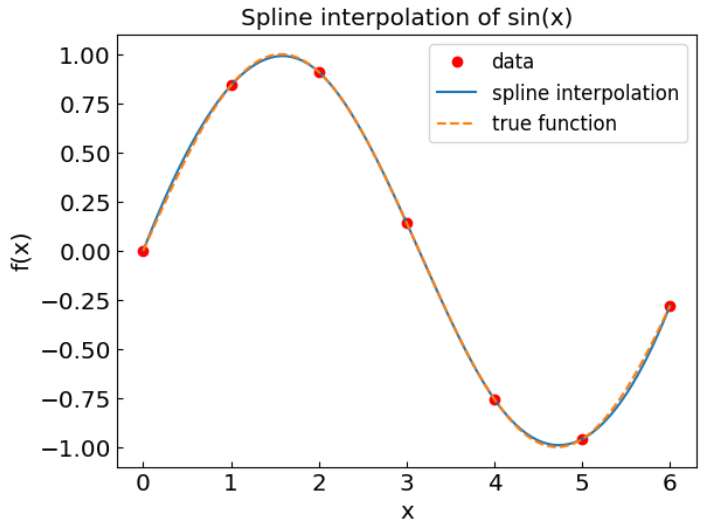
- n+1 data points
- continuity of first and second derivatives at nodes
- Boundary conditions for first derivative

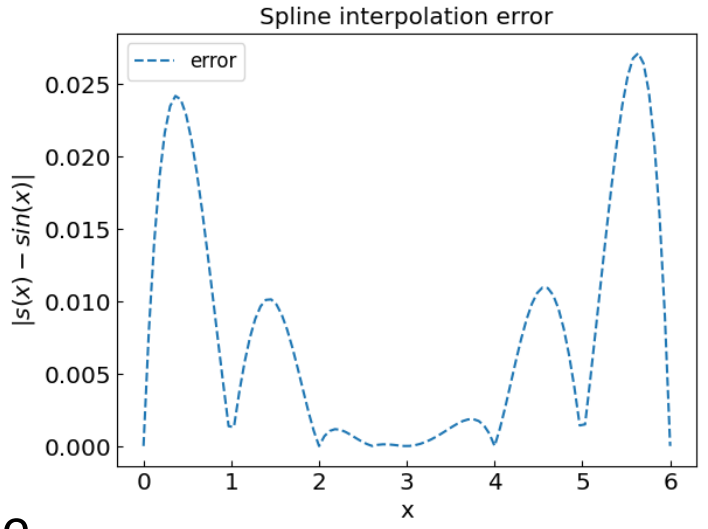
Advantages:

- More accurate than linear interpolation
- Derivatives are continuous
- Avoids issues with polynomials of high degree

Disadvantages:

- Implementation not so simple
- Artefacts like large oscillations between nodes are possible





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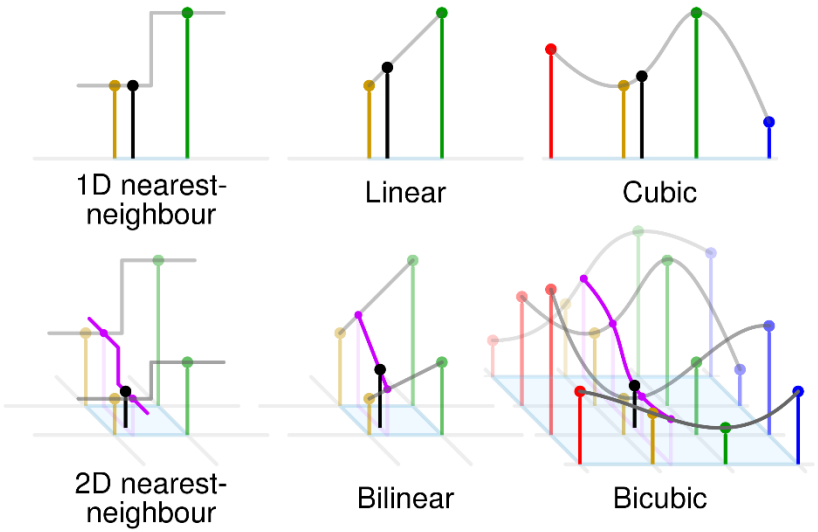
Multiple dimensions

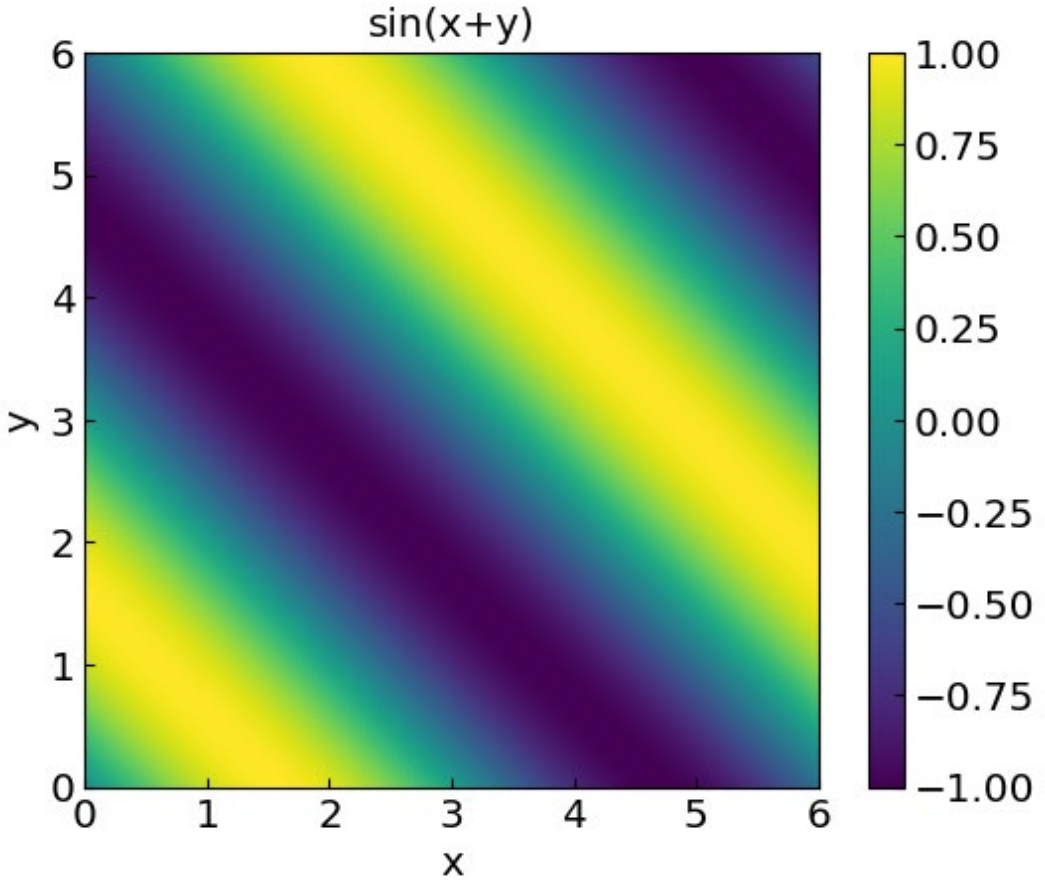
Functions of more than one variable, e.g. f(x,y) = sin(x+y)

Data points: (x_i, y_i, f_i)

Main methods:

- Nearest-neighbor
- Successive 1D interpolations





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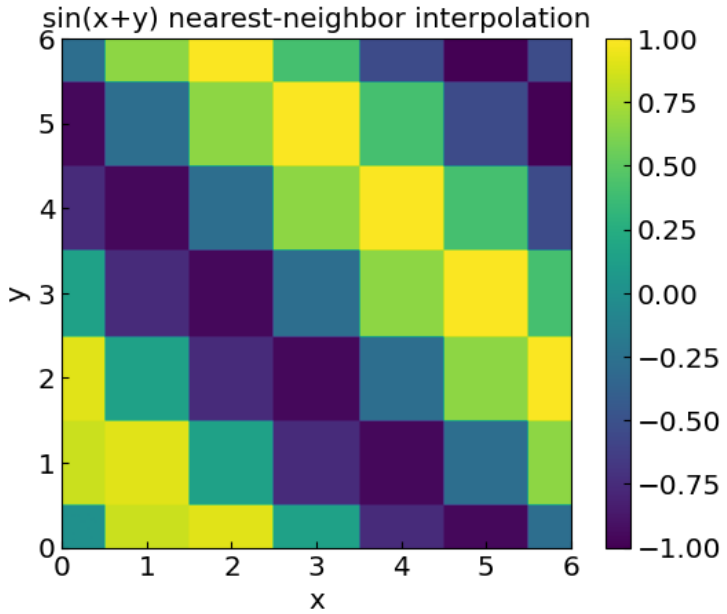
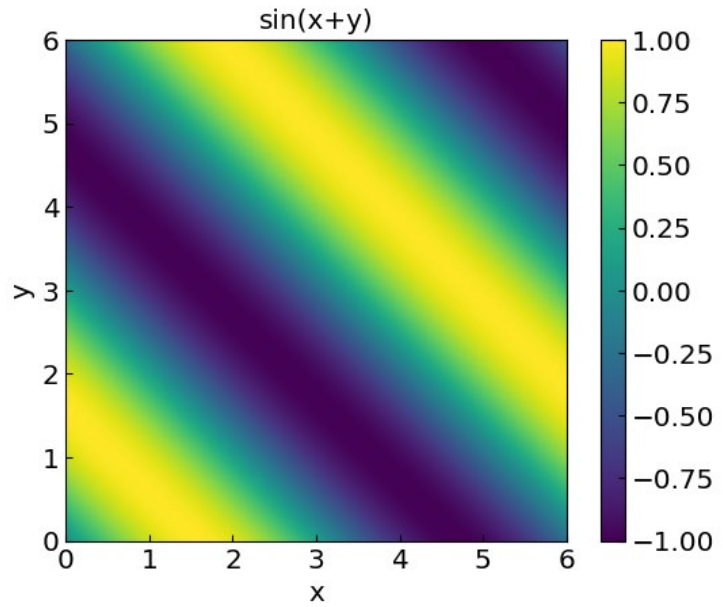
2D nearest-neighbor

2D nearest-neighbor:
Simply assign the value of the closest data point to *(x,y)* in the plane

Consider f(x,y) = sin(x+y)

Data points at integer values x,y=0,1,…6 (*regular grid*)





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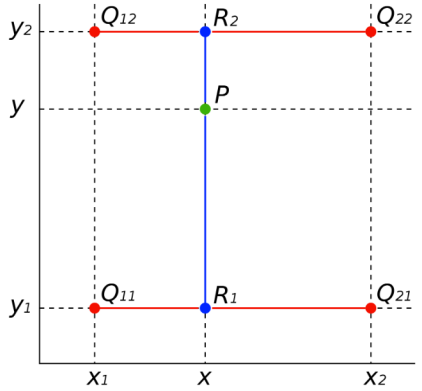
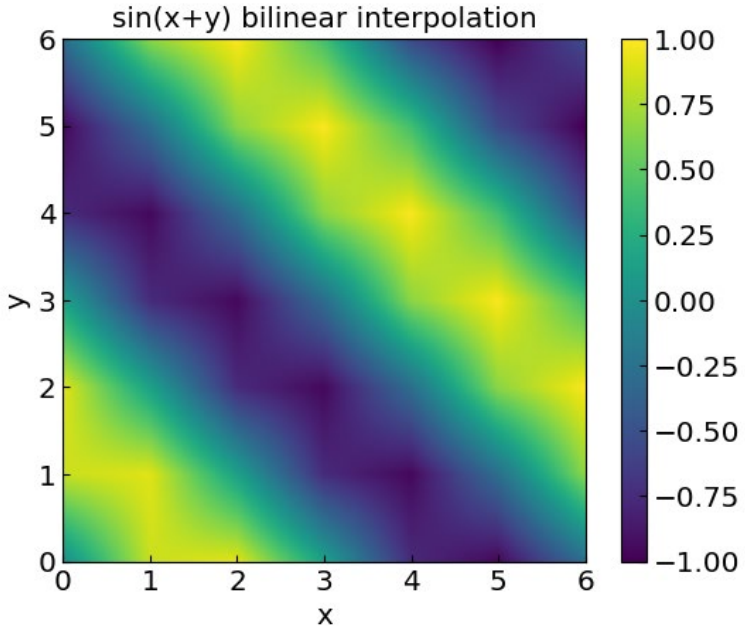
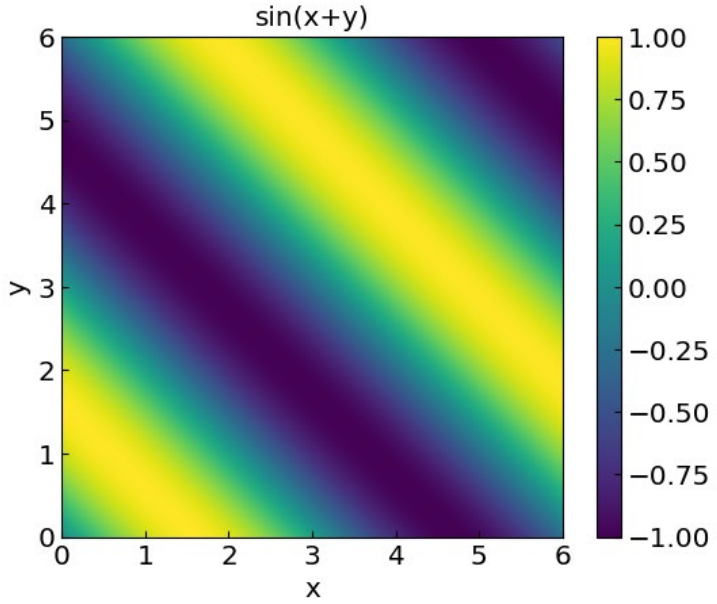
Bilinear interpolation

Bilinear interpolation: apply linear interpolation twice



1. Find (x_1, x_2) and (y_1, y_2) such that $x \in (x_1, x_2)$ and $y \in (y_1, y_2)$
2. Calculate R_1 and R_2 for $y = y_1$ and $y = y_2$, respectively, by applying linear interpolation in x
3. Calculate the interpolated function value at (x, y) by performing linear interpolation in y using the computed values of R_1 and R_2





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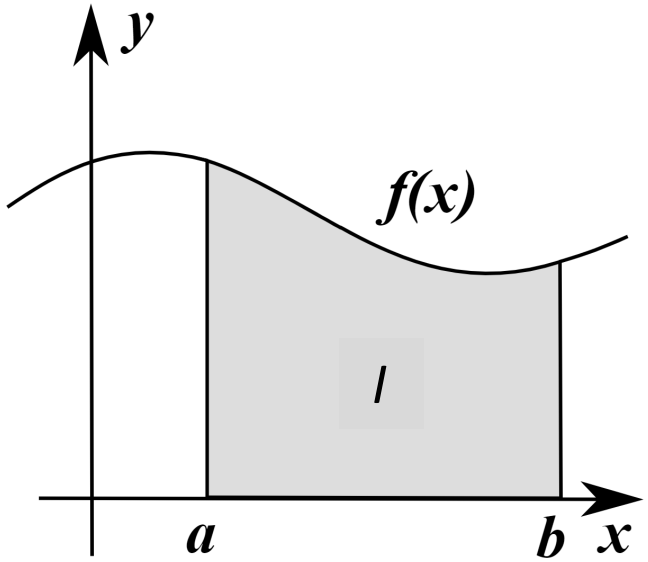
Numerical integration

Generic problem: evaluate

$$I = \int_a^b f(x)dx$$



We need numerical integration when

- Cannot/difficult integrate analytically
- Only know the integrand *f(x)* at certain points

References: Chapter 5 of *Computational Physics* by Mark Newman

Chapter 4 of *Numerical Recipes Third Edition* by W.H. Press et al.

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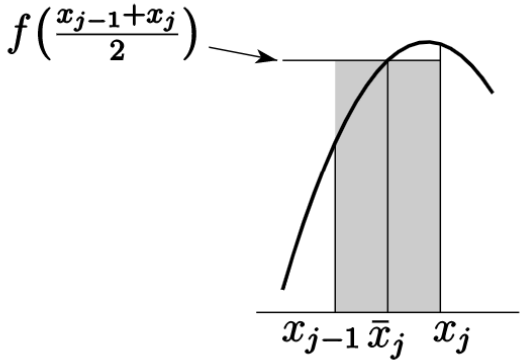
Numerical integration: rectangular (midpoint) rule

Interpret the integral as the area under the curve and approximate by a rectangle evaluated at midpoint

$$\int_a^b f(x)\,dx \approx (b-a)\,f\left(\frac{a+b}{2}\right)$$



Error (from Euler-McLaurin formula):

$$\int_a^b f(x)dx - (b-a)\,f\left(\frac{a+b}{2}\right) \approx \frac{(b-a)^3}{24} f''(a)$$

The rule is exact for the integration of linear functions

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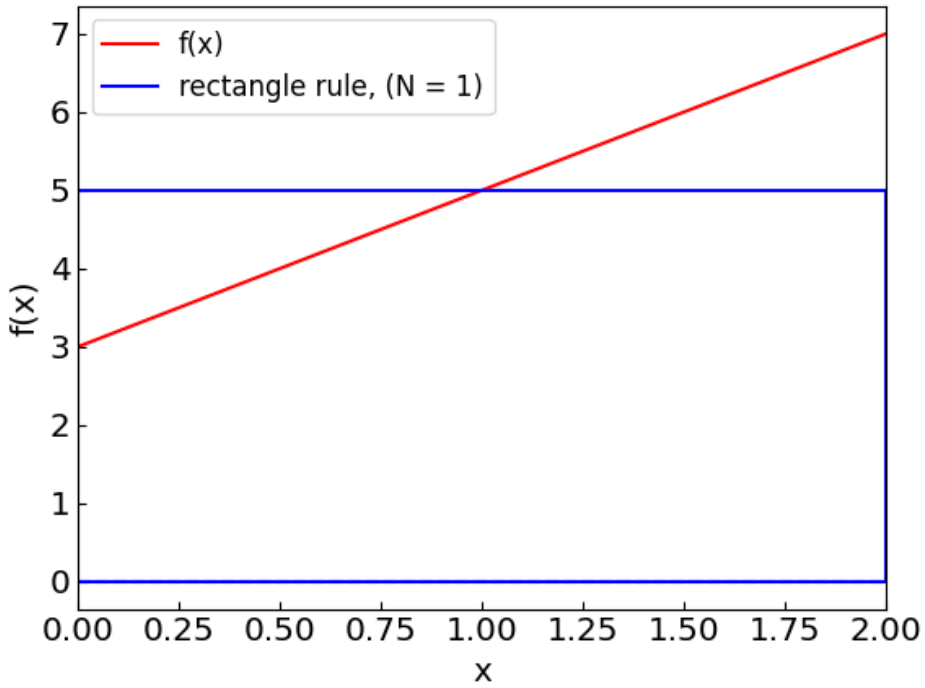
Numerical integration: rectangular (midpoint) rule

Example:

$$I = \int_0^2 2x + 3dx = 10$$



Although the rectangle is a poor approximate of the line (which is a trapezoid here), the errors cancel out

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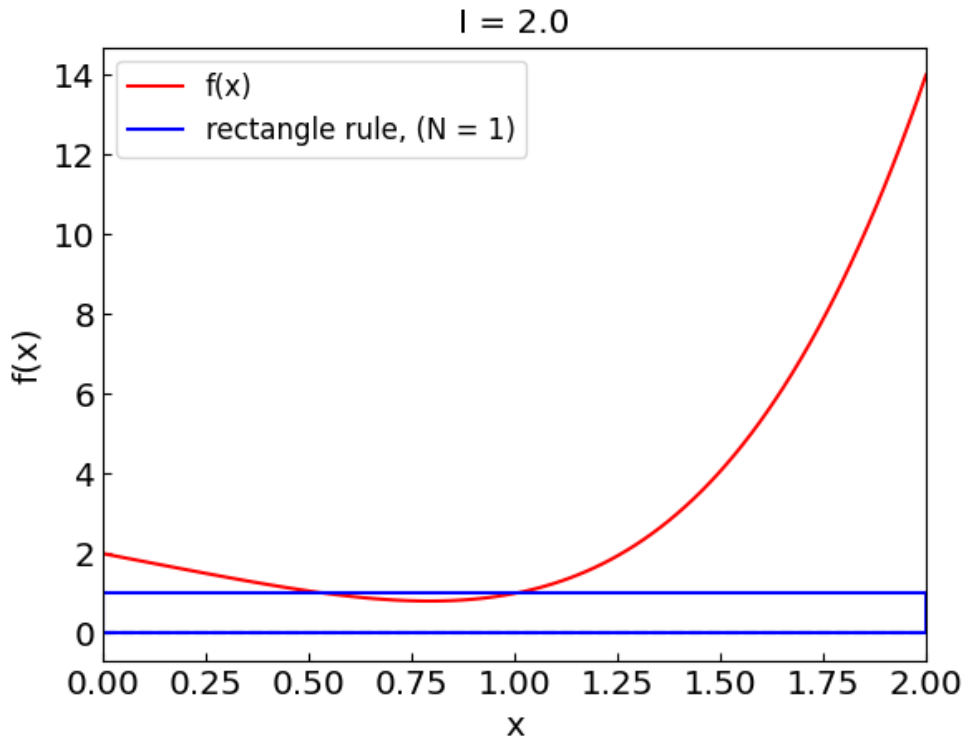
Numerical integration: rectangular (midpoint) rule

