Chem/BioE C142/242 Spring 2024 - Tutorial 1

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Outline:

- Visualizing univariate and multivariate functions
- Time your function
- Minimization using CG/BFGS
- Golden section example

Visualizing univariate and multivariate functions

```
In [1]: import numpy as np
import matplotlib.pyplot as plt

%matplotlib inline

In [2]: # Prior to Matplotlib 3.2.0, you will have to explicitly import Axes3D
    # to enable 3d plot
    from mpl_toolkits.mplot3d import Axes3D
```

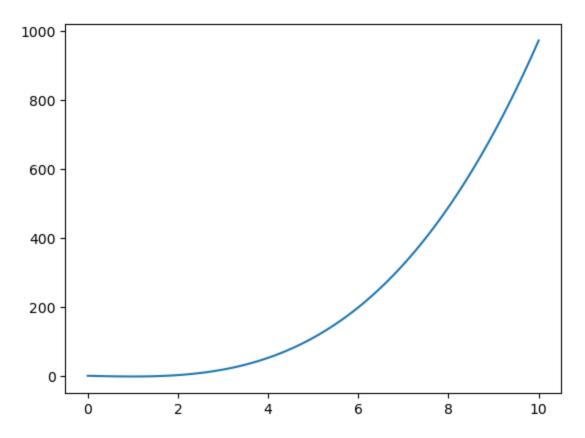
Univariate function

$$f(x) = x^3 - 3x + 2$$

```
In [3]: def func2d(x):
    f = x ** 3 - 3 * x + 2
    return f

In [4]: # to plot func
    x = np.linspace(0, 10, 100)
    y = func2d(x)
    plt.plot(x, y)
```

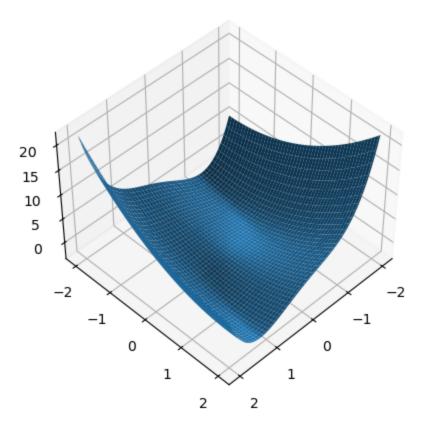
Out[4]: [<matplotlib.lines.Line2D at 0x19dd2e5cec0>]



Multivariate function

$$f(x,y) = x^4 - x^2 + y^2 - 2xy - 2$$

```
In [5]:    def func3d(x, y):
        return x ** 4 - x ** 2 + y ** 2 - 2 * x * y - 2
In [6]:    a = np.linspace(-2, 2, 100)
    x, y = np.meshgrid(a, a) # generate x, y grid
    fig = plt.figure()
    ax = fig.add_subplot(projection='3d')
    ax.plot_surface(x, y, func3d(x,y))
    ax.view_init(45,45)
```



Time your function

With a magic method

```
In [7]: def add(a, b):
    return a + b

%timeit add(1, 2)
```

55.4 ns \pm 2.04 ns per loop (mean \pm std. dev. of 7 runs, 10,000,000 loops each)

With decorators

Decorators wrap a function, and modify its behavior.

```
In [8]: import time

def timeit(f):

    def timed(*args, **kw):

        ts = time.time()
        result = f(*args, **kw)
        te = time.time()

        print(f'func:{f.__name__}} took: {te-ts:.4f} sec')
        return result
```

```
return timed

In [9]:  @timeit # equivalent to mysleep = timeit(mysleep)
def mysleep(sec):
    print("Sleeping...")
    time.sleep(sec)
    print("Wake up!")

mysleep(2)

Sleeping...
Wake up!
func:mysleep took: 2.0005 sec
```

Minimization using CG/BFGS

The multivariate Rosenbrock function is given below:

$$f(ec{x}) = \sum_{i=1}^{N-1} 100(x_{i+1} - x_i^2)^2 + (1 - x_i^2)^2$$

```
In [10]: def rosenbrock(X):
             Rosenbrock function
             Parameters
             X: np.ndarray
                  Input values
             Returns
             y: float
                 Output of Rosenbrock function with given X
             X2=X**2
             y = np.sum(100*(X[1:] - X2[:-1])**2 + (1 - X2[:-1])**2)
             return y
         def test rosenbrock():
             testX = np.array([1.0, 2.0])
             if rosenbrock(testX) == 100.0:
                  print("Well done!")
             else:
                  raise ValueError("Bad implementation")
         test_rosenbrock()
```

Well done!