Another example: $I = \int_0^2 x^4 - 2x + 2 = 6.4$



Rectangle rule gives I_{rect} = 2 which is way off

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Extended (composite) rectangular rule

Split the integration interval into *N* sub-intervals and apply the rectangle rule separately to each one

$$\int_0^2 x^4 - 2x + 2$$

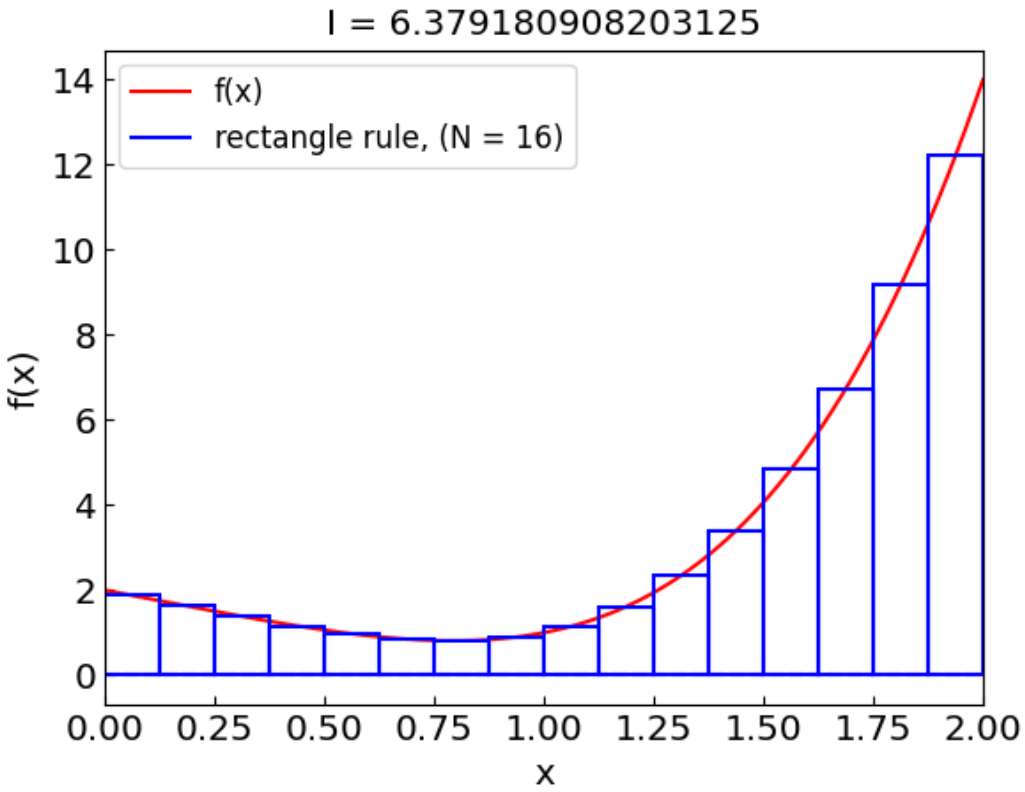
$$\int_a^b f(x) \approx h \sum_{k=1}^{N} f(x_k), \qquad k = 1, \ldots, N$$

$$x_k = a + \frac{2k-1}{2} h \,.$$

$$h = (b-a)/N$$

Error estimate:

$$I - I_{\text{rect}} = (b-a)\frac{h^2}{24} f''(a) + \mathcal{O}(h^4)$$



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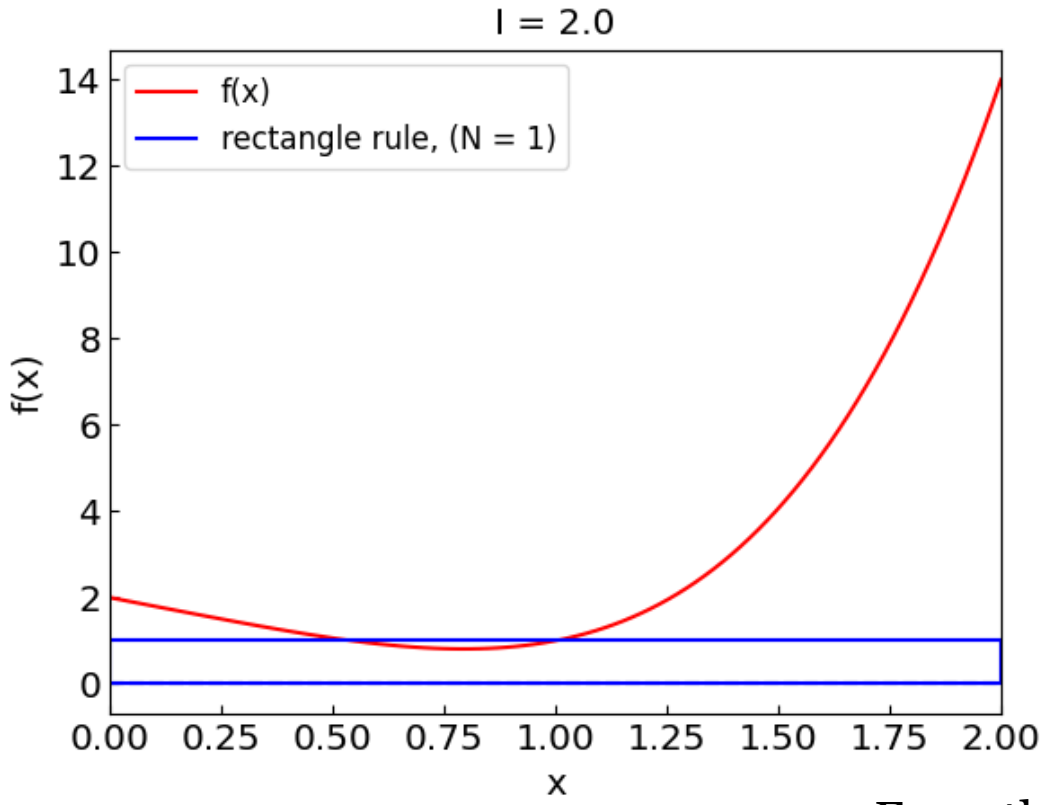
Extended (composite) rectangular rule

$$I = \int_0^2 x^4 - 2x + 2 = 6.4$$



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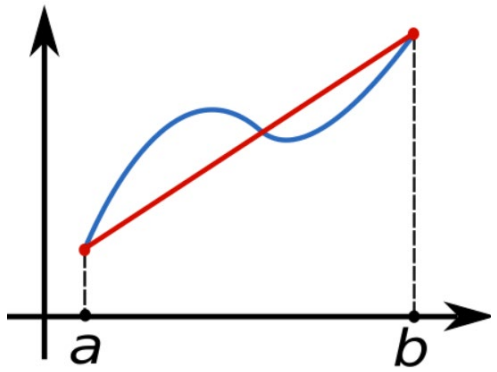
Numerical integration: trapezoidal rule

Approximate the integral by a trapezoid

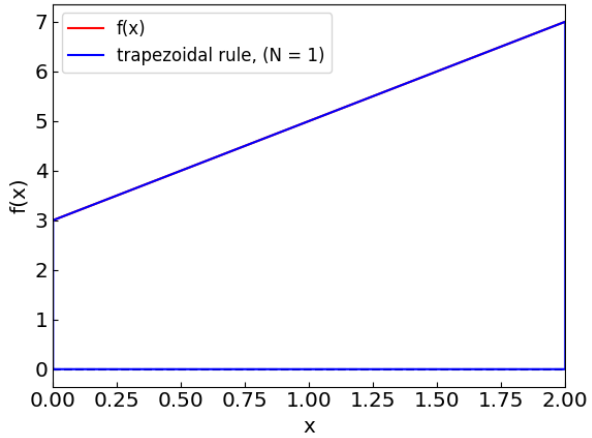
$$\int_a^b f(x)\,dx \approx (b-a)\,\frac{f(a)+f(b)}{2}$$



Error:

$$\int_a^b f(x)dx \;-\; (b-a)\,\frac{f(a)+f(b)}{2} \approx -\frac{(b-a)^3}{12}f''(a)$$

The rule is exact for the integration of linear functions



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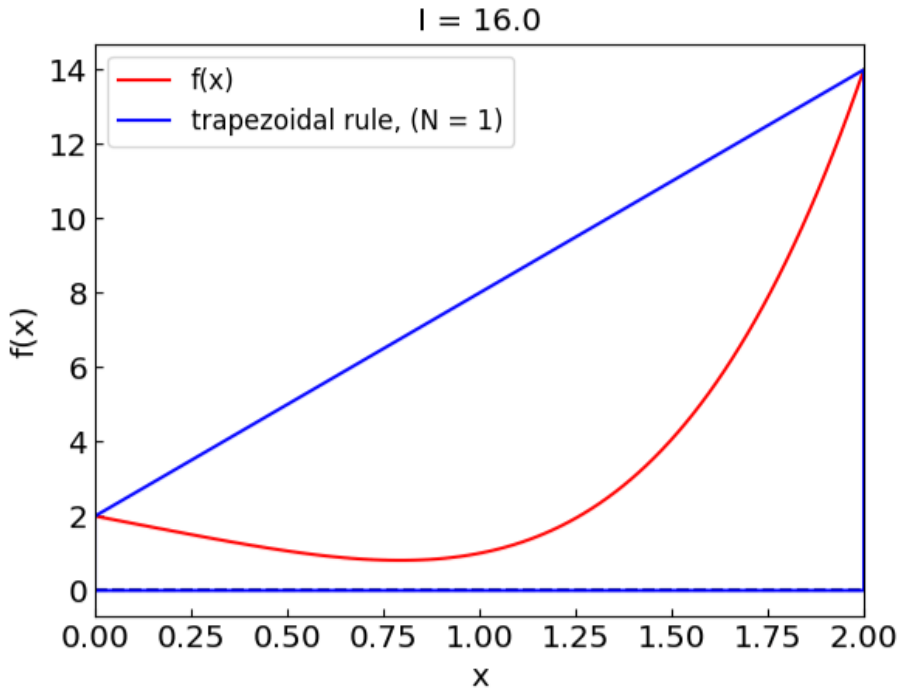
Numerical integration: trapezoidal rule

$$I = \int_0^2 x^4 - 2x + 2 = 6.4$$



Trapezoidal rule gives I_{trap} = 16, way off and in the opposite direction relative to rectangle rule

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Extended trapezoidal rule

$$\int_a^b f(x) \approx h \sum_{k=0}^{N} \frac{f(x_k) + f(x_{k+1})}{2}, \qquad i = 0, \ldots, N$$

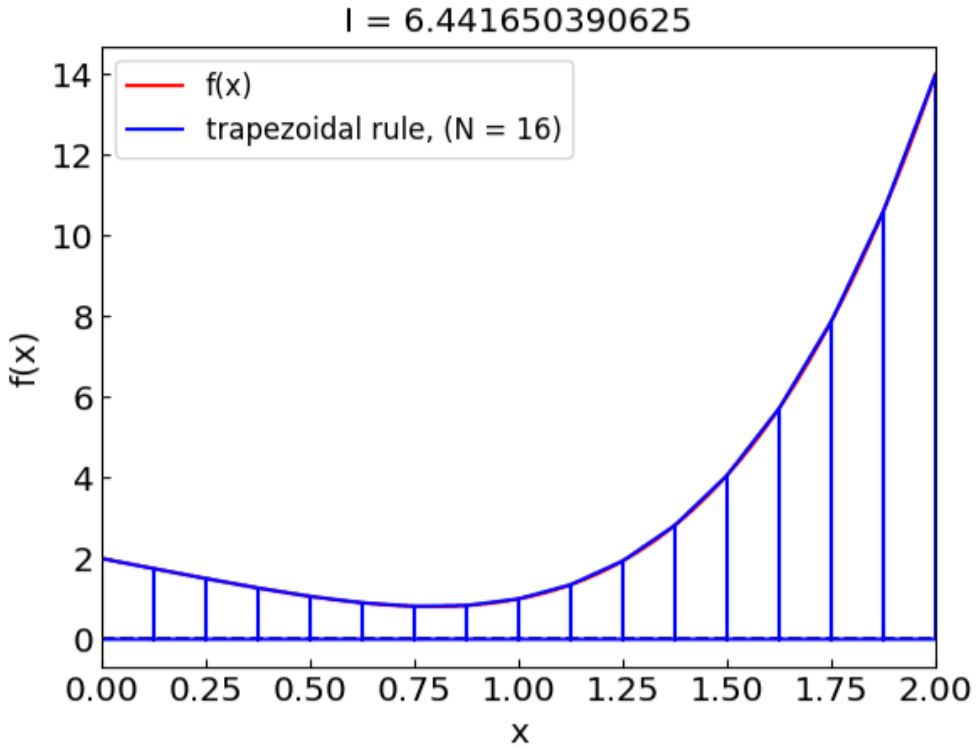
$$x_k = a + kh \, .$$

$$h = (b - a)/N$$

Error estimate:

$$I - I_{\text{trap}} = -(b-a)\frac{h^2}{12} f''(a) + \mathcal{O}(h^4)$$

$$\int_0^2 x^4 - 2x + 2$$



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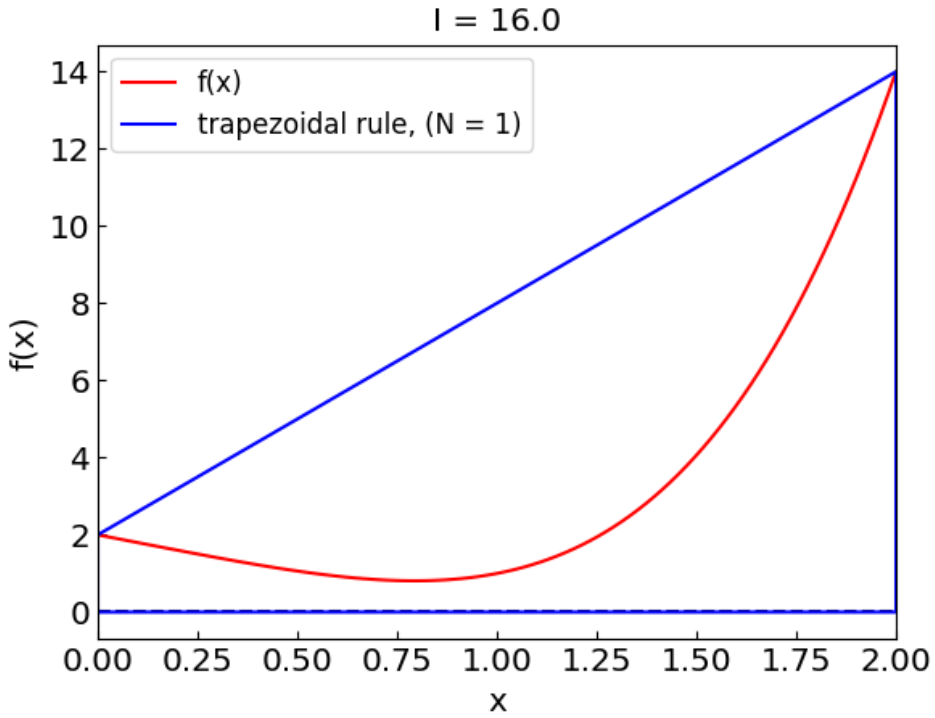
Extended (composite) trapezoidal rule

$$I = \int_0^2 x^4 - 2x + 2 = 6.4$$



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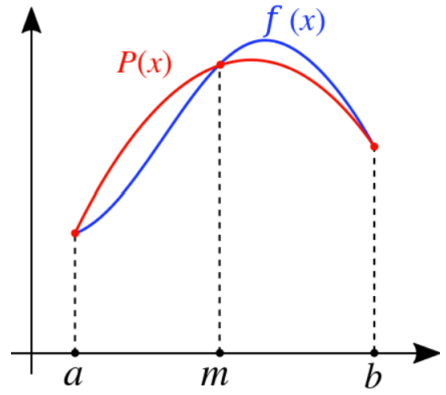
Numerical integration: Simpson's rule

Recall the error estimates for rectangular and trapezoidal rules

$$I - I_{\text{rect}} = (b-a)\frac{h^2}{24} f''(a) + \mathcal{O}(h^4) \qquad I - I_{\text{trap}} = -(b-a)\frac{h^2}{12} f''(a) + \mathcal{O}(h^4)$$



Combine them to eliminate the O(h^2) error term:

$$I_S = \frac{2I_{\text{rect}} + I_{\text{trap}}}{3}$$

i.e.

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

An equivalent way to obtain the rule: replace the integrand by the parabolic interpolation

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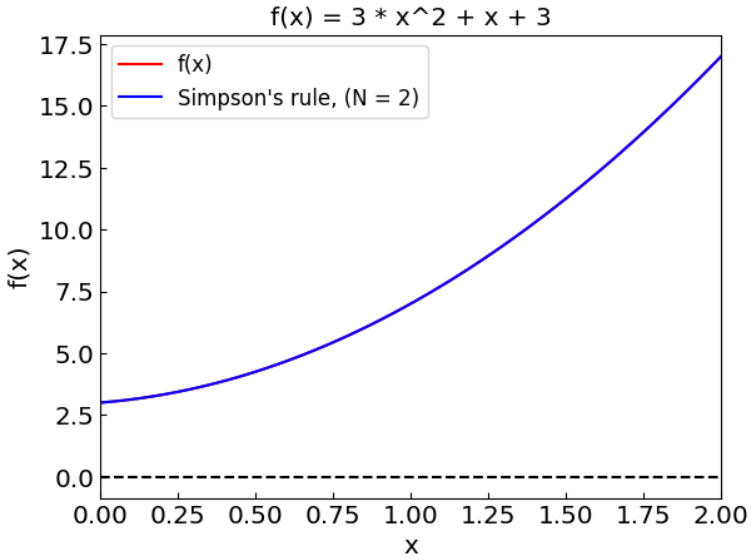
Numerical integration: Simpson's rule

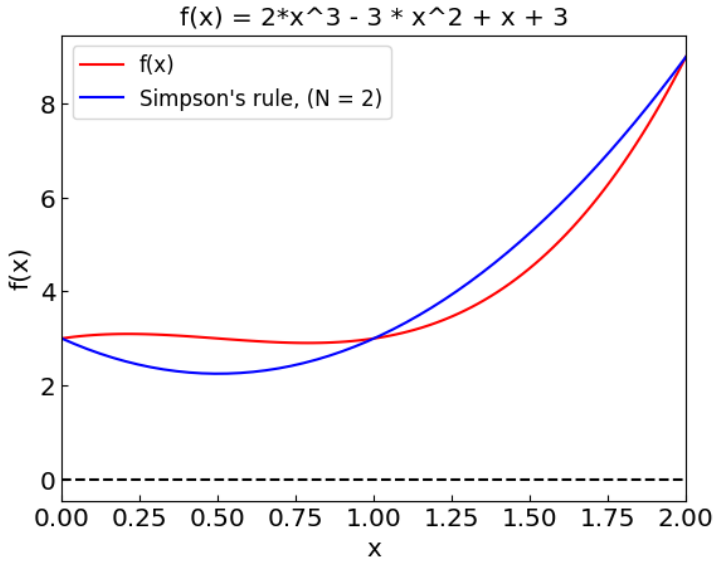
$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

The error for the Simpson's rule is

$$I - I_S = C\,h^4 + \mathcal{O}(h^6)$$

The method is exact for polynomials up to third order





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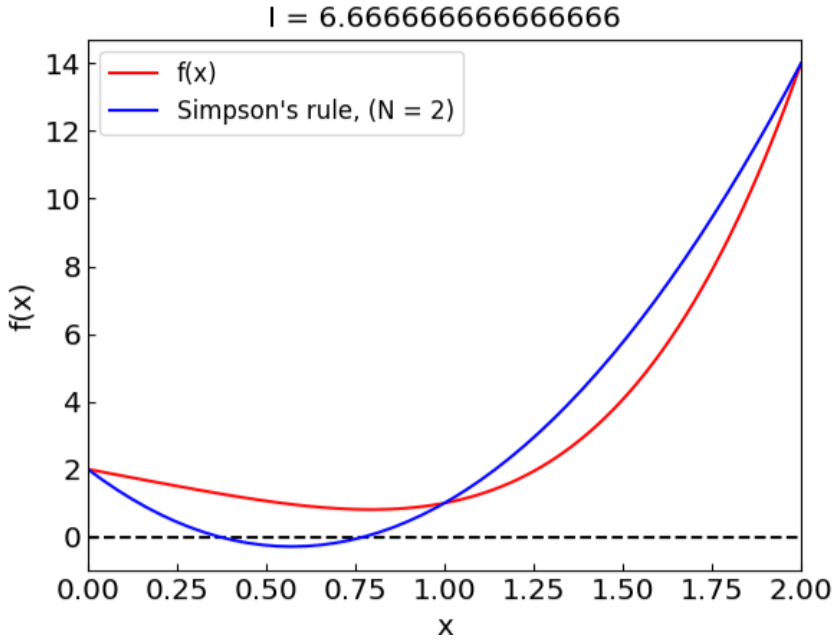
Numerical integration: Simpson's rule

$$I = \int_0^2 x^4 - 2x + 2 = 6.4$$



Simpson's rule gives I_{trap} = 6.66 using three points, which is already not too bad!