Use x0 = np.array([1.3, 0.7, 0.8, 1.9, 1.2]) as a starting porint and find minimum

In [11]: from scipy.optimize import minimize

In [12]: ?minimize

```
Signature:
minimize(
    fun.
    x0,
    args=(),
   method=None,
    jac=None,
   hess=None,
   hessp=None,
    bounds=None,
    constraints=(),
   tol=None,
    callback=None,
    options=None,
Docstring:
Minimization of scalar function of one or more variables.
Parameters
-----
fun : callable
    The objective function to be minimized.
        ``fun(x, *args) -> float``
   where ``x`` is a 1-D array with shape (n,) and ``args``
    is a tuple of the fixed parameters needed to completely
    specify the function.
x0 : ndarray, shape (n,)
    Initial guess. Array of real elements of size (n,),
    where ``n`` is the number of independent variables.
args: tuple, optional
    Extra arguments passed to the objective function and its
    derivatives (`fun`, `jac` and `hess` functions).
method : str or callable, optional
    Type of solver. Should be one of
        - 'Nelder-Mead' :ref:`(see here) <optimize.minimize-neldermead>`
        - 'Powell' :ref:`(see here) <optimize.minimize-powell>`
        - 'CG'
                      :ref:`(see here) <optimize.minimize-cg>`
        - 'BFGS'
                      :ref:`(see here) <optimize.minimize-bfgs>`
        - 'Newton-CG' :ref:`(see here) <optimize.minimize-newtoncg>`
        - 'L-BFGS-B' :ref:`(see here) <optimize.minimize-lbfgsb>`
        - 'TNC'
                       :ref:`(see here) <optimize.minimize-tnc>`
        - 'COBYLA'
                      :ref:`(see here) <optimize.minimize-cobyla>`
        - 'SLSQP'
                      :ref:`(see here) <optimize.minimize-slsqp>`
        - 'trust-constr':ref:`(see here) <optimize.minimize-trustconstr>`
        - 'dogleg'
                   :ref:`(see here) <optimize.minimize-dogleg>`
        - 'trust-ncg'
                       :ref:`(see here) <optimize.minimize-trustncg>`
        - 'trust-exact' :ref:`(see here) <optimize.minimize-trustexact>`
        - 'trust-krylov' :ref:`(see here) <optimize.minimize-trustkrylov>`
        - custom - a callable object, see below for description.
    If not given, chosen to be one of ``BFGS``, ``L-BFGS-B``, ``SLSQP``,
    depending on whether or not the problem has constraints or bounds.
jac : {callable, '2-point', '3-point', 'cs', bool}, optional
```

Method for computing the gradient vector. Only for CG, BFGS, Newton-CG, L-BFGS-B, TNC, SLSQP, dogleg, trust-ncg, trust-krylov, trust-exact and trust-constr.

If it is a callable, it should be a function that returns the gradient vector:

```
``jac(x, *args) -> array like, shape (n,)``
```

where ``x`` is an array with shape (n,) and ``args`` is a tuple with the fixed parameters. If `jac` is a Boolean and is True, `fun` is assumed to return a tuple ``(f, g)`` containing the objective function and the gradient.

Methods 'Newton-CG', 'trust-ncg', 'dogleg', 'trust-exact', and 'trust-krylov' require that either a callable be supplied, or that `fun` return the objective and gradient.

If None or False, the gradient will be estimated using 2-point finite difference estimation with an absolute step size.

Alternatively, the keywords {'2-point', '3-point', 'cs'} can be used to select a finite difference scheme for numerical estimation of the gradient with a relative step size. These finite difference schemes obey any specified `bounds`.

hess: {callable, '2-point', '3-point', 'cs', HessianUpdateStrategy}, optional Method for computing the Hessian matrix. Only for Newton-CG, dogleg, trust-ncg, trust-krylov, trust-exact and trust-constr.

If it is callable, it should return the Hessian matrix:

```
``hess(x, *args) -> {LinearOperator, spmatrix, array}, (n, n)``
```

where ``x`` is a (n,) ndarray and ``args`` is a tuple with the fixed parameters.

The keywords {'2-point', '3-point', 'cs'} can also be used to select a finite difference scheme for numerical estimation of the hessian. Alternatively, objects implementing the `HessianUpdateStrategy` interface can be used to approximate the Hessian. Available quasi-Newton methods implementing this interface are:

- `BFGS`;
- `SR1`.