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Extended Simpson's rule

$$\int_a^b f(x) \approx \frac{h}{3}\left[f(x_0) + 4\sum_{k=1}^{N/2} f(x_{2k-1}) + 2\sum_{k=1}^{N/2-1} f(x_{2k}) + f(x_N)\right], \qquad i = 0, \ldots, N$$

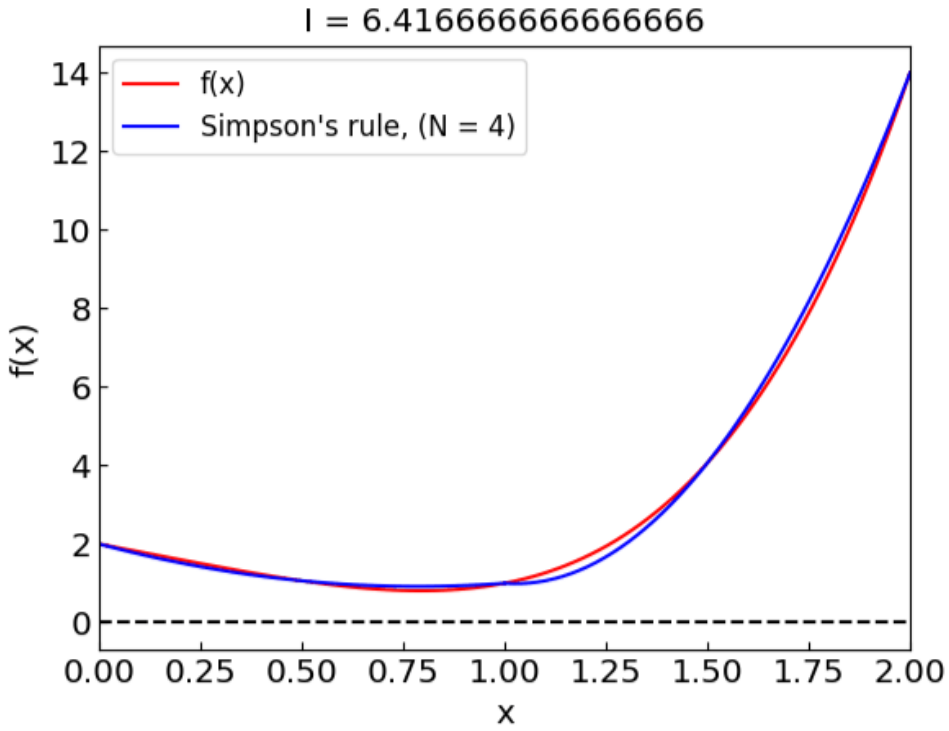
$$\int_0^2 x^4 - 2x + 2$$

$$h = (b - a)/N$$

N must be even!

Error estimate:

$$I - I_S = C\,h^4 + \mathcal{O}(h^6)$$



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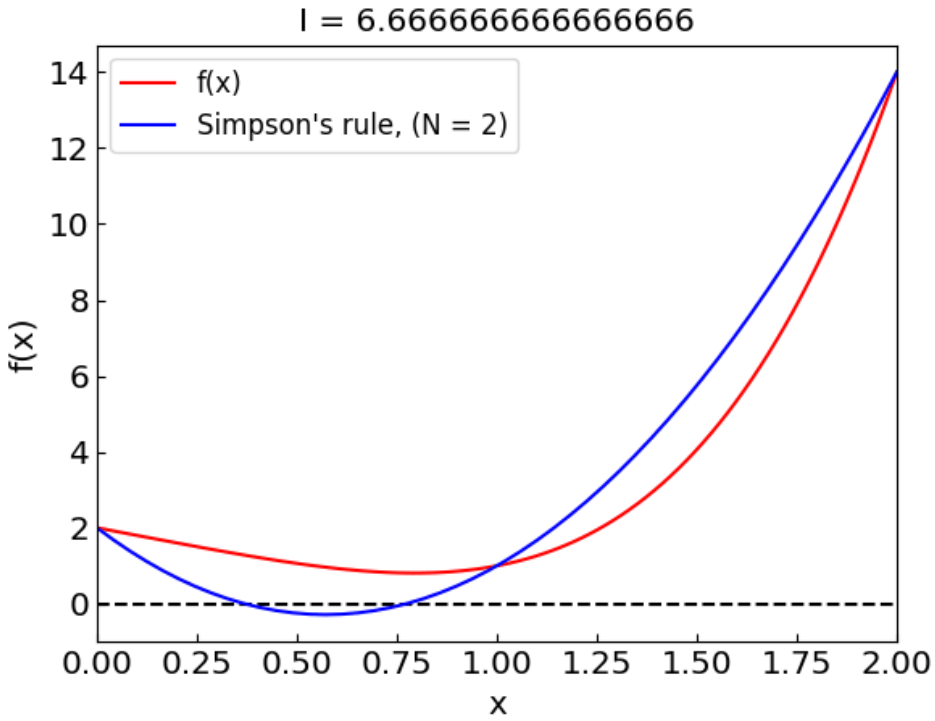
Extended Simpson's rule

$$I = \int_0^2 x^4 - 2x + 2 = 6.4$$



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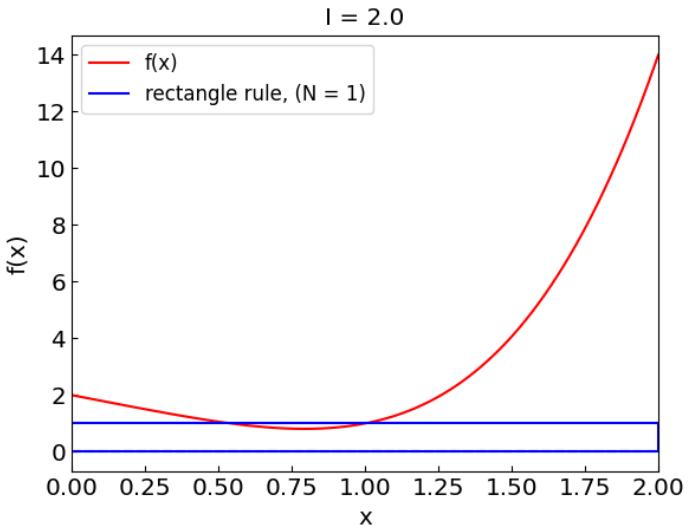
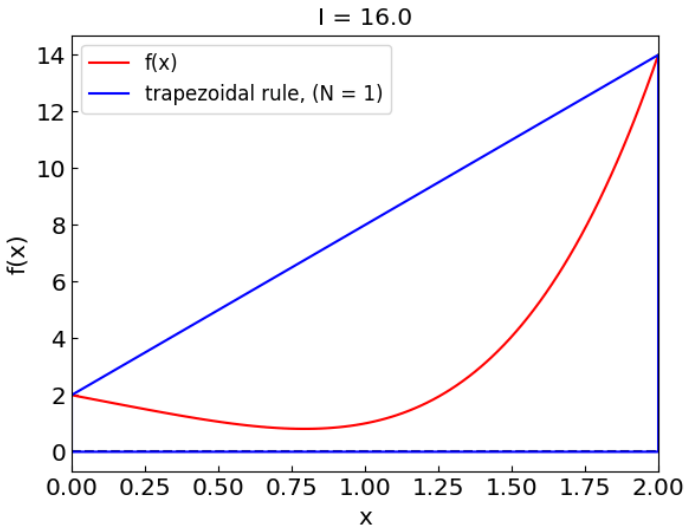
Comparing the methods

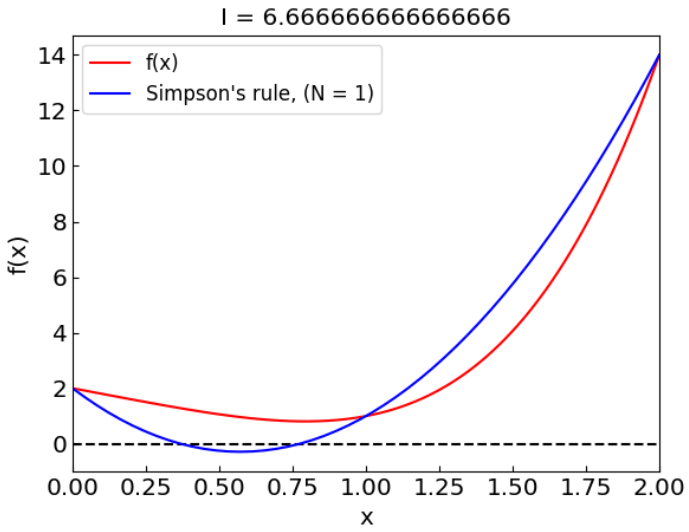
Rectangle



Trapezoid



Simpson



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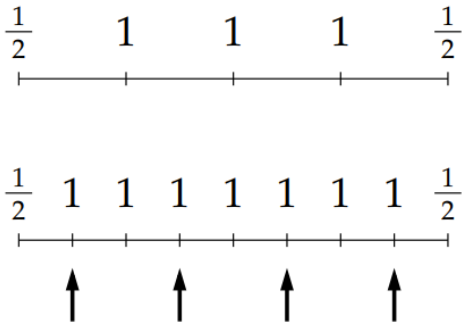
Adaptive quadrature

We would like to control the error in our calculation



This can be achieved by doubling the number of subintervals and keeping track of the error estimate

Recall that in the rectangle/trapezoidal rule the error is proportional to h^2

$$I - I_{\text{trap}} \approx ch^2$$

At step k we have $h_k = h_{k-1}/2$ therefore $\quad I - I^k_{\text{trap}} \approx ch_k^2, \qquad I - I^{k-1}_{\text{trap}} \approx 4ch_k^2,$
and the error at step k is estimated as

$$\varepsilon_k \simeq (I^k_{\text{trap}} - I^{k-1}_{\text{trap}})/3$$

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Adaptive trapezoidal rule

```
# Trapezoidal rule for numerical integration with adaptive step
def trapezoidal_rule_adaptive(f, a, b, nst = 1, tol = 1.e-8, max_iterations = 16):
    Iprev = 0.
    n = nst
    Iprev = trapezoidal_rule(f, a, b, n)
    print("Iteration: {0:5}, I = {1:20.15f}".format(1, Iprev))
    for k in range(1, max_iterations):
        n *= 2
        Inew = trapezoidal_rule(f, a, b, n)
        ek = (Inew - Iprev) / 3.
        print("Iteration: {0:5}, I = {1:20.15f}, error estimate = {2:10.15f}".format(k+1, Inew, ek))
        if (abs(ek) < tol):
            return Inew
        Iprev = Inew

    print("Failed to achiev
    return Inew
```

```
Computing the integral of x^4 - 2x + 2 over the interval ( 0.0 , 2.0 ) using adaptive trapezoidal rule
Iteration:     1, I =   16.000000000000000
Iteration:     2, I =    9.000000000000000, error estimate = -2.333333333333333
Iteration:     3, I =    7.062500000000000, error estimate = -0.645833333333333
Iteration:     4, I =    6.566406250000000, error estimate = -0.165364583333333
Iteration:     5, I =    6.441650390625000, error estimate = -0.041585286458333
Iteration:     6, I =    6.410415649414062, error estimate = -0.010411580403646
Iteration:     7, I =    6.402604103088379, error estimate = -0.002603848775228
Iteration:     8, I =    6.400651037693024, error estimate = -0.000651021798452
Iteration:     9, I =    6.400162760168314, error estimate = -0.000162759174903
Iteration:    10, I =    6.400040690088645, error estimate = -0.000040690026556
Iteration:    11, I =    6.400010172525072, error estimate = -0.000010172521191
Iteration:    12, I =    6.400002543131352, error estimate = -0.000002543131240
Iteration:    13, I =    6.400000635782950, error estimate = -0.000000635782801
Iteration:    14, I =    6.400000158945742, error estimate = -0.000000158945736
Iteration:    15, I =    6.400000039736406, error estimate = -0.000000039736446
Iteration:    16, I =    6.400000009934106, error estimate = -0.000000009934100
```

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Adaptive Simpson rule

For Simpson's rule $\varepsilon_k \simeq (I_S^k - I_S^{k-1})/15$ (understand why 15 and not 3?)

```python
# Simpson's rule for numerical integration with adaptive step
def simpson_rule_adaptive(f, a, b, nst = 2, tol = 1.e-8, max_iterations = 16):
    Iprev = 0.
    n = nst
    Iprev = simpson_rule(f, a, b, n)
    print("Iteration: {0:5}, I = {1:20.15f}".format(1, Iprev))
    for k in range(1, max_iterations):
        n *= 2
        Inew = simpson_rule(f, a, b, n)
        ek = (Inew - Iprev) / 15.

        print("Iteration: {0:5}, I = {1:20.15f}, error estimate = {2:10.15f}".format(k+1, Inew, ek))
        if (abs(ek) < tol):
            return Inew
        Iprev = Inew

    print("Failed to achieve
    return Inew
```

```
Computing the integral of x^4 - 2x + 2 over the interval ( 0.0 , 2.0 ) using adaptive Simpson's rule
Iteration:     1, I =    6.666666666666666
Iteration:     2, I =    6.416666666666666, error estimate = -0.016666666666667
Iteration:     3, I =    6.401041666666666, error estimate = -0.001041666666667
Iteration:     4, I =    6.400065104166666, error estimate = -0.000065104166667
Iteration:     5, I =    6.400004069010416, error estimate = -0.000004069010417
Iteration:     6, I =    6.400000254313150, error estimate = -0.000000254313151
Iteration:     7, I =    6.400000015894571, error estimate = -0.000000015894572
Iteration:     8, I =    6.400000000993410, error estimate = -0.000000000993411
```

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Adaptive quadratures: Romberg method

Recall that we obtained error estimate for trapezoidal method at step k

$$\varepsilon_k \simeq (I^k_{\text{trap}} - I^{k-1}_{\text{trap}})/3$$

On the other hand, by definition, $\varepsilon_k = I - I^k_{\text{trap}}$

Therefore, we can improve our estimate of the integral as

$$I = R_{k,1} = I^k_{\text{trap}} + \frac{I^k_{\text{trap}} - I^{k-1}_{\text{trap}}}{3} + \mathcal{O}(h^4)$$

Romberg method: continue this procedure iteratively

$$R_{k,m+1} = R_{k,m} + \frac{R_{k,m} - R_{k-1,m}}{4^m - 1} \ .$$

until the desired accuracy is reached

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Romberg method

```
def romberg(
    f,
    a,
    b,
    accuracy=1e-8,
    max_order=10
):
    R = np.zeros((max_order, max_order))
    h = (b - a) / 2.
    R[0, 0] = h * (f(a) + f(b)) # The initial trapezoidal rule
    for n in range(1, max_order):
        trapezoid = 0.0
        for j in range(2**(n-1)):
            trapezoid += f(a + (2*j+1)*h)
        R[n, 0] = 0.5 * R[n-1, 0] + h * trapezoid # The trapezoidal rule
        l = 1
        # The Romberg iterations
        for m in range(1, n+1):
            l *= 4
            R[n, m] = (l * R[n, m-1] - R[n-1, m-1]) / (l-1)
        print("Iteration: {0:5}, I = {1:20.15f}, error estimate = {2:10.15f}".format(n, R[n, m], abs(R[n, m] - R[n-1, m-1])))
        if abs(R[n, m] - R[n-1, m-1]) < accuracy:
            return R[n, m]
        h /= 2.
    print("Romberg method did not converge to required accuracy")
    return R[-1, -1]
```

```
Computing the integral of x^4 - 2x + 2 over the interval ( 0.0 , 2.0 ) using Romberg method
Iteration:     1, I =    6.666666666666667, error estimate = 9.333333333333332
Iteration:     2, I =    6.400000000000000, error estimate = 0.266666666666667
Iteration:     3, I =    6.400000000000000, error estimate = 0.000000000000000
```

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Improper integrals

- Contain integrable singularities (typically at the endpoints)

$$\int_0^1 \frac{1}{\sqrt{x}} dx = 2\sqrt{x}\Big|_0^1 = 2$$

- (Semi-)infinite integration range

$$\int_0^\infty e^{-x} dx = 1$$

$$\int_{-\infty}^\infty e^{-x^2} dx = \sqrt{\pi}$$

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Improper integrals: Singularities at endpoints

- Even though if the singularities at integration endpoints are integrable, the trapezoidal, Simpson, etc. methods will fail because they evaluate the integrand at the endpoints

$$\int_0^1 \frac{1}{\sqrt{x}} dx = 2\sqrt{x}\Big|_0^1 = 2$$

```
def fsing1(x):
    return 1./np.sqrt(x)

trapezoidal_rule(fsing1,0.,1.,10)
```

```
/tmp/ipykernel_31240/847063500.py:2: RuntimeWarning: divide by zero encountered in double_scalars
  return 1./np.sqrt(x)
```

- **Solution:** use method that does use the endpoints (e.g. **rectangle rule**)

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Improper integrals: Singularities at endpoints

$$\int_0^1 \frac{1}{\sqrt{x}} dx = 2\sqrt{x}\Big|_0^1 = 2$$

```
def fsing1(x):
    return 1./np.sqrt(x)
```

```
print('Using rectangle rule to evaluate \int_0^1 1/\sqrt{x} dx')
nst = 1
rectangle_rule_adaptive(fsing1,0.,1.,1,1.e-3,20)
```

```
Using rectangle rule to evaluate \int_0^1 1/\sqrt{x} dx
Iteration:     1, I =    1.414213562373095
Iteration:     2, I =    1.577350269189626, error estimate = 0.054378902272177
Iteration:     3, I =    1.698844079579673, error estimate = 0.040497936796682
Iteration:     4, I =    1.786461001734842, error estimate = 0.029205640718390
Iteration:     5, I =    1.848856684639738, error estimate = 0.020798560968299
Iteration:     6, I =    1.893088359706383, error estimate = 0.014743891688882
Iteration:     7, I =    1.924392755699513, error estimate = 0.010434798664376
Iteration:     8, I =    1.946535279970520, error estimate = 0.007380841423669
Iteration:     9, I =    1.962194152677056, error estimate = 0.005219624235512
Iteration:    10, I =    1.973267083679453, error estimate = 0.003690977000799
Iteration:    11, I =    1.981096937261288, error estimate = 0.002609951193945
Iteration:    12, I =    1.986633507070365, error estimate = 0.001845523269692
Iteration:    13, I =    1.990548459938304, error estimate = 0.001304984289313
Iteration:    14, I =    1.993316751362098, error estimate = 0.000922763807931
```

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Improper integrals: (Semi-)infinite intervals

Solution: map to a finite interval [e.g. (0,1)] by a change of variables

- Semi-infinite:

$$\int_a^\infty f(x)dx \quad \Rightarrow \quad x = a + \frac{t}{1-t} \quad \Rightarrow \quad \int_a^\infty f(x)dx = \int_0^1 f\left(a + \frac{t}{1-t}\right)\frac{dt}{1-t^2} = \int_0^1 g(t)dt$$