Not all of the options are available for each of the methods; for availability refer to the notes.

hessp : callable, optional

Hessian of objective function times an arbitrary vector p. Only for Newton-CG, trust-ncg, trust-krylov, trust-constr.

Only one of `hessp` or `hess` needs to be given. If `hess` is provided, then `hessp` will be ignored. `hessp` must compute the Hessian times an arbitrary vector:

```
``hessp(x, p, *args) -> ndarray shape (n,)``
```

where ``x`` is a (n,) ndarray, ``p`` is an arbitrary vector with dimension (n,) and ``args`` is a tuple with the fixed parameters.

bounds : sequence or `Bounds`, optional

Bounds on variables for Nelder-Mead, L-BFGS-B, TNC, SLSQP, Powell, trust-constr, and COBYLA methods. There are two ways to specify the

bounds:

1. Instance of `Bounds` class.

2. Sequence of ``(min, max)`` pairs for each element in `x`. None is used to specify no bound.

constraints : {Constraint, dict} or List of {Constraint, dict}, optional
 Constraints definition. Only for COBYLA, SLSQP and trust-constr.

Constraints for 'trust-constr' are defined as a single object or a list of objects specifying constraints to the optimization problem. Available constraints are:

- `LinearConstraint`
- `NonlinearConstraint`

Constraints for COBYLA, SLSQP are defined as a list of dictionaries. Each dictionary with fields:

type : str
 Constraint type: 'eq' for equality, 'ineq' for inequality.
fun : callable
 The function defining the constraint.
jac : callable, optional
 The Jacobian of `fun` (only for SLSQP).
args : sequence, optional
 Extra arguments to be passed to the function and Jacobian.

Equality constraint means that the constraint function result is to be zero whereas inequality means that it is to be non-negative. Note that COBYLA only supports inequality constraints.

tol : float, optional

Tolerance for termination. When `tol` is specified, the selected minimization algorithm sets some relevant solver-specific tolerance(s) equal to `tol`. For detailed control, use solver-specific options.

options : dict, optional

A dictionary of solver options. All methods except `TNC` accept the following generic options:

maxiter : int

Maximum number of iterations to perform. Depending on the method each iteration may use several function evaluations.

For `TNC` use `maxfun` instead of `maxiter`. disp : bool
Set to True to print convergence messages.

For method-specific options, see :func:`show_options()`.
callback : callable, optional

A callable called after each iteration.

All methods except TNC, SLSQP, and COBYLA support a callable with the signature:

``callback(intermediate result: OptimizeResult)``

where ``intermediate_result`` is a keyword parameter containing an `OptimizeResult` with attributes ``x`` and ``fun``, the present values of the parameter vector and objective function. Note that the name of the parameter must be ``intermediate_result`` for the callback to be passed an `OptimizeResult`. These methods will also terminate if the callback raises ``StopIteration``.

All methods except trust-constr (also) support a signature like:

```
``callback(xk)``
```

where ``xk`` is the current parameter vector.

Introspection is used to determine which of the signatures above to invoke.

Returns

res: OptimizeResult

The optimization result represented as a ``OptimizeResult`` object. Important attributes are: ``x`` the solution array, ``success`` a Boolean flag indicating if the optimizer exited successfully and ``message`` which describes the cause of the termination. See `OptimizeResult` for a description of other attributes.

See also

minimize_scalar : Interface to minimization algorithms for scalar univariate functions show options : Additional options accepted by the solvers

Notes

_ _ _ _

This section describes the available solvers that can be selected by the 'method' parameter. The default method is *BFGS*.

Unconstrained minimization

Method :ref:`CG <optimize.minimize-cg>` uses a nonlinear conjugate gradient algorithm by Polak and Ribiere, a variant of the Fletcher-Reeves method described in [5]_ pp.120-122. Only the first derivatives are used.

Method :ref:`BFGS <optimize.minimize-bfgs>` uses the quasi-Newton method of Broyden, Fletcher, Goldfarb, and Shanno (BFGS) [5]_pp. 136. It uses the first derivatives only. BFGS has proven good performance even for non-smooth optimizations. This method also returns an approximation of the Hessian inverse, stored as `hess inv` in the OptimizeResult object.

Method :ref:`Newton-CG <optimize.minimize-newtoncg>` uses a Newton-CG algorithm [5]_ pp. 168 (also known as the truncated Newton method). It uses a CG method to the compute the search direction. See also *TNC* method for a box-constrained minimization with a similar algorithm. Suitable for large-scale

problems.

Method :ref:`dogleg <optimize.minimize-dogleg>` uses the dog-leg trust-region algorithm [5]_ for unconstrained minimization. This algorithm requires the gradient and Hessian; furthermore the Hessian is required to be positive definite.

Method :ref:`trust-ncg <optimize.minimize-trustncg>` uses the Newton conjugate gradient trust-region algorithm [5]_ for unconstrained minimization. This algorithm requires the gradient and either the Hessian or a function that computes the product of the Hessian with a given vector. Suitable for large-scale problems.

Method :ref:`trust-krylov <optimize.minimize-trustkrylov>` uses
the Newton GLTR trust-region algorithm [14]_, [15]_ for unconstrained
minimization. This algorithm requires the gradient
and either the Hessian or a function that computes the product of
the Hessian with a given vector. Suitable for large-scale problems.
On indefinite problems it requires usually less iterations than the
`trust-ncg` method and is recommended for medium and large-scale problems.

Method :ref:`trust-exact <optimize.minimize-trustexact>`
is a trust-region method for unconstrained minimization in which
quadratic subproblems are solved almost exactly [13]_. This
algorithm requires the gradient and the Hessian (which is
not required to be positive definite). It is, in many
situations, the Newton method to converge in fewer iterations
and the most recommended for small and medium-size problems.

Bound-Constrained minimization

Method :ref:`Nelder-Mead <optimize.minimize-neldermead>` uses the Simplex algorithm [1]_, [2]_. This algorithm is robust in many applications. However, if numerical computation of derivative can be trusted, other algorithms using the first and/or second derivatives information might be preferred for their better performance in general.

Method :ref:`L-BFGS-B <optimize.minimize-lbfgsb>` uses the L-BFGS-B algorithm [6]_, [7]_ for bound constrained minimization.

Method :ref:`Powell <optimize.minimize-powell>` is a modification of Powell's method [3]_, [4]_ which is a conjugate direction method. It performs sequential one-dimensional minimizations along each vector of the directions set (`direc` field in `options` and `info`), which is updated at each iteration of the main minimization loop. The function need not be differentiable, and no derivatives are taken. If bounds are not provided, then an unbounded line search will be used. If bounds are provided and the initial guess is within the bounds, then every function evaluation throughout the minimization procedure will be within the bounds. If bounds are provided, the initial guess is outside the bounds, and `direc` is full rank (default has full rank), then some function evaluations during the first iteration may be outside the bounds, but every function evaluation after the first iteration will be within the bounds. If `direc` is not full rank,

then some parameters may not be optimized and the solution is not guaranteed to be within the bounds.

Method :ref:`TNC <optimize.minimize-tnc>` uses a truncated Newton algorithm [5]_, [8]_ to minimize a function with variables subject to bounds. This algorithm uses gradient information; it is also called Newton Conjugate-Gradient. It differs from the *Newton-CG* method described above as it wraps a C implementation and allows each variable to be given upper and lower bounds.

Constrained Minimization

Method :ref:`COBYLA <optimize.minimize-cobyla>` uses the Constrained Optimization BY Linear Approximation (COBYLA) method [9]_, [10]_, [11]_. The algorithm is based on linear approximations to the objective function and each constraint. The method wraps a FORTRAN implementation of the algorithm. The constraints functions 'fun' may return either a single number or an array or list of numbers.

Method :ref:`SLSQP <optimize.minimize-slsqp>` uses Sequential Least SQuares Programming to minimize a function of several variables with any combination of bounds, equality and inequality constraints. The method wraps the SLSQP Optimization subroutine originally implemented by Dieter Kraft [12]_. Note that the wrapper handles infinite values in bounds by converting them into large floating values.

Method :ref:`trust-constr <optimize.minimize-trustconstr>` is a trust-region algorithm for constrained optimization. It switches between two implementations depending on the problem definition. It is the most versatile constrained minimization algorithm implemented in SciPy and the most appropriate for large-scale problems. For equality constrained problems it is an implementation of Byrd-Omojokun Trust-Region SQP method described in [17]_ and in [5]_, p. 549. When inequality constraints are imposed as well, it switches to the trust-region interior point method described in [16]_. This interior point algorithm, in turn, solves inequality constraints by introducing slack variables and solving a sequence of equality-constrained barrier problems for progressively smaller values of the barrier parameter. The previously described equality constrained SQP method is used to solve the subproblems with increasing levels of accuracy as the iterate gets closer to a solution.