- Infinite:

$$\int_{-\infty}^\infty f(x)dx \quad \Rightarrow \quad x = \frac{t}{1-t^2} \quad \Rightarrow \quad \int_{-\infty}^\infty f(x)dx = \int_{-1}^1 f\left(\frac{t}{1-t^2}\right)\frac{1+t^2}{(1-t^2)^2}dt = \int_{-1}^1 g(t)dt$$

Then apply a standard method (e.g. rectangle rule to avoid endpoint singularities) to g(t)

NB: Other options for the change of variable are possible

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Improper integrals: Semi-infinite intervals

$$\int_0^\infty e^{-x} dx = 1$$

```
def fexp(x):
    return np.exp(-x)

def g(t, f, a = 0.):
    return f(a + t / (1. - t)) / (1. - t)**2
```

```
a = 0.
def frect(x):
    return g(x, fexp, a)

print('Using change of variable and the rectangle rule to evaluate \int_0^\infty \exp(-x) dx')
rectangle_rule_adaptive(frect,0.,1.,1,1.e-6,20)
```

```
Using change of variable and the rectangle rule to evaluate \int_0^\infty \exp(-x) dx
Iteration:     1, I =    1.471517764685769
Iteration:     2, I =    1.035213267452946, error estimate = -0.145434832410941
Iteration:     3, I =    0.984670579385046, error estimate = -0.016847562689300
Iteration:     4, I =    1.001784913275257, error estimate = 0.005704777963404
Iteration:     5, I =    1.000155714391028, error estimate = -0.000543066294743
Iteration:     6, I =    1.000040642390661, error estimate = -0.000038357333456
Iteration:     7, I =    1.000010172618432, error estimate = -0.000010156590743
Iteration:     8, I =    1.000002543136036, error estimate = -0.000002543160799
Iteration:     9, I =    1.000000635783161, error estimate = -0.000000635784292
```

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Improper integrals: Infinite intervals

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} = 1.772454\ldots$$

```
def fexp2(x):
    return np.exp(-x**2)

def g2(t, f):
    return f(t / (1. - t**2)) * (1.+t**2) / (1. - t**2)**2
```

```
def frect2(x):
    return g2(x, fexp2)

print('Using change of variable and the rectangle rule to evaluate \int_{-\infty}^\infty \exp(-x^2) dx')
rectangle_rule_adaptive(frect2,-1.,1.,1,1.e-6,20)

print('Expected value: \sqrt{\pi} =', np.sqrt(np.pi))
```

```
Using change of variable and the rectangle rule to evaluate \int_{-\infty}^\infty \exp(-x^2) dx
Iteration:     1, I =    2.000000000000000
Iteration:     2, I =    2.849690615244243, error estimate = 0.283230205081414
Iteration:     3, I =    1.557994553948652, error estimate = -0.430565353765197
Iteration:     4, I =    1.808005109208286, error estimate = 0.083336851753211
Iteration:     5, I =    1.770118560572371, error estimate = -0.012628849545305
Iteration:     6, I =    1.772492101507391, error estimate = 0.000791180311673
Iteration:     7, I =    1.772453880915058, error estimate = -0.000012740197444
Iteration:     8, I =    1.772453850905505, error estimate = -0.000000010003185
Expected value: \sqrt{\pi} = 1.7724538509055159
```

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Numerical integration so far

- Rectangle rule

$$\int_a^b f(x)\,dx \approx (b-a)\,f\left(\frac{a+b}{2}\right)$$

- Trapezoidal rule

$$\int_a^b f(x)\,dx \approx (b-a)\,\frac{f(a)+f(b)}{2}$$

- Simpson's rule

$$\int_a^b f(x)\,dx \approx \frac{(b-a)}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

All can be written as

$$\int_a^b f(x)\,dx \approx \sum_k w_k\,f(x_k)$$

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Integrating the interpolating polynomial

There is a systematic way to derive a numerical integration scheme

$$\int_a^b f(x)\,dx \approx \sum_k w_k f(x_k)$$

which will give an exact result when f(x) is a polynomial up to a certain degree.

Recall the interpolating polynomial through N+1 points where f(x) can be evaluated

$$f(x) \approx p_N(x) = \sum_{k=0}^{N} f(x_k)\, L_{N,k}(x) \qquad L_{N,k}(x) = \prod_{j \neq k} \frac{x - x_j}{x_k - x_j}$$

Then, the integral reads

$$\int_a^b f(x)\,dx \approx \int_a^b p_N(x)\,dx = \sum_{k=0}^{N} w_k f(x_k) \qquad \text{where} \qquad w_k = \int_a^b L_{N,k}(x)dx$$

This expression is exact when f(x) is a polynomial up to degree N

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Quadrature methods

- Newton-Cotes: equidistant spacing
- Clenshaw-Curtis: minimize Runge phenomenon
- Gauss-Legendre quadrature: use Legendre polynomials

Summary of integration

- Rectangle/trapezoidal rule
  - Good for quick calculations not requiring great accuracy
  - Does not rely on the integrand being smooth; a good choice for noisy/singular integrands, equally spaced points

- Romberg method
  - Control over error
  - Good for relatively smooth functions evaluated at equidistant nodes

- Gaussian quadrature
  - Theoretically most accurate if the function is relatively smooth
  - Good for many repeated calculations of the same type of integral
  - Requires unequally spaced nodes
  - Error can be challenging to control, especially for non-smooth functions

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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

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

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

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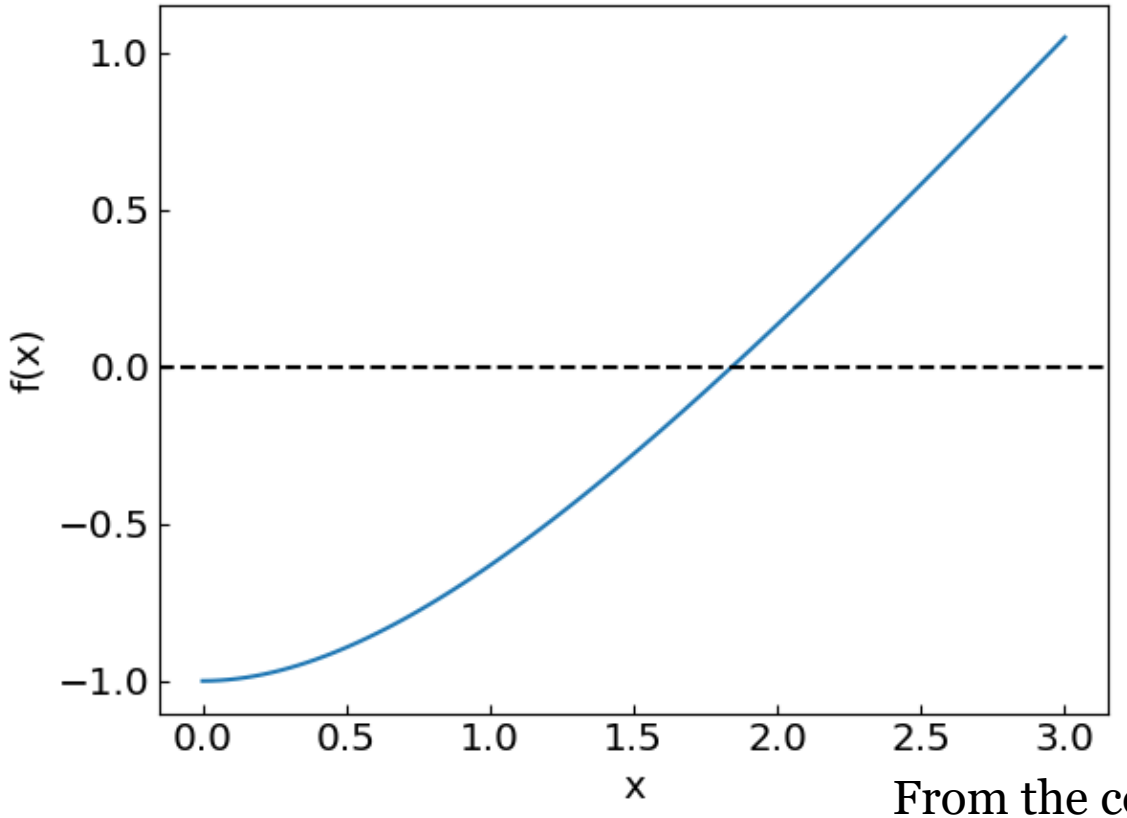
Non-linear equations

Consider an equation

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



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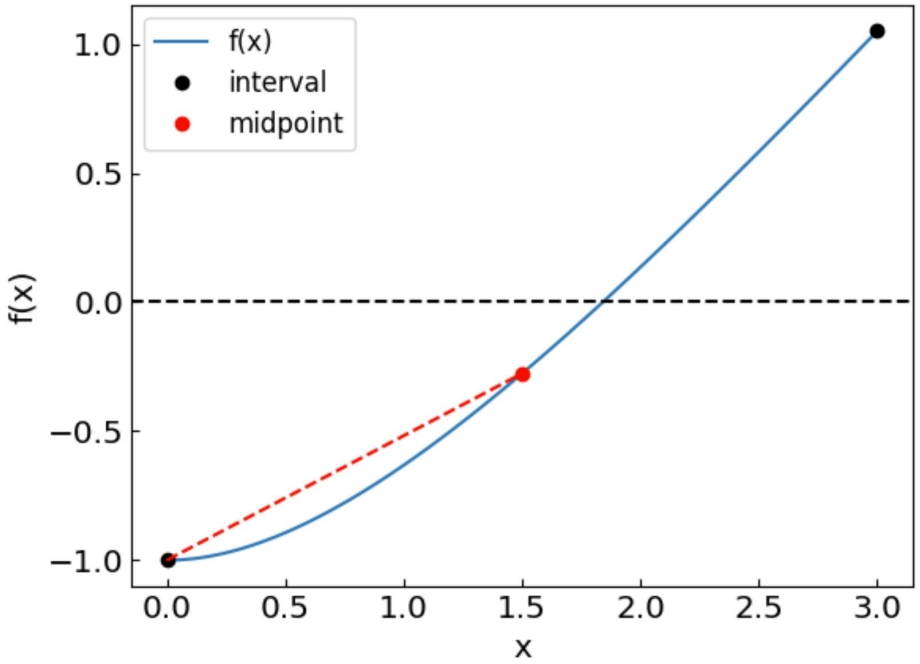
Bisection method

Bisection method:

1. Find an interval (a,b) which brackets the root x*
   - x* ∈ (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



Method is guaranteed to converge to the root
The error is halved at each step – “linear” convergence

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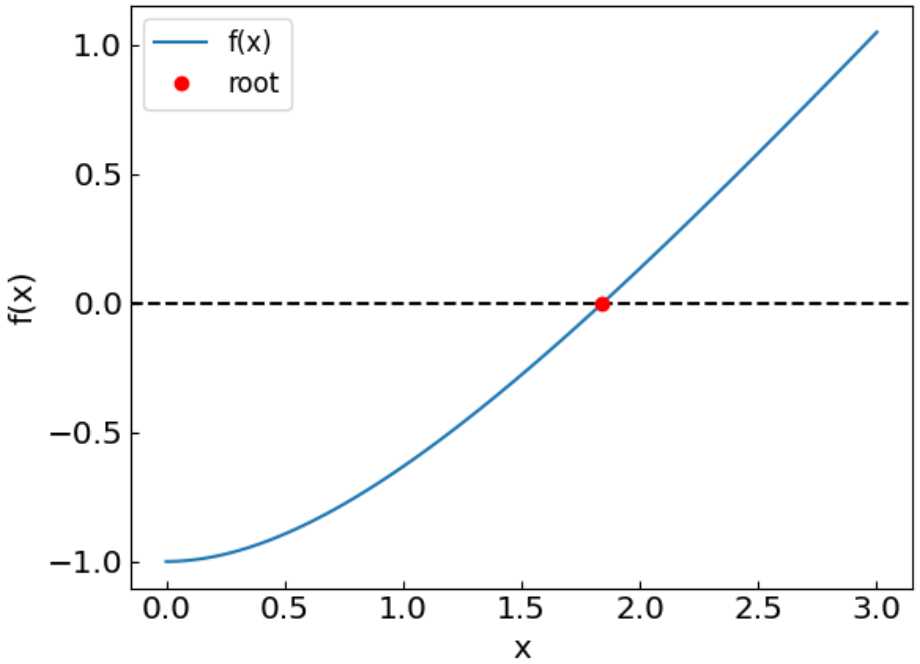
Bisection method

```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
```

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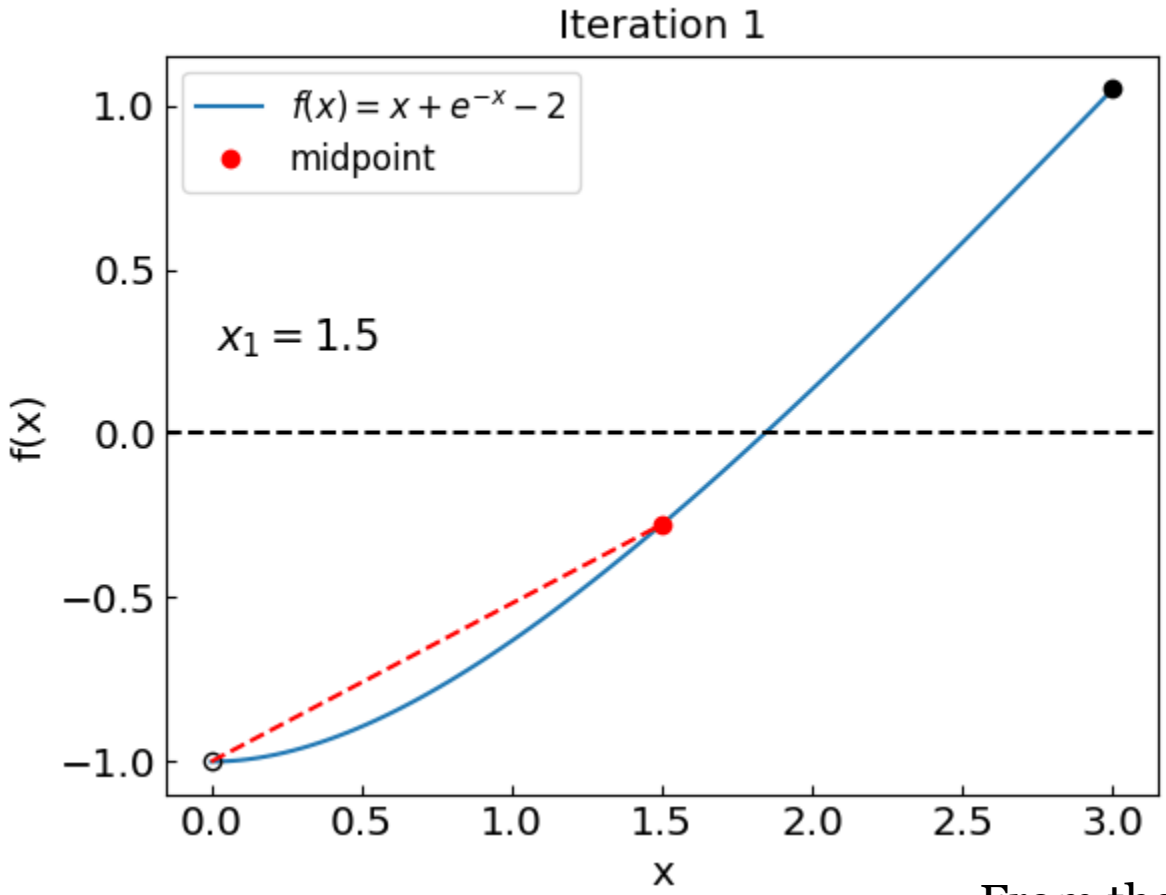
Bisection method: how the iterations look like

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



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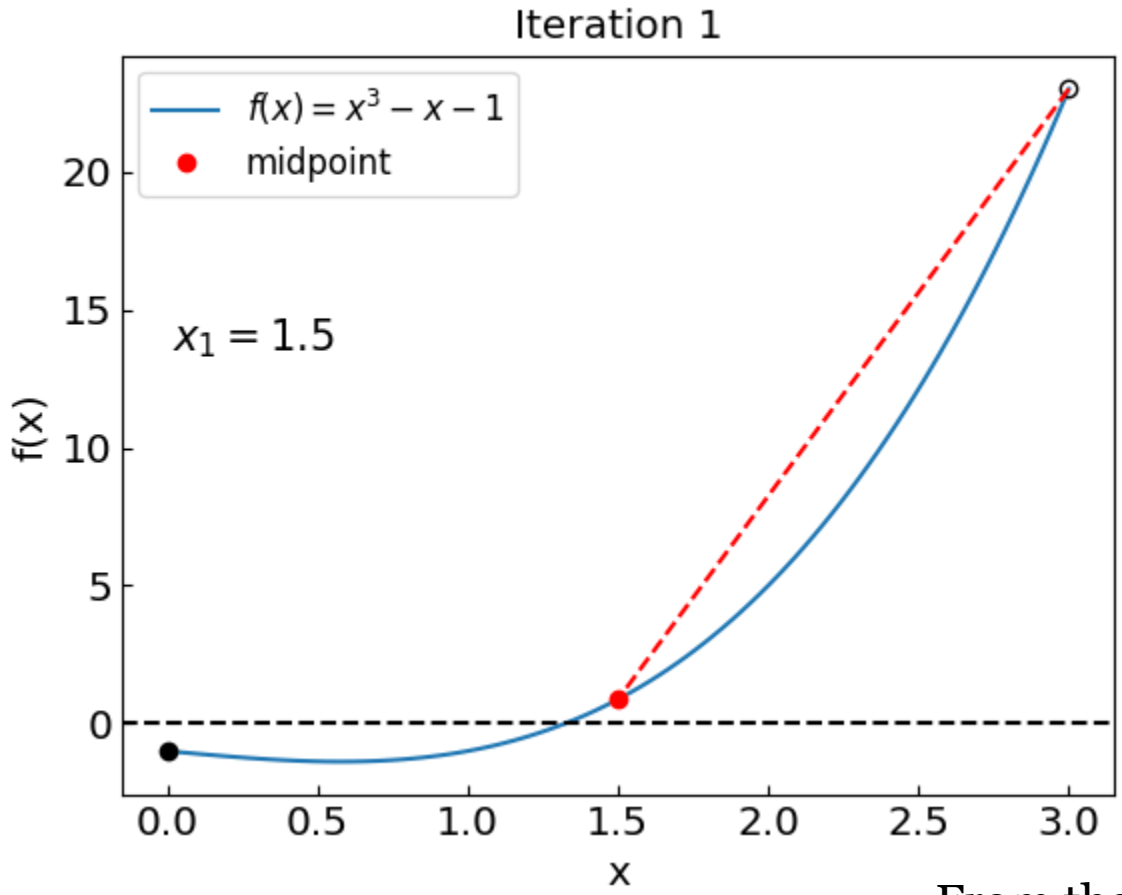
Bisection method: another example

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



35 iterations in both cases

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False position method

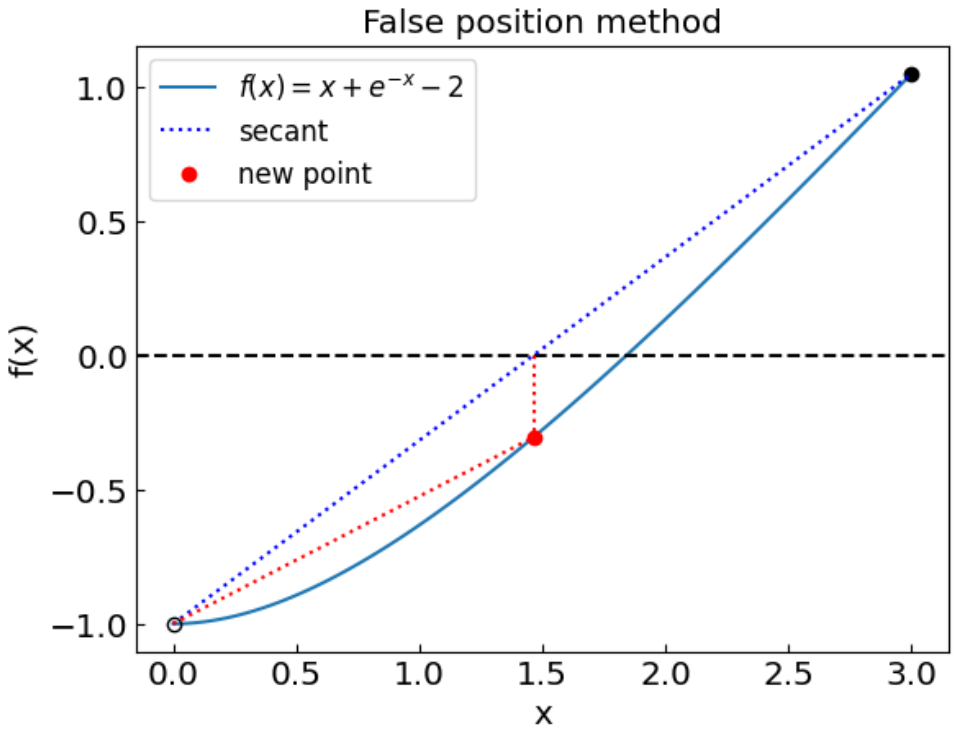
False position method:

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

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



Method is guaranteed to converge to the root
"Linear" convergence; typically faster than bisection, but not always

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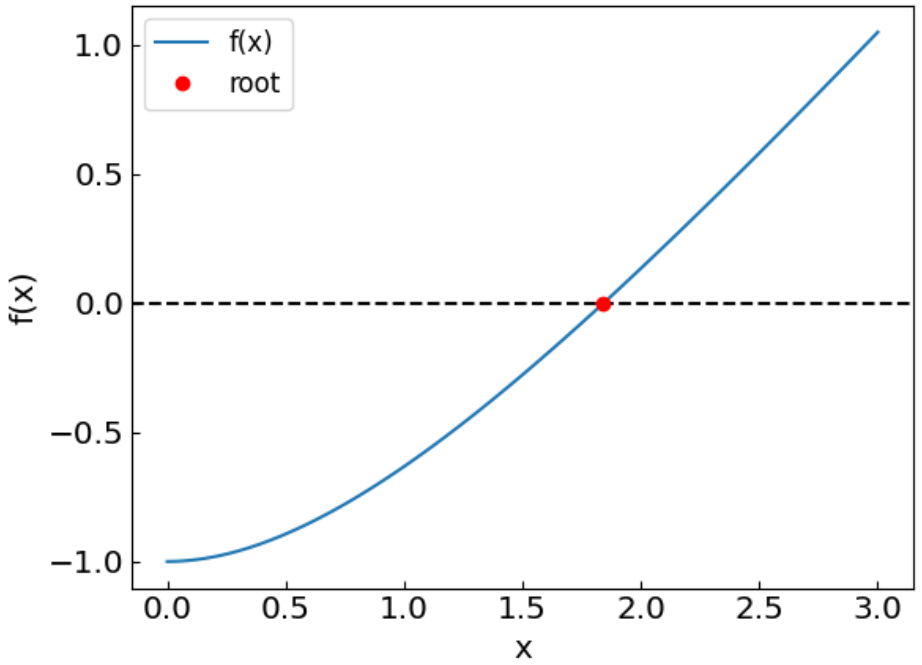
False position method

```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
```

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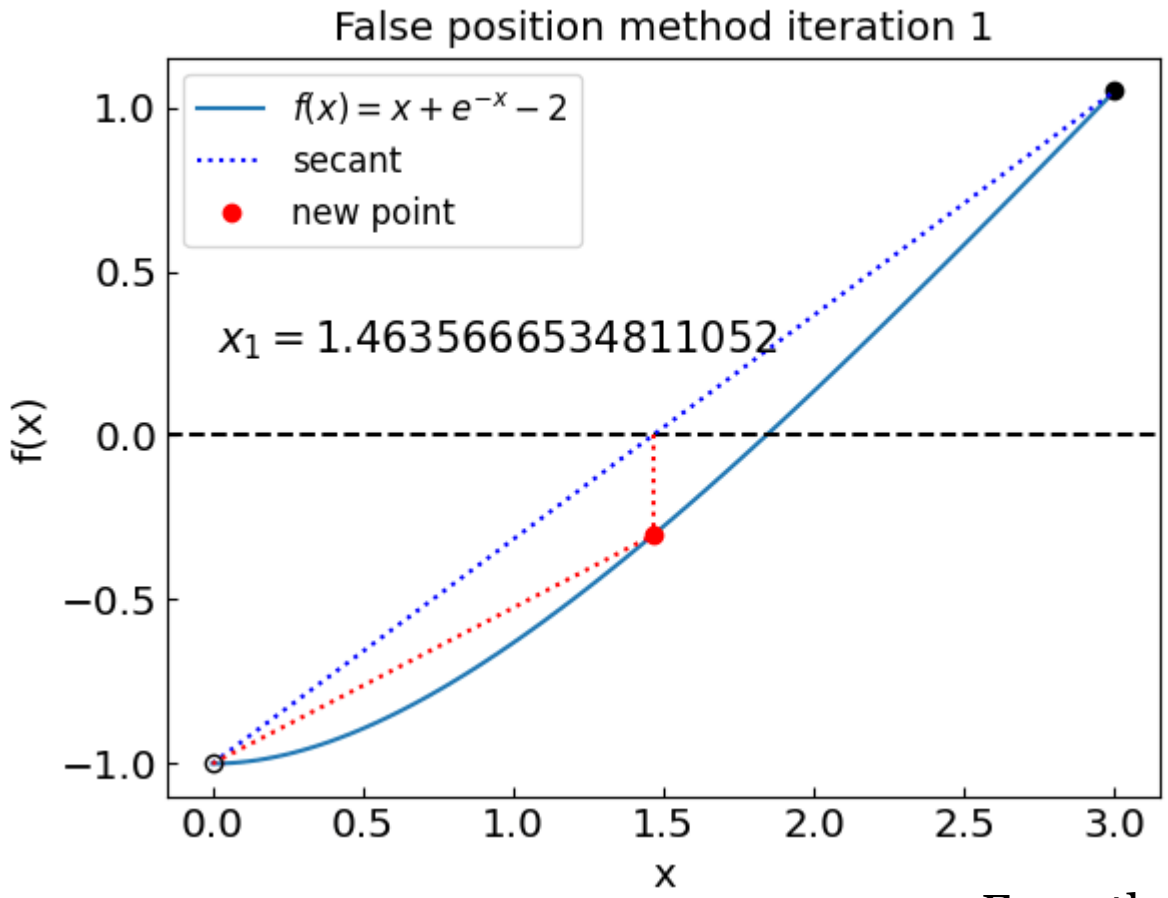
False position method

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



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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
```

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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
```

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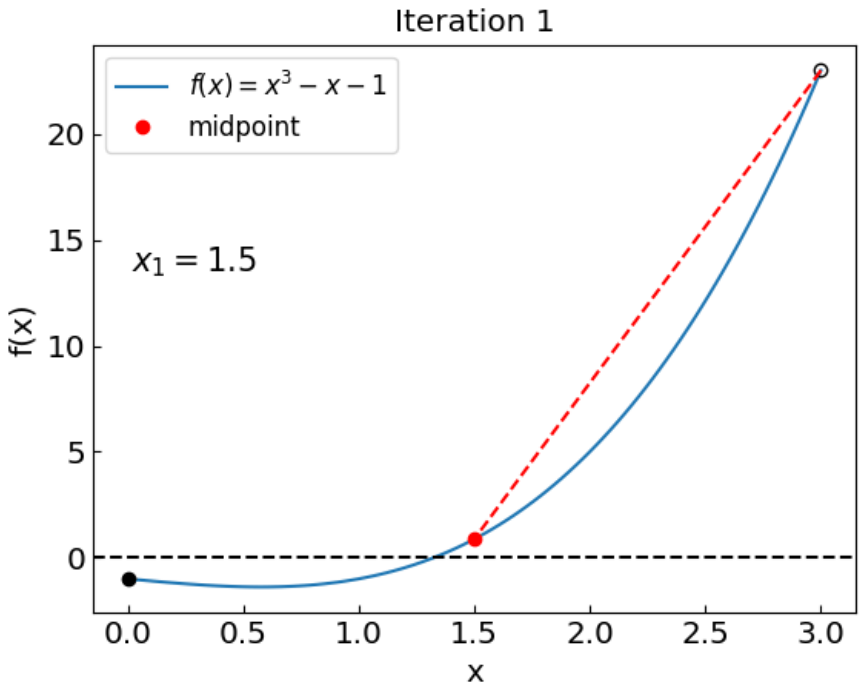
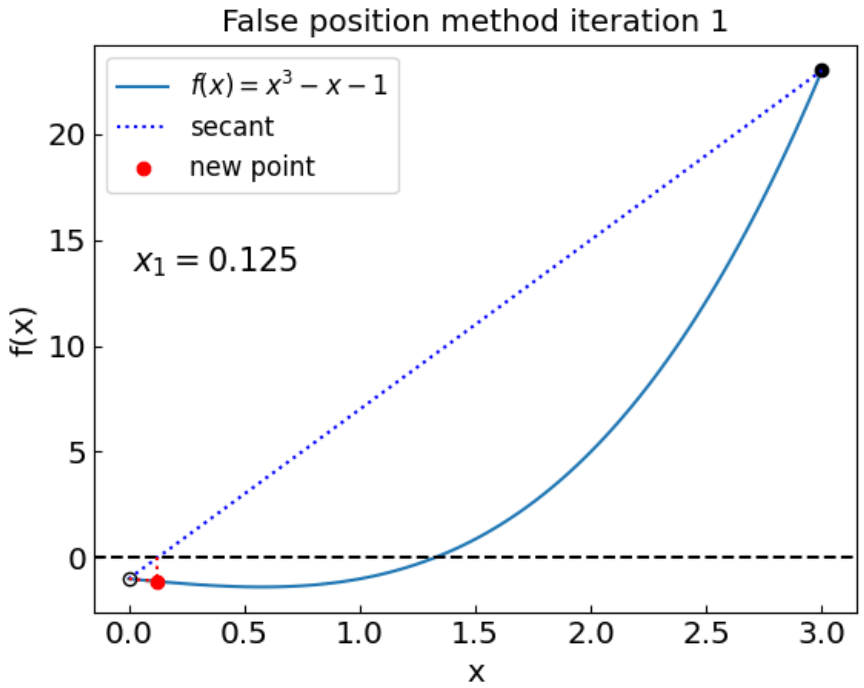
False position vs bisection: not always clear who wins

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

Bisection method:



False position method:



More advanced methods combine the two and add other refinements*

- Ridders' method
- Brent method

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

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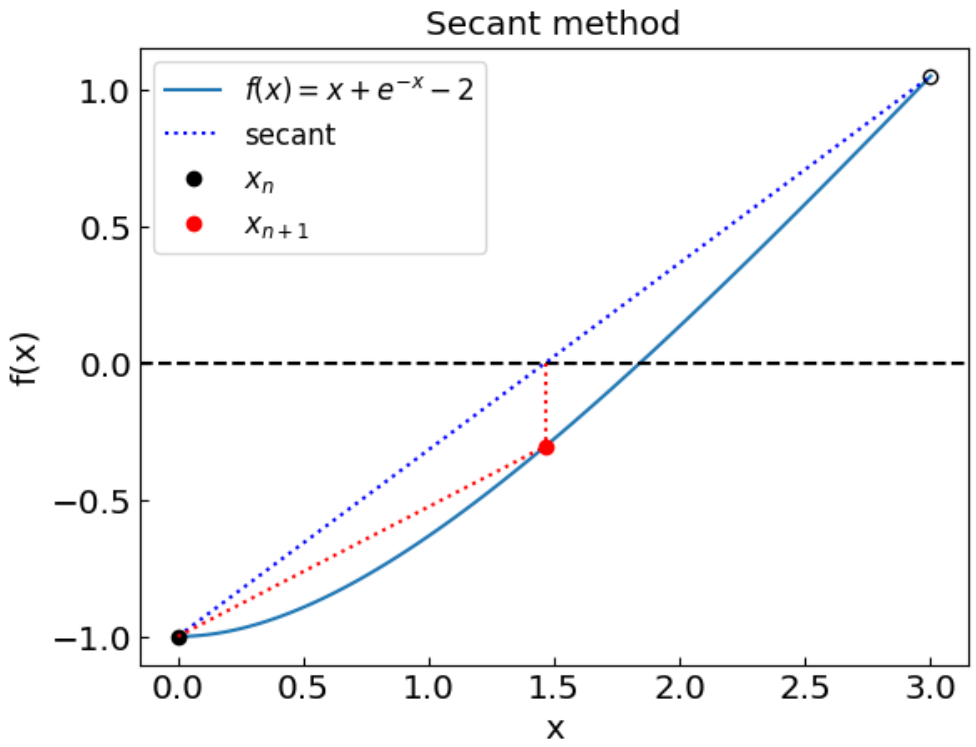
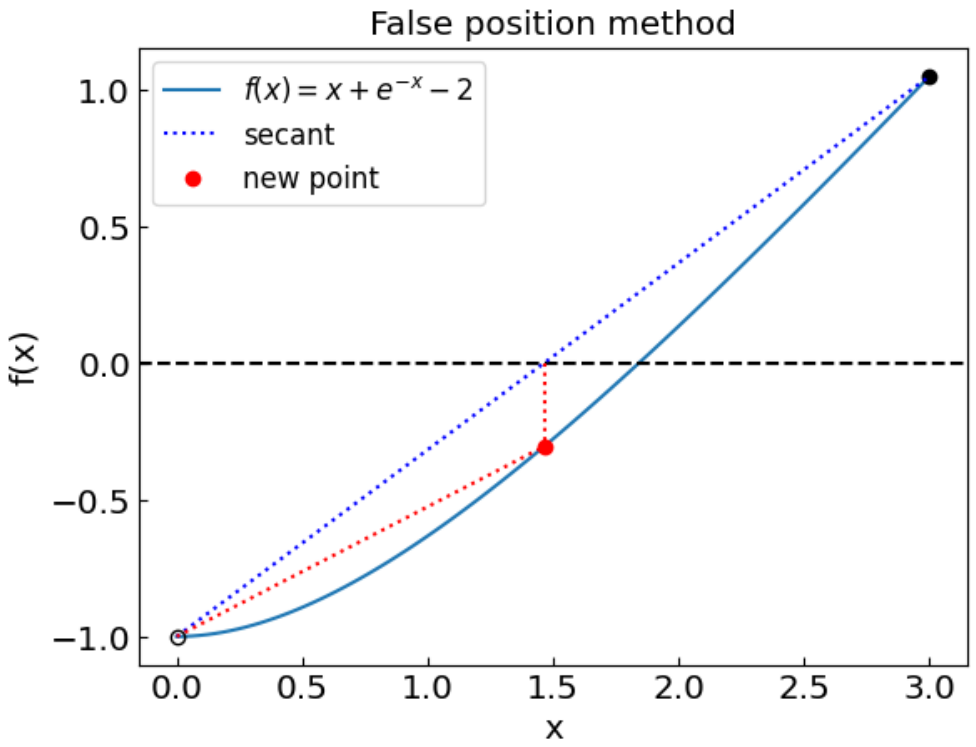
Secant method

Secant method: similar to false position, but the interval *need not bracket the root*

Always uses the last two points



vs



Typically “superlinear” convergence when works

Can still be slower than bisection or not converge at all (e.g. secant is parallel to y = 0 axis)

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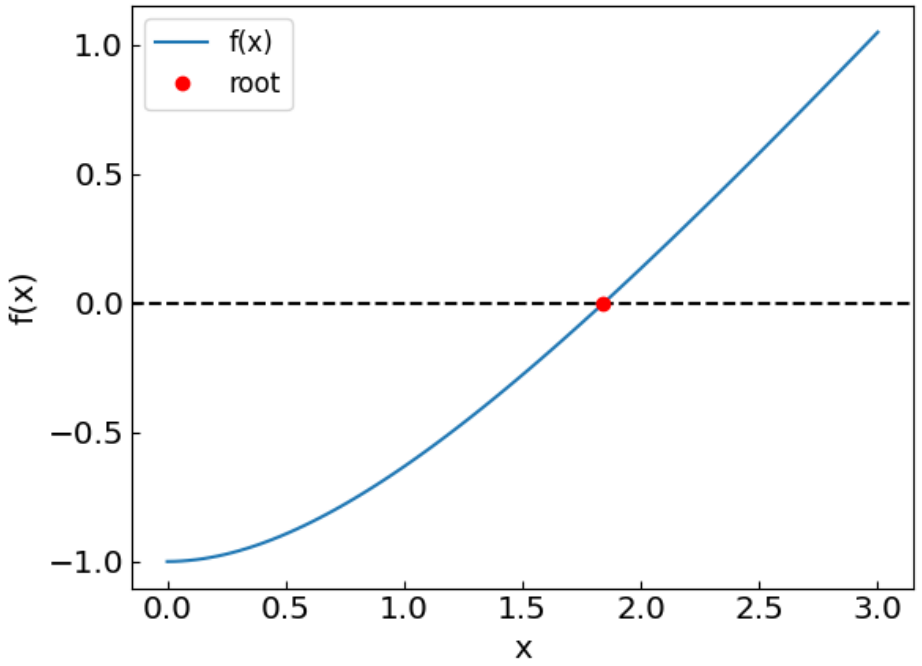
Secant method

```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
```

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




```
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
```

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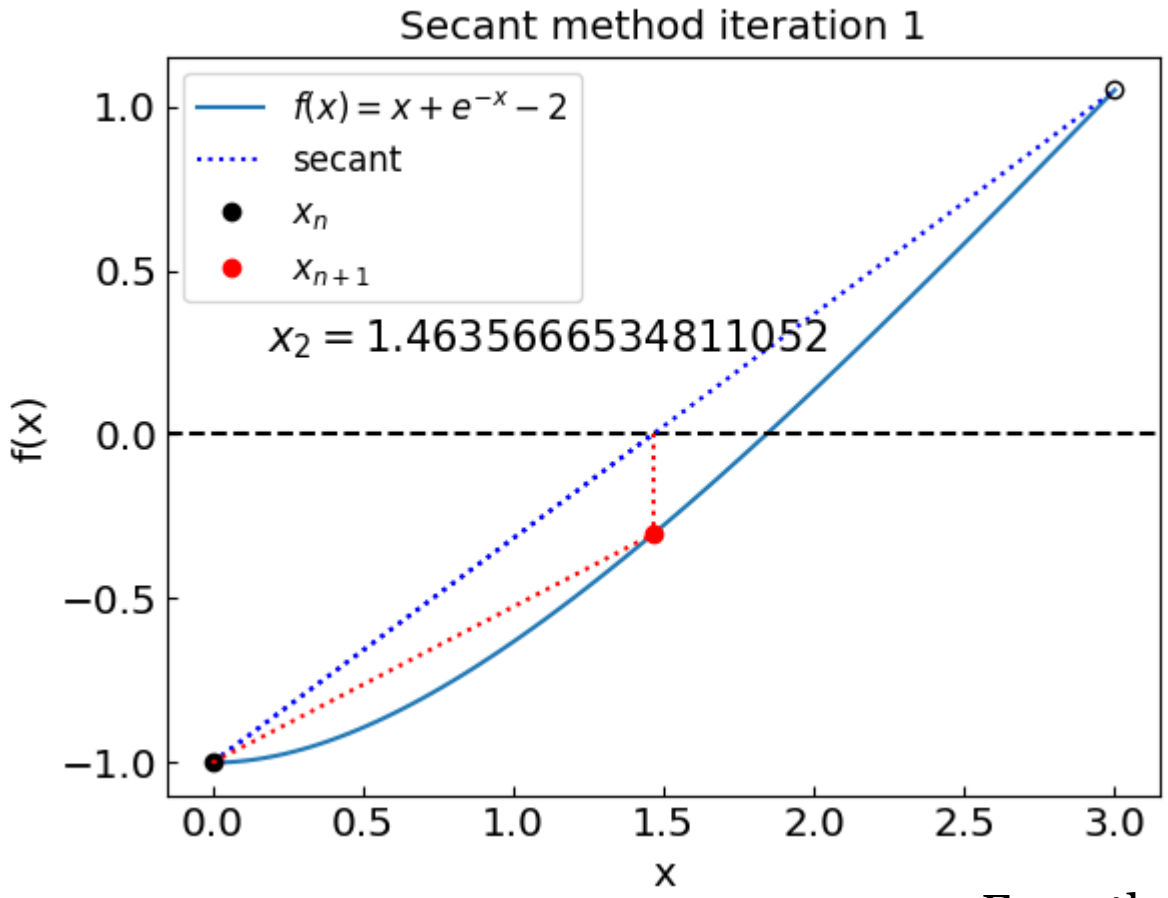
Secant method

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



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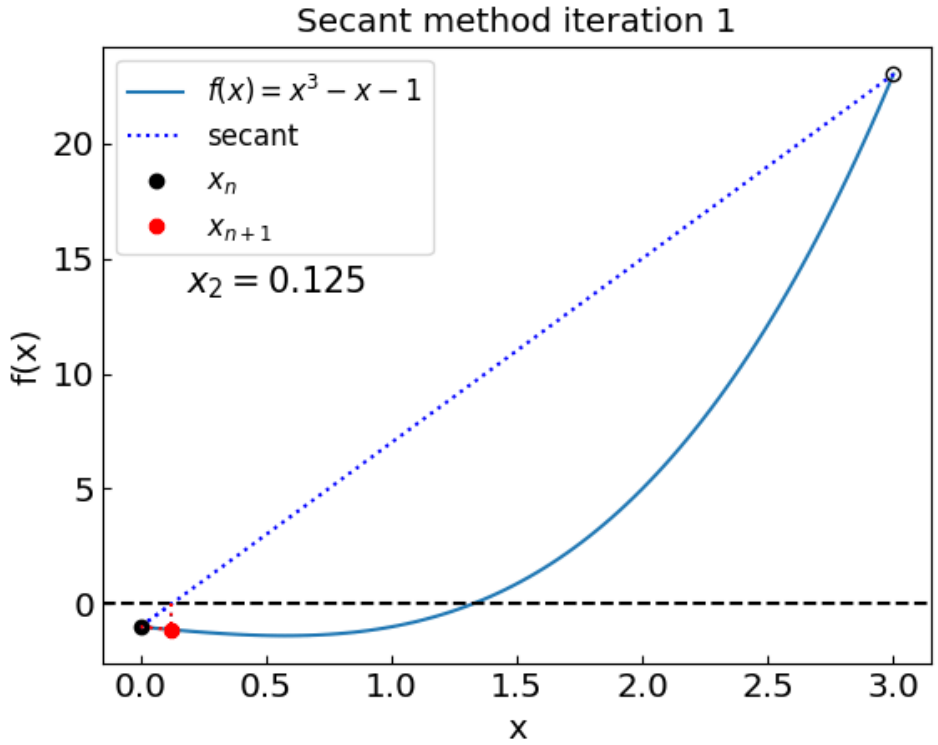
Secant method

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

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



Because the method does not bracket the root, it is not guaranteed to converge

In this case, it managed to recover

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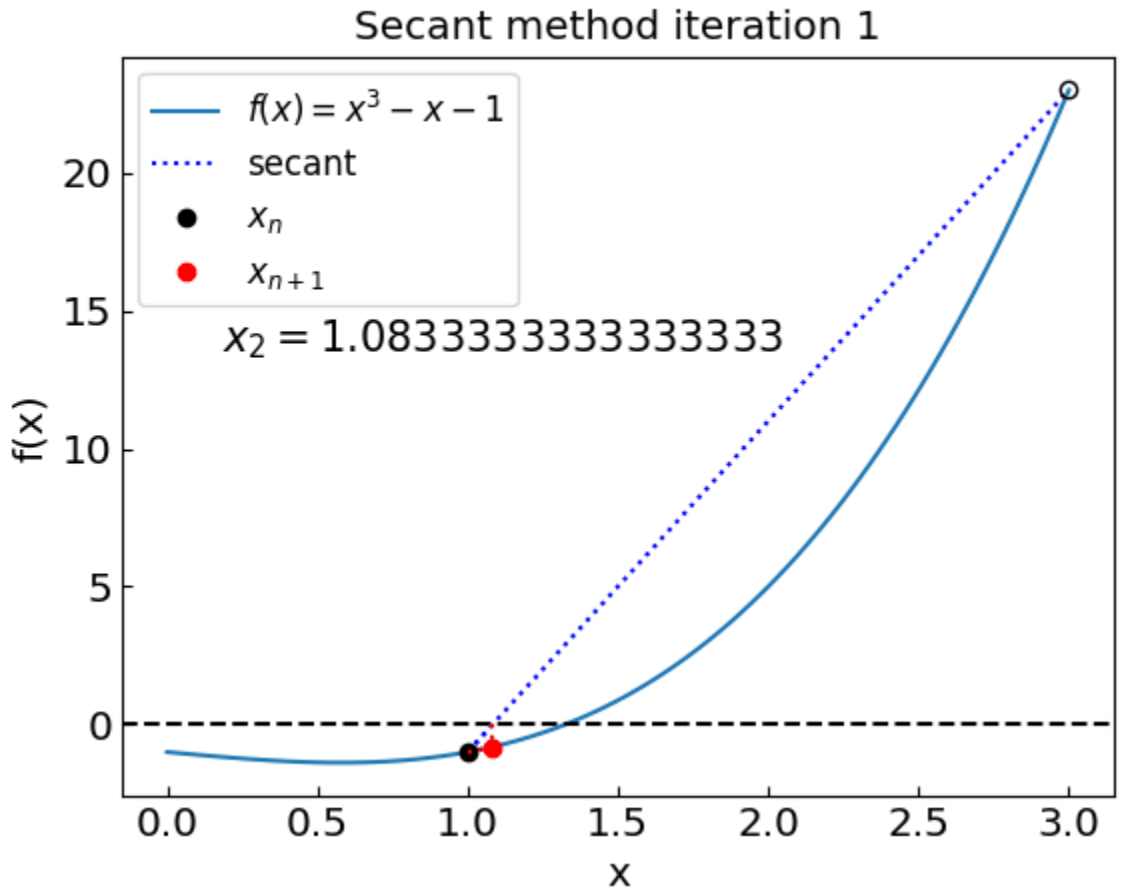
Secant method

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

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



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Newton-Raphson method

Newton-Raphson method:

- Local method (uses only the current estimate to get the next one)
- Requires the evaluation of derivative

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

Then

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

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

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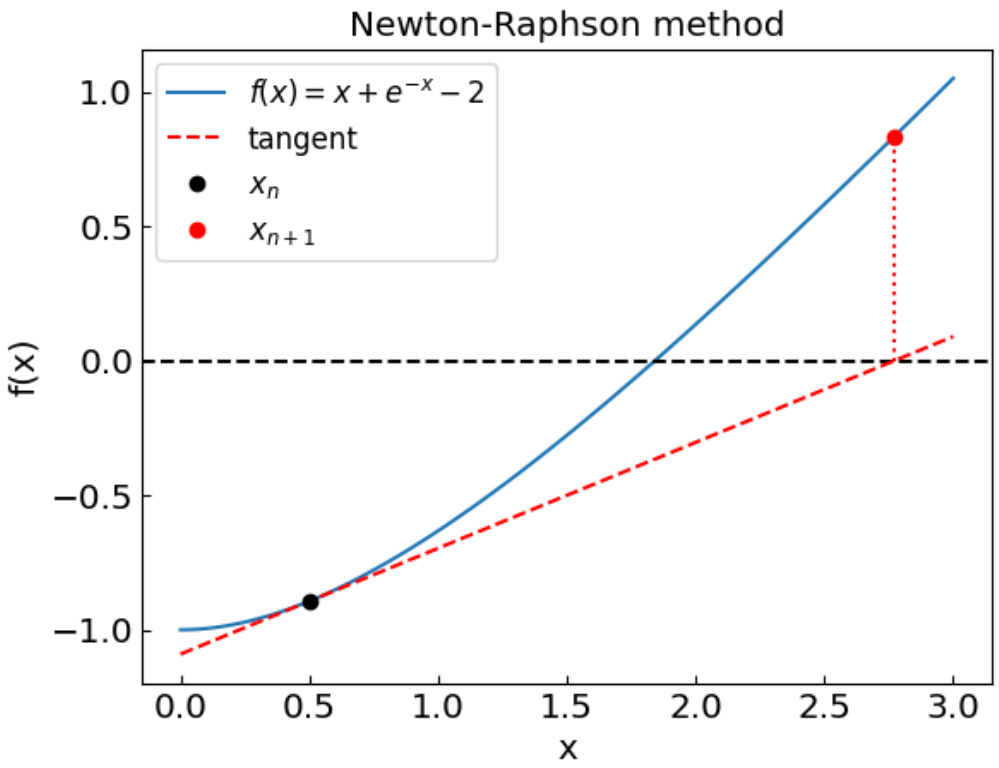
Newton-Raphson method

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



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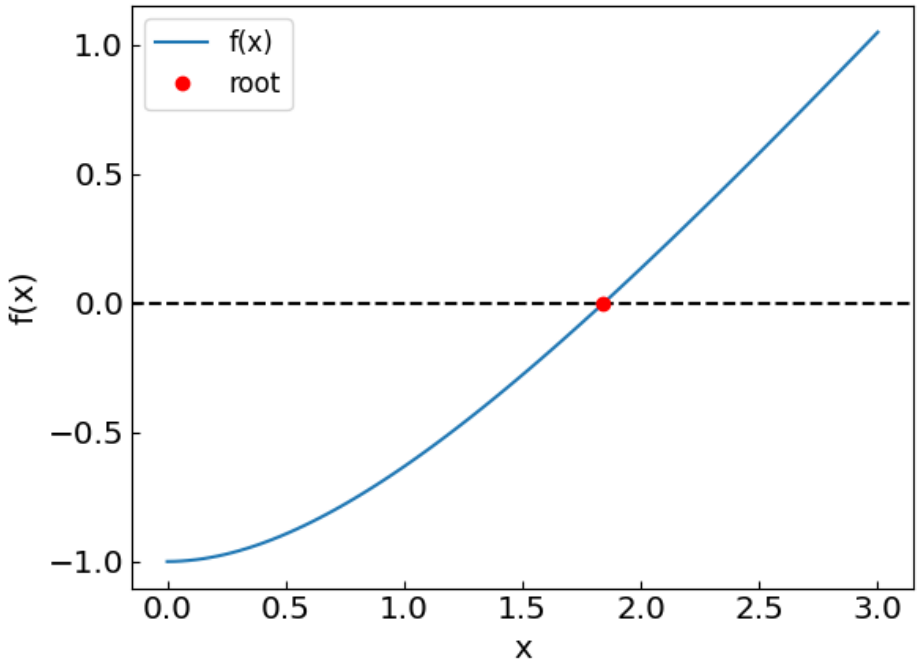
"Quadratic" convergence when works

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

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
```

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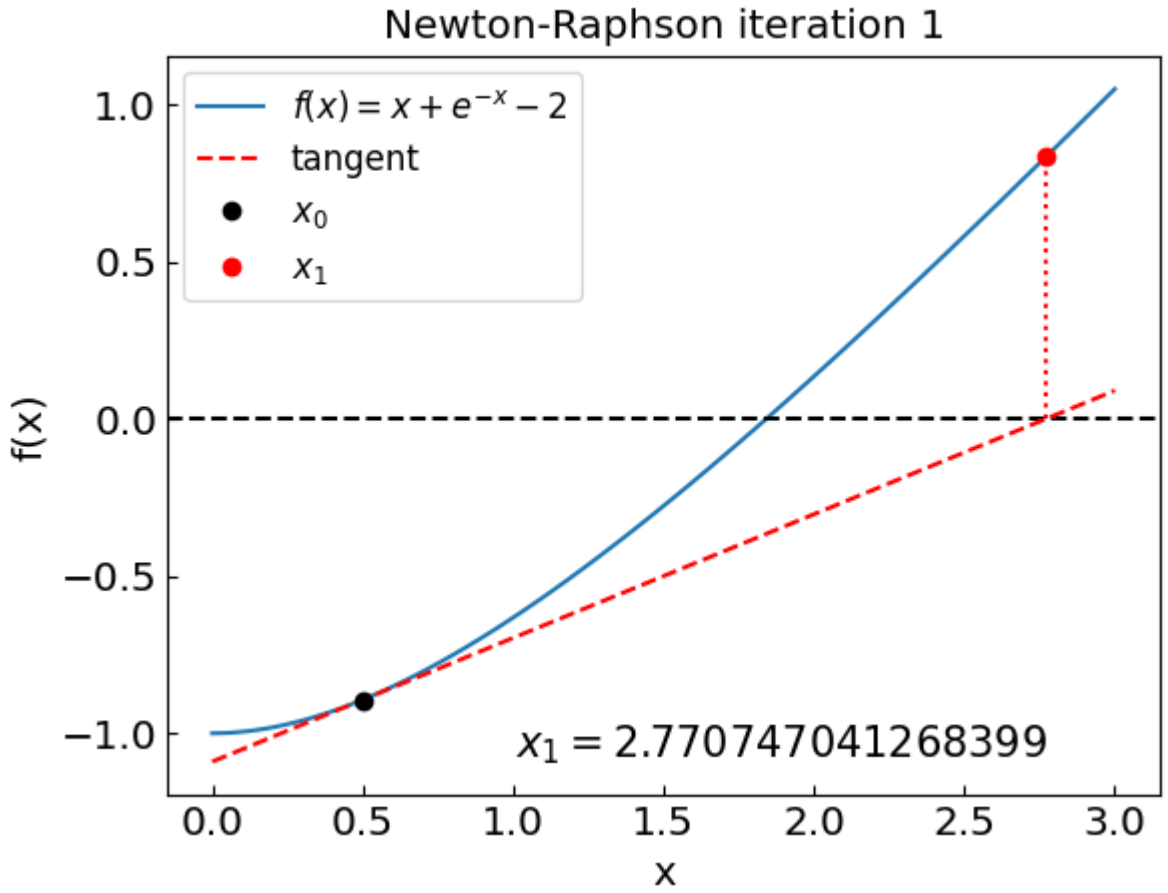
Newton-Raphson method

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



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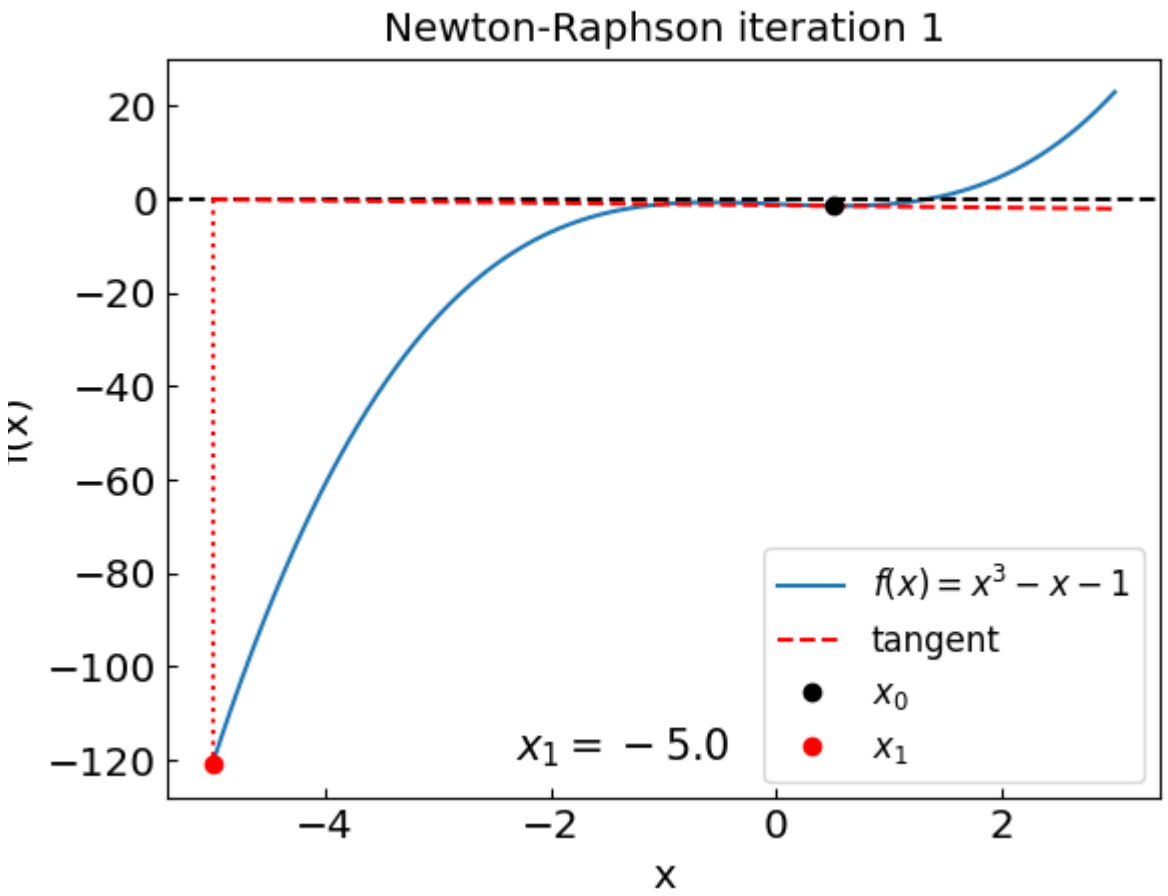
Newton-Raphson method: issues

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



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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 $x_0 = 0$

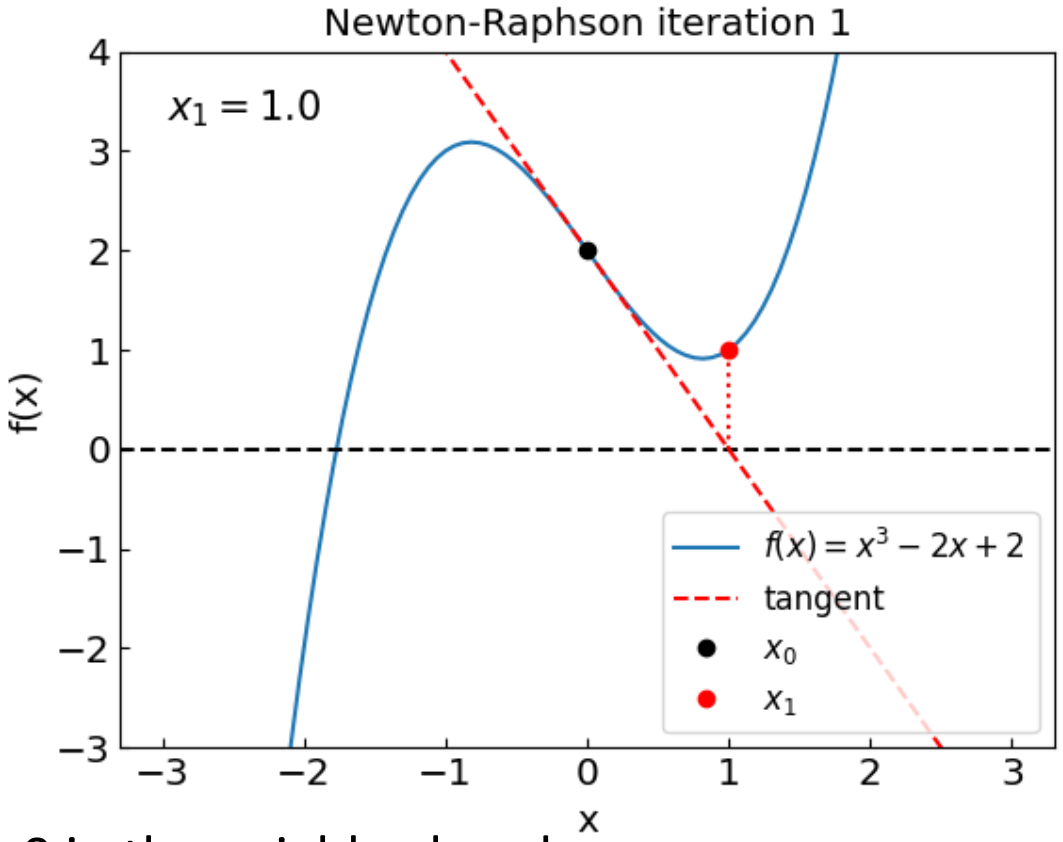
Iteration 1: $f(x_0) = 2, \quad f'(x_0) = -2$

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

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

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Relaxation method

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:

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

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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
```

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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