Finite-Difference Options

For Method :ref:`trust-constr <optimize.minimize-trustconstr>`
the gradient and the Hessian may be approximated using
three finite-difference schemes: {'2-point', '3-point', 'cs'}.
The scheme 'cs' is, potentially, the most accurate but it
requires the function to correctly handle complex inputs and to
be differentiable in the complex plane. The scheme '3-point' is more
accurate than '2-point' but requires twice as many operations. If the
gradient is estimated via finite-differences the Hessian must be
estimated using one of the quasi-Newton strategies.

Method specific options for the `hess` **keyword**

+ method/Hess	None	callable	+ '2-point/'3-point'/'cs'	++ HUS
Newton-CG	j i	(n, n) LO		x
		(n, n)		
trust-ncg		(n, n)	x	x
trust-krylov		(n, n)	x	x
trust-exact		(n, n)		
trust-constr			x 	x

where LO=LinearOperator, sp=Sparse matrix, HUS=HessianUpdateStrategy

It may be useful to pass a custom minimization method, for example when using a frontend to this method such as `scipy.optimize.basinhopping` or a different library. You can simply pass a callable as the ``method`` parameter.

The callable is called as ``method(fun, x0, args, **kwargs, **options)`` where ``kwargs`` corresponds to any other parameters passed to `minimize` (such as `callback`, `hess`, etc.), except the `options` dict, which has its contents also passed as `method` parameters pair by pair. Also, if `jac` has been passed as a bool type, `jac` and `fun` are mangled so that `fun` returns just the function values and `jac` is converted to a function returning the Jacobian. The method shall return an `OptimizeResult` object.

The provided `method` callable must be able to accept (and possibly ignore) arbitrary parameters; the set of parameters accepted by `minimize` may expand in future versions and then these parameters will be passed to the method. You can find an example in the scipy.optimize tutorial.

References

- .. [1] Nelder, J A, and R Mead. 1965. A Simplex Method for Function Minimization. The Computer Journal 7: 308-13.
- .. [2] Wright M H. 1996. Direct search methods: Once scorned, now respectable, in Numerical Analysis 1995: Proceedings of the 1995 Dundee Biennial Conference in Numerical Analysis (Eds. D F Griffiths and G A Watson). Addison Wesley Longman, Harlow, UK. 191-208.
- .. [3] Powell, M J D. 1964. An efficient method for finding the minimum of a function of several variables without calculating derivatives. The Computer Journal 7: 155-162.

^{**}Custom minimizers**

.. [4] Press W, S A Teukolsky, W T Vetterling and B P Flannery. Numerical Recipes (any edition), Cambridge University Press.

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- .. [8] Nash, S G. Newton-Type Minimization Via the Lanczos Method. 1984. SIAM Journal of Numerical Analysis 21: 770-778.
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- .. [13] Conn, A. R., Gould, N. I., and Toint, P. L. Trust region methods. 2000. Siam. pp. 169-200.
- .. [14] F. Lenders, C. Kirches, A. Potschka: "trlib: A vector-free implementation of the GLTR method for iterative solution of the trust region problem", :arxiv:`1611.04718`
- .. [15] N. Gould, S. Lucidi, M. Roma, P. Toint: "Solving the Trust-Region Subproblem using the Lanczos Method", SIAM J. Optim., 9(2), 504--525, (1999).
- .. [16] Byrd, Richard H., Mary E. Hribar, and Jorge Nocedal. 1999. An interior point algorithm for large-scale nonlinear programming. SIAM Journal on Optimization 9.4: 877-900.
- .. [17] Lalee, Marucha, Jorge Nocedal, and Todd Plantega. 1998. On the implementation of an algorithm for large-scale equality constrained optimization. SIAM Journal on Optimization 8.3: 682-706.

Examples

_ _ _ _ _ _ _

Let us consider the problem of minimizing the Rosenbrock function. This function (and its respective derivatives) is implemented in `rosen` (resp. `rosen_der`, `rosen_hess`) in the `scipy.optimize`.