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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) = -588715871622705914576896000.000000000000000
Iteration:     6, x = -588715871622705914576896000.000000000000000, phi(x) = -204040901322752646989478259680513109526757826056202557355691431285390611316736
6202557355691431285390611316736.000000000000000
Iteration:     7, x = -204040901322752646989478259680513109526757826056202557355691431285390611316736.000000000000000, phi
(x) = -849477147223738769124261153859947219933304503407088864329587058315002861225858314510130211954336728493261609772281413
112710427529099370666994394355751882504172013925675175629651436351046350178280569616740709679141494327303316334182 4.00000000
0000000
```

Divergent!

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

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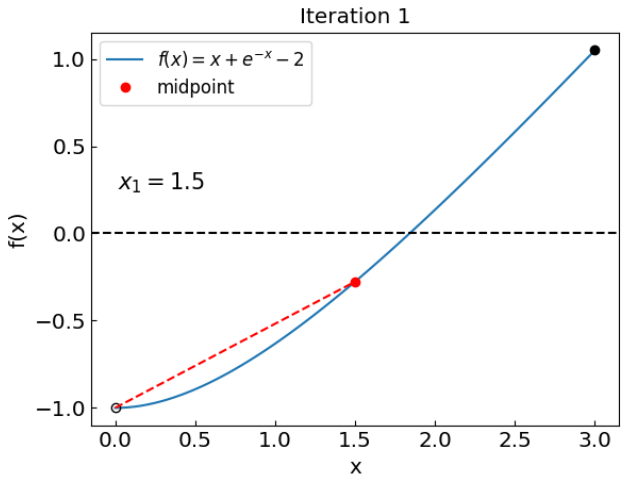
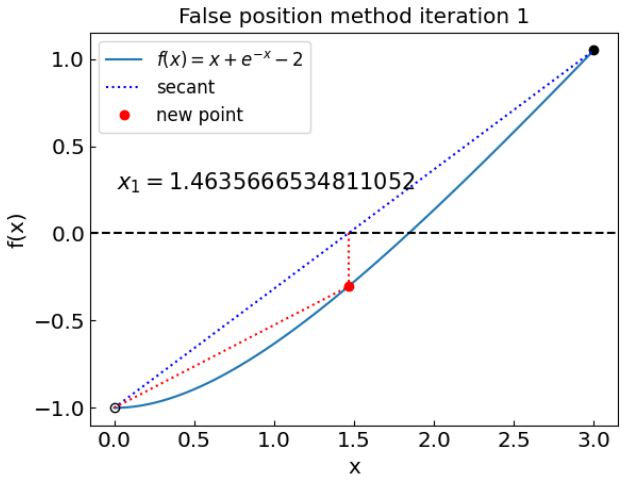
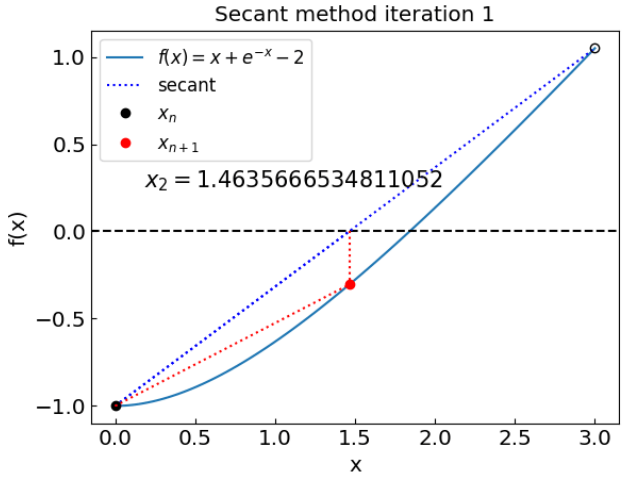
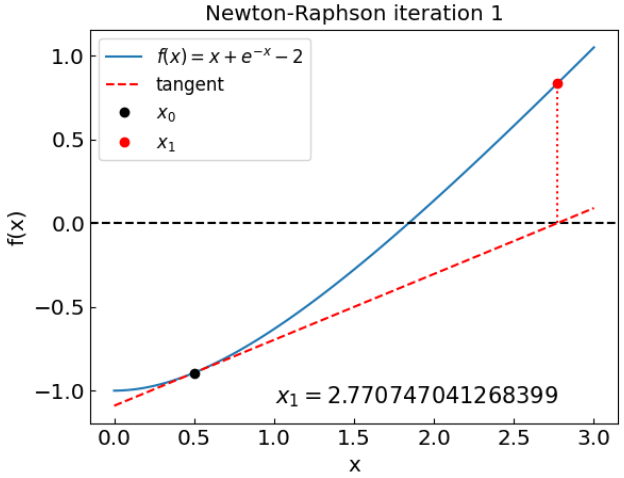
Summary


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

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

Secant method:
- Typically faster than bisection and false position
- May not always converge

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

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Systems of non-linear equations

$$
\begin{aligned}
f_1(x_1, \ldots, x_N) &= 0, \\
f_2(x_1, \ldots, x_N) &= 0, \\
&\ldots \\
f_N(x_1, \ldots, x_N) &= 0
\end{aligned}
$$

References: Chapter 9.6 of *Numerical Recipes Third Edition* by W.H. Press et al.

Systems of non-linear equations

Sometimes we need to solve a system of non-linear equations, e.g.

$$
\begin{aligned}
f_1(x_1, \ldots, x_N) &= 0, \\
f_2(x_1, \ldots, x_N) &= 0, \\
&\ldots \\
f_N(x_1, \ldots, x_N) &= 0
\end{aligned}
$$

Denoting $\mathbf{f} = (f_1, \ldots, f_N)$ and $\mathbf{x} = (x_1, \ldots, x_N)$ this can be written in compact form as

$$\mathbf{f}(\mathbf{x}) = 0 \, .$$

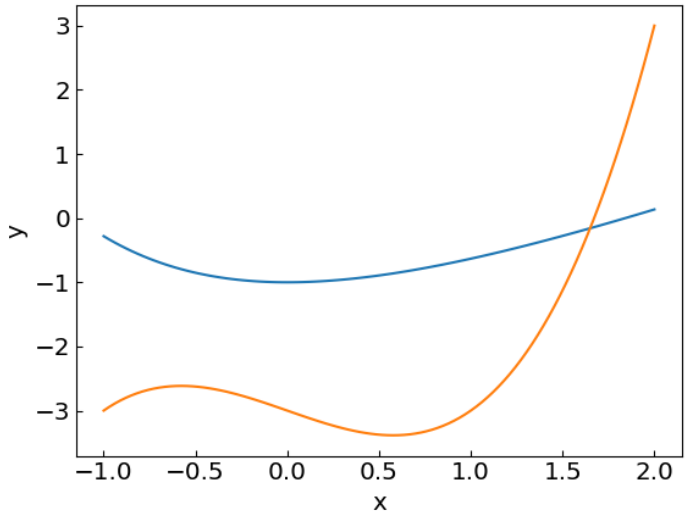
For example:

$$
\begin{aligned}
x + \exp(-x) - 2 - y &= 0, \\
x^3 - x - 3 - y &= 0.
\end{aligned}
$$

i.e.

$$f_1(x_1, x_2) = x_1 + \exp(-x_1) - 2 - x_2$$

$$f_2(x_1, x_2) = x_1^3 - x_1 - 3 - x_2$$



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Newton-Raphson method in multiple dimensions

Recall the Taylor expansion of function f around the root x^* in one-dimensional case:

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

The multi-dimensional version of this expansion reads

$$\mathbf{f}(\mathbf{x}^*) \approx \mathbf{f}(\mathbf{x}) + J(\mathbf{x})(\mathbf{x}^* - \mathbf{x})$$

Here $J(\mathbf{x})$ is the Jacobian, i.e. a $N \times N$ matrix of derivatives evaluated at $\mathbf{x}$

$$J_{ij}(\mathbf{x}) = \frac{\partial f_i}{\partial x_j} \ .$$

Given that $\mathbf{f}(\mathbf{x}^*) = 0$, we have

$$J(\mathbf{x})(\mathbf{x}^* - \mathbf{x}) \approx -\mathbf{f}(\mathbf{x}),$$

which is a system of linear equations for $\mathbf{x}^* - \mathbf{x}$. Solving this system yields

$$\mathbf{x}^* \approx \mathbf{x} - J^{-1}(\mathbf{x})\,\mathbf{f}(\mathbf{x}) \ .$$

Here $J^{-1}(\mathbf{x})$ is the inverse Jacobian matrix.

The multi-dimensional Newton's method is an iterative procedure

$$\mathbf{x_{n+1}} = \mathbf{x_n} - J^{-1}(\mathbf{x_n})\,\mathbf{f}(\mathbf{x_n}) \ .$$

Reduces to Newton's method in 1D $\quad x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$

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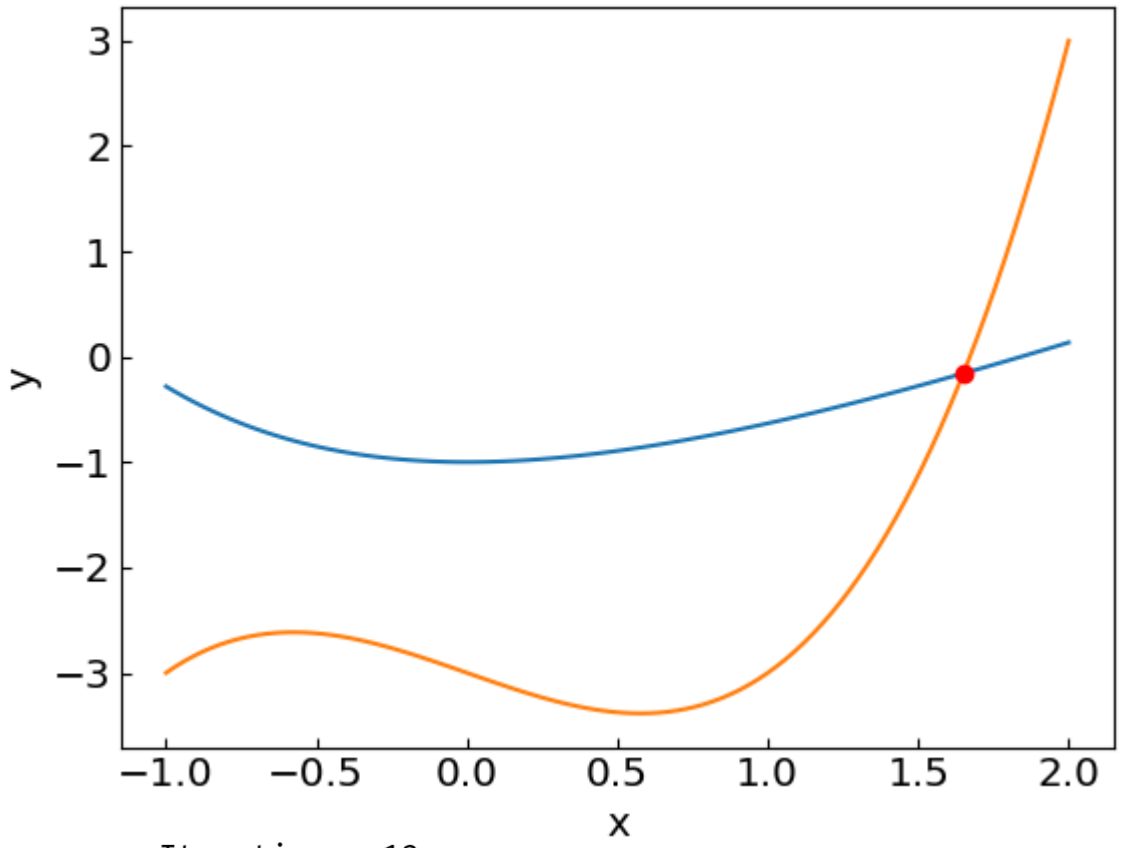
Newton-Raphson method in multiple dimensions

```python
def newton_method_multi(
    f,
    jacobian,
    x0,
    accuracy=1e-8,
    max_iterations=100):
    x = x0
    global last_newton_iterations
    last_newton_iterations = 0

    if newton_verbose:
        print("Iteration: ", last_newton_iterations)
        print("x = ", x0)
        print("f = ", f(x0))
        print("|f| = ", ftil(f(x0)))

    for i in range(max_iterations):
        last_newton_iterations += 1
        f_val = f(x)
        jac = jacobian(x)
        jinv = np.linalg.inv(jac)
        delta = np.dot(jinv, -f_val)
        x = x + delta

        if np.linalg.norm(delta, ord=2) < accuracy:
            return x
    return x
```




```
Iteration:  12
x =  [ 1.64998819 -0.15795963]
f =  [ 0.00000000e+00 -6.66133815e-16]
|f| =  2.2186712959340957e-31
```

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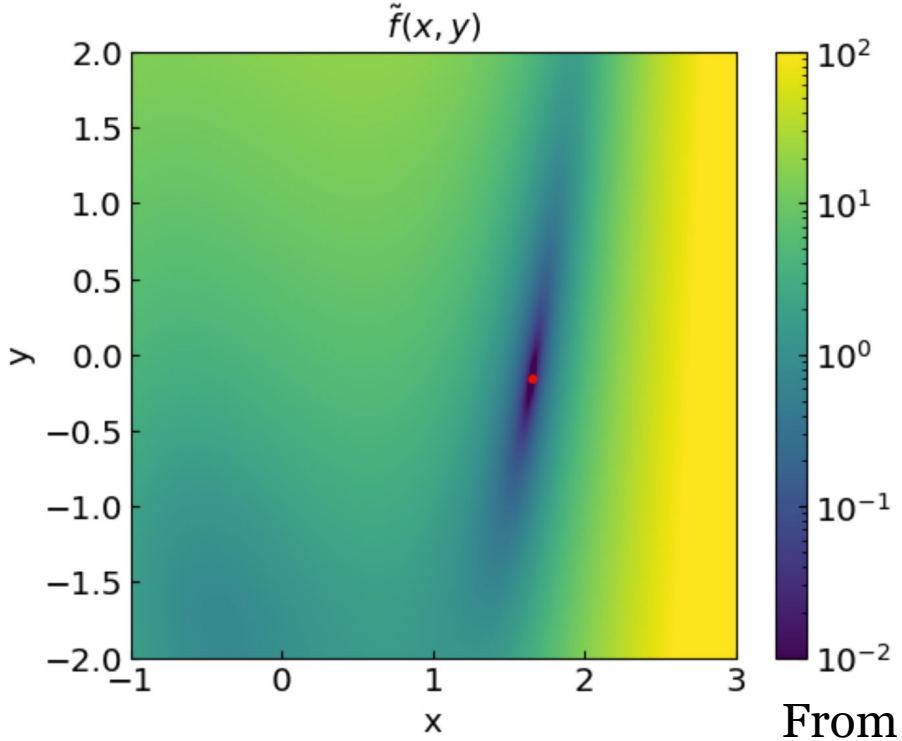
Newton-Raphson method in multiple dimensions

Introduce an objective function

$$\tilde{f}(\mathbf{x}) = \frac{\mathbf{f}(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x})}{2}$$

Its value is equal to zero (minimized) at the root



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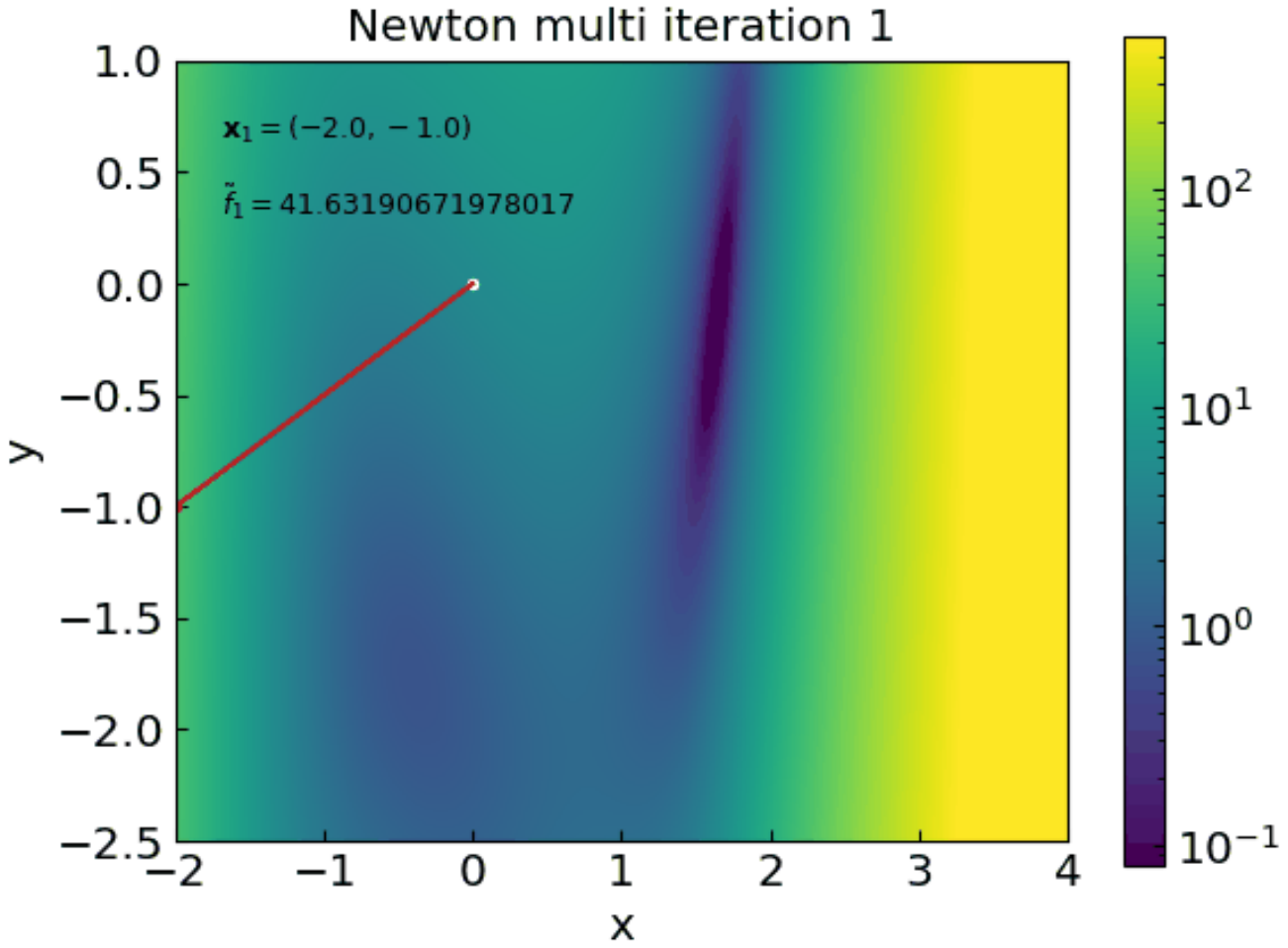
Newton-Raphson method in multiple dimensions



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Broyden method

Broyden method is a multi-dimensional generalization of the secant method

Secant method: $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$ with $f'(x_n) \simeq \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$

Broyden method: $\mathbf{x_{n+1}} = \mathbf{x_n} - J^{-1}(\mathbf{x_n})\,\mathbf{f}(\mathbf{x_n})$ with

The solution to $J(\mathbf{x_n})\,(\mathbf{x_n} - \mathbf{x_{n-1}}) \simeq \mathbf{f}(\mathbf{x_n}) - \mathbf{f}(\mathbf{x_{n-1}})$ is not unique

Broyden: $\mathbf{J}_n = \mathbf{J}_{n-1} + \frac{\Delta\mathbf{f}_n - \mathbf{J}_{n-1}\Delta\mathbf{x}_n}{\|\Delta\mathbf{x}_n\|^2}\Delta\mathbf{x}_n^{\mathrm{T}}$ with

$$\begin{aligned}\mathbf{f}_n &= \mathbf{f}(\mathbf{x}_n),\\ \Delta\mathbf{x}_n &= \mathbf{x}_n - \mathbf{x}_{n-1},\\ \Delta\mathbf{f}_n &= \mathbf{f}_n - \mathbf{f}_{n-1},\end{aligned}$$

For J_0 one can take the identity matrix or full Jacobian calculated once

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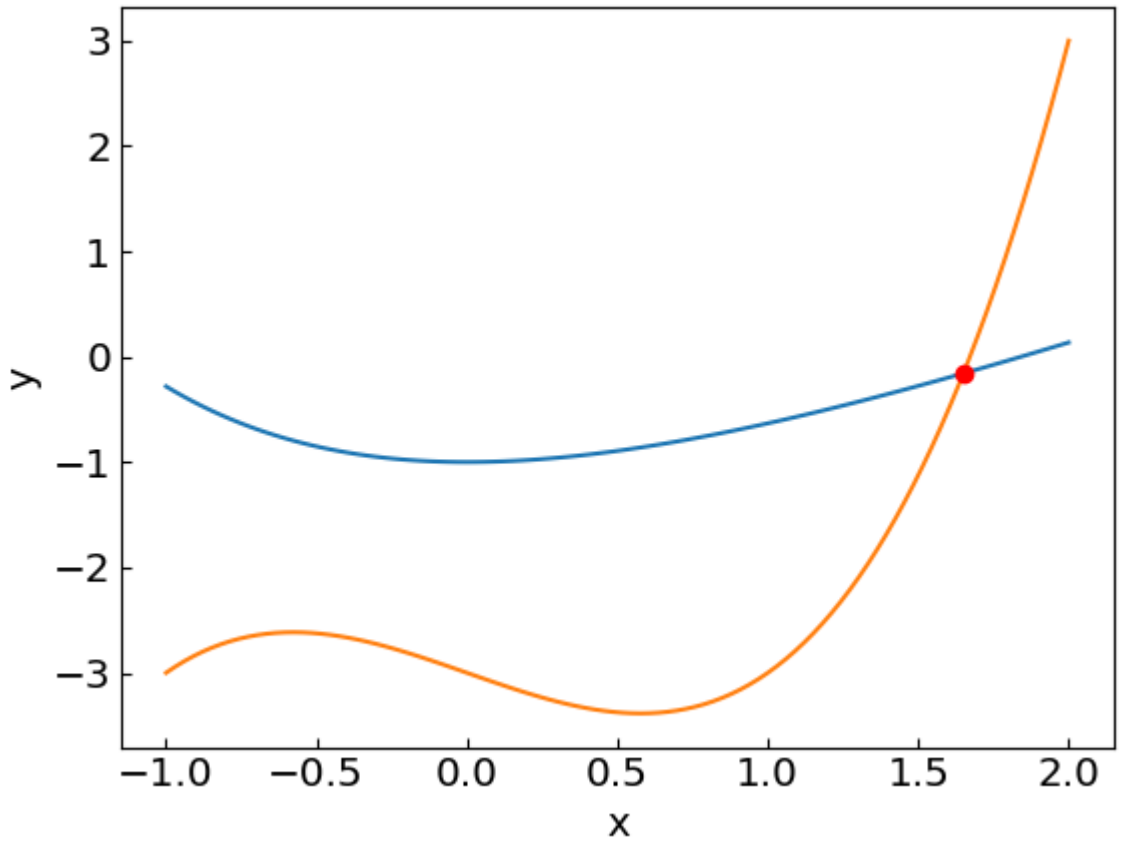
Broyden method (direct)

```python
# Direct implementation of Broyden's method
# (using matrix inversion at each step)
def broyden_method_direct(
    f,
    x0,
    accuracy=1e-8,
    max_iterations=100):
    global last_broyden_iterations
    last_broyden_iterations = 0
    x = x0
    n = x0.shape[0]
    J = np.eye(n)


    for i in range(max_iterations):
        last_broyden_iterations += 1
        f_val = f(x)
        Jinv = np.linalg.inv(J)
        delta = np.dot(Jinv, -f_val)
        x = x + delta
        if np.linalg.norm(delta, ord=2) < accuracy:
            return x
        f_new = f(x)
        u = f_new - f_val
        v = delta
        J = J + np.outer(u - J.dot(v), v) / np.dot(v, v)

    return x
```




```
Iteration:  54
x =  [ 1.64998819 -0.15795963]
f =  [ 2.97817326e-14 -4.50097265e-10]
|f| =  1.0129377443026415e-19
```

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Broyden method: avoid matrix inversion

$$\mathbf{J}_n = \mathbf{J}_{n-1} + \frac{\Delta \mathbf{f}_n - \mathbf{J}_{n-1}\Delta \mathbf{x}_n}{\|\Delta \mathbf{x}_n\|^2} \Delta \mathbf{x}_n^{\mathrm{T}}$$

Sherman-Morrison formula:

$$\mathbf{J}_n^{-1} = \mathbf{J}_{n-1}^{-1} + \frac{\Delta \mathbf{x}_n - \mathbf{J}_{n-1}^{-1}\Delta \mathbf{f}_n}{\Delta \mathbf{x}_n^{\mathrm{T}} \mathbf{J}_{n-1}^{-1} \Delta \mathbf{f}_n} \Delta \mathbf{x}_n^{\mathrm{T}} \mathbf{J}_{n-1}^{-1}$$

Update the inverse Jacobian directly!

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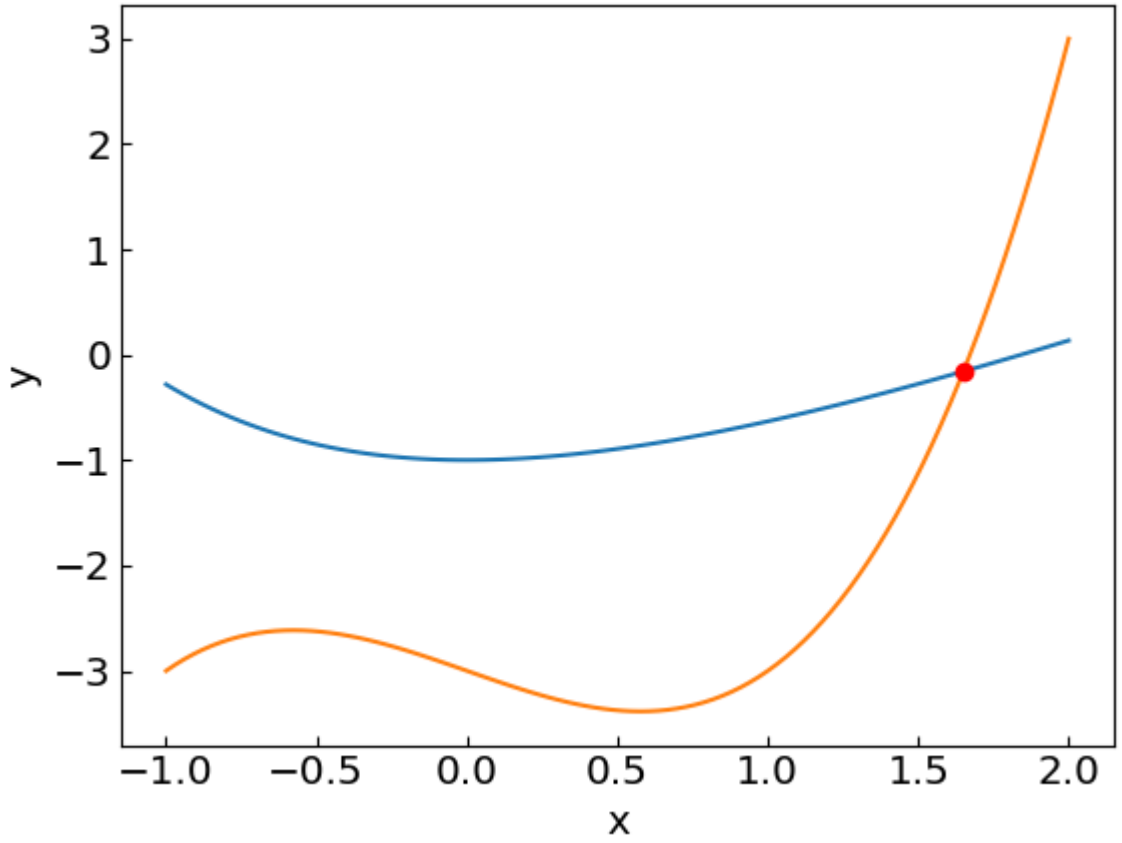
Broyden method (Sherman-Morrison)

```python
def broyden_method(
    f,
    x0,
    accuracy=1e-8,
    max_iterations=100):
    global last_broyden_iterations
    last_broyden_iterations = 0
    x = x0
    n = x0.shape[0]
    Jinv = np.eye(n)

    for i in range(max_iterations):
        last_broyden_iterations += 1
        f_val = f(x)
        delta = -Jinv.dot(f_val)
        x = x + delta
        if np.linalg.norm(delta, ord=2) < accuracy:
            return x
        f_new = f(x)
        df = f_new - f_val
        dx = delta
        Jinv = Jinv + np.outer(dx - Jinv.dot(df), dx.T.dot(Jinv))
        / np.dot(dx.T, Jinv.dot(df))

    return x
```




```
Iteration:  54
x =  [ 1.64998819 -0.15795963]
f =  [ 2.8255176e-14 -3.8877096e-10]
|f| =  7.557143001803891e-20
```

From the course by Volodymyr Vovchenko,
https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Broyden method vs Newton-Raphson method

Broyden method converges somewhat slower (e.g. 54 vs 12 iterations in our example) but:

- Does not involve the calculation of Jacobian
- Does not involve matrix inversion

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Broyden method vs Newton-Raphson method

Broyden method converges somewhat slower (e.g. 54 vs 12 iterations in our example) but:

- Does not involve the calculation of Jacobian
- Does not involve matrix inversion

Possible refinement: improve the initial estimate for the Jacobian

```
Iteration:  54
x =  [ 1.64998819 -0.15795963]
f =  [ 2.8255176e-14 -3.8877096e-10]
|f| =  7.557143001803891e-20
```

```
Iteration:  15
x =  [ 1.64998819 -0.15795963]
f =  [1.02683695e-11 1.31871458e-11]
|f| =  1.3967011340731408e-22
```

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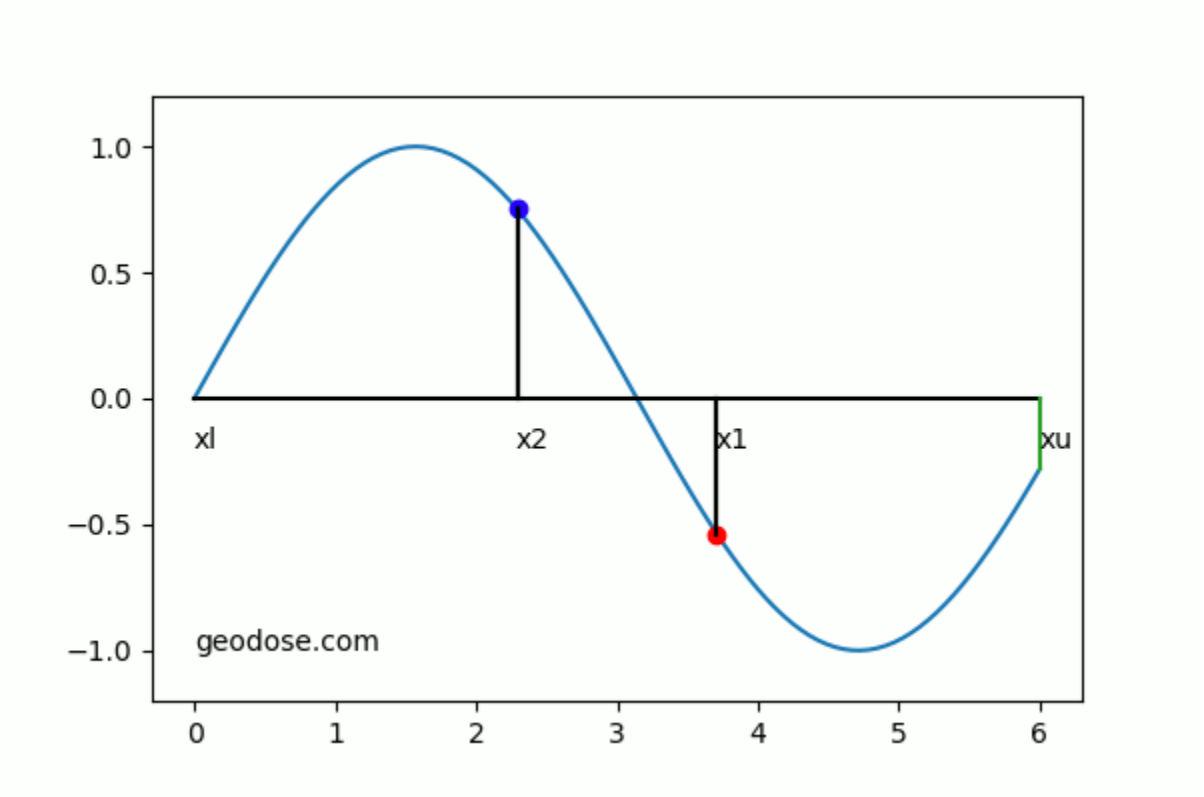
Function minimization/maximization



References: Chapter 6.4 of *Computational Physics* by Mark Newman
Chapter 10 of *Numerical Recipes Third Edition* by W.H. Press et al.

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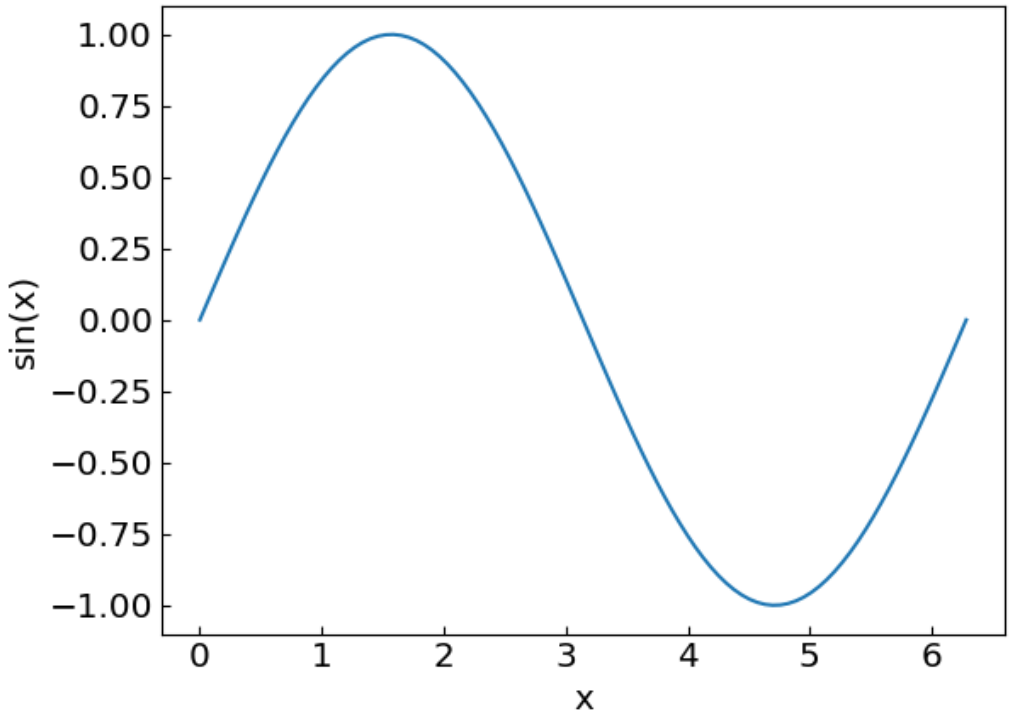
Function extrema

Often we are interested to find the minimum of a function (e.g. energy minimization)

Consider the minimum of f(x)=sin(x) on interval 0..2π



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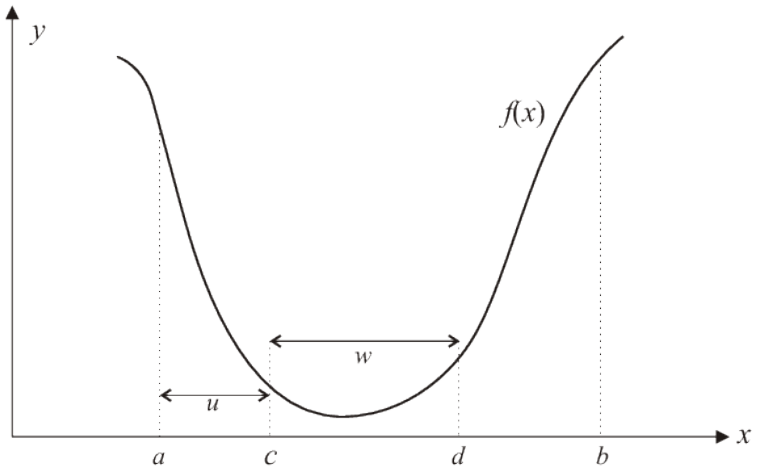
Golden section search

- Bracket the minimum x_{min} in (a,b)
- Take c = b – (b-a)/φ and d = a + (b-a)/φ
- if f(c)<f(d), take b = d as new right endpoint
- Otherwise, take a = c as new left endpoint
- Repeat over the new interval (a,b) until the desired accuracy is reached



$$\varphi = \frac{1+\sqrt{5}}{2} = 1.618\ldots$$ is the **golden ratio**

This value ensures that the interval decreases by factor φ no matter what

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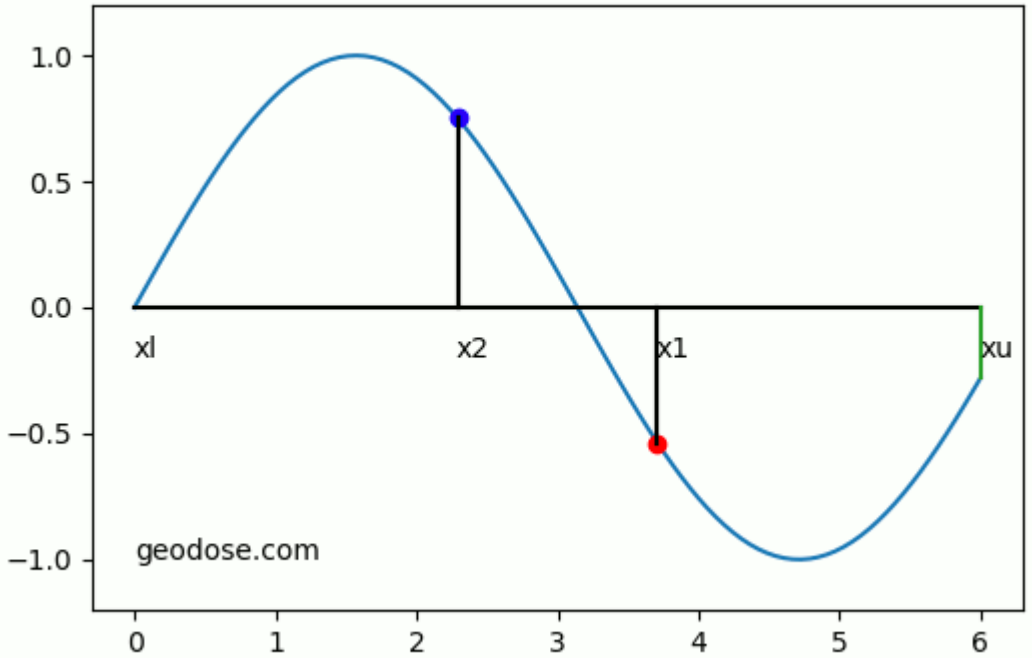
Golden section search

```
def gss(f, a, b, accuracy=1e-7):
    c = b - (b - a) / phi
    d = a + (b - a) / phi
    while abs(b - a) > accuracy:
        if f(c) < f(d):
            b = d
        else:
            a = c

        c = b - (b - a) / phi
        d = a + (b - a) / phi

    return (b + a) / 2
```




```
The minimum of sin(x) over the interval ( 0.0 , 6.283185307179586 ) is 4.712388990891052
```

To search for maximum of f(x) look for minimum of –f(x)

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Newton method

The extremum of f(x) is the root of the derivative, $f'(x) = 0$

Simply apply Newton-Raphson method for finding the root of $f'(x)$

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

$f''(x) > 0, \quad \rightarrow \quad$ minimum

$f''(x) < 0, \quad \rightarrow \quad$ maximum

```
def newton_extremum(f, df, d2f, x0, accuracy=1e-7, max_iterations=100):
    xprev = xnew = x0
    for i in range(max_iterations):
        xnew = xprev - df(xprev) / d2f(xprev)

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

        xprev = xnew
    return xnew
```

```
An extremum of sin(x) using Newton's method starting from x0 =  5.0  is ( 0.0 , 6.283185307179586 ) is 4.71238898038469
```

Gradient descent method

Replace, $f''(x)$ by a descent factor $1/\gamma_n$

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

```
def gradient_descent(f, df, x0, gam = 0.01, accuracy=1e-7, max_iterations=100):
    xprev  = x0
    for i in range(max_iterations):
        xnew = xprev - gam * df(xprev)

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

        xprev2 = xprev
        xprev = xnew
    return xnew
```

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Freedom in choosing γ_n

Can be generalized to multi-variable function $F(x_1,x_2,...)$

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \gamma_n \nabla F(\mathbf{x}_n)$$