>>> from scipy.optimize import minimize, rosen, rosen_der

A simple application of the *Nelder-Mead* method is:

```
>>> x0 = [1.3, 0.7, 0.8, 1.9, 1.2]
>>> res = minimize(rosen, x0, method='Nelder-Mead', tol=1e-6)
>>> res.x
array([ 1.,  1.,  1.,  1.])
```

Now using the *BFGS* algorithm, using the first derivative and a few

```
options:
        >>> res = minimize(rosen, x0, method='BFGS', jac=rosen der,
                           options={'gtol': 1e-6, 'disp': True})
        Optimization terminated successfully.
                 Current function value: 0.000000
                 Iterations: 26
                 Function evaluations: 31
                 Gradient evaluations: 31
        >>> res.x
        array([ 1., 1., 1., 1.])
        >>> print(res.message)
        Optimization terminated successfully.
        >>> res.hess_inv
        array([
            [ 0.00749589, 0.01255155, 0.02396251, 0.04750988, 0.09495377], # may vary
            [0.01255155, 0.02510441, 0.04794055, 0.09502834, 0.18996269],
            [0.02396251, 0.04794055, 0.09631614, 0.19092151, 0.38165151],
            [ 0.04750988, 0.09502834, 0.19092151, 0.38341252, 0.7664427 ],
            [ 0.09495377, 0.18996269, 0.38165151, 0.7664427, 1.53713523]
        ])
        Next, consider a minimization problem with several constraints (namely
        Example 16.4 from [5]_). The objective function is:
        >>> fun = lambda x: (x[0] - 1)**2 + (x[1] - 2.5)**2
        There are three constraints defined as:
        >>> cons = ({'type': 'ineq', 'fun': lambda x: x[0] - 2 * x[1] + 2},
                    {'type': 'ineq', 'fun': lambda x: -x[0] - 2 * x[1] + 6},
                    {'type': 'ineq', 'fun': lambda x: -x[0] + 2 * x[1] + 2})
        And variables must be positive, hence the following bounds:
        >>> bnds = ((0, None), (0, None))
        The optimization problem is solved using the SLSQP method as:
        >>> res = minimize(fun, (2, 0), method='SLSQP', bounds=bnds,
                           constraints=cons)
        It should converge to the theoretical solution (1.4, 1.7).
        File:
                   c:\users\artui\miniforge3\envs\c242\lib\site-packages\scipy\optimize\_min
        imize.py
        Type:
                   function
         More on optimization: Scipy tutorial on optimization
In [13]: @timeit
         def minimize_rosenbrock(x0, method):
             Minimize Rosenbrock function
             Parameters
```

```
x0: np.ndarray
                 Starting point
             method: str
                 Method for minimization
             Returns
              _ _ _ _ _ _
             res: OptimzizeResult
                  Result object of scipy optimization
             res = minimize(rosenbrock, x0, method=method, options={"gtol": 1e-5, "disp": Tr
             return res
In [14]: x0 = np.array([1.3, 0.7, 0.8, 1.9, 1.2])
In [15]: res = minimize_rosenbrock(x0, "CG")
         print(res.nit)
                 Current function value: 0.000000
                 Iterations: 54
                 Function evaluations: 882
                 Gradient evaluations: 145
        func:minimize_rosenbrock took: 0.0515 sec
        C:\Users\artui\miniforge3\envs\c242\Lib\site-packages\scipy\optimize\_minimize.py:70
        6: OptimizeWarning: Desired error not necessarily achieved due to precision loss.
          res = _minimize_cg(fun, x0, args, jac, callback, **options)
In [16]: res = minimize_rosenbrock(x0, "BFGS")
         print(res.nit)
        Optimization terminated successfully.
                 Current function value: 0.000000
                 Iterations: 21
                 Function evaluations: 150
                 Gradient evaluations: 25
        func:minimize_rosenbrock took: 0.0130 sec
        21
```

Golden section example

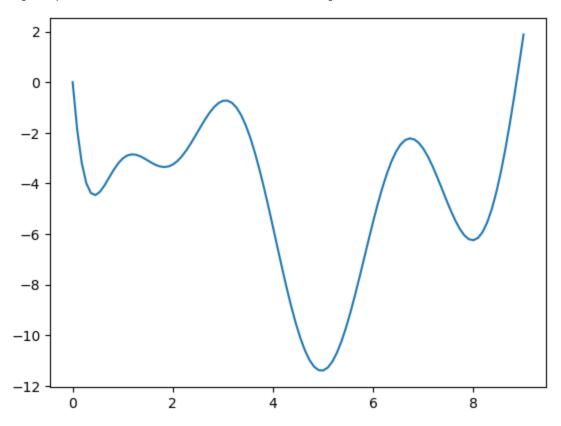
Given the following function, can you find its minimum value in range $\left[0,9\right]$ using golden section?

```
In [17]: def func(x):
    isarray = type(x) is np.ndarray
    coefs = np.array([
        8.0013714770, -24.06731415, 37.07604400, 0.00000000000, -43.86909846,
        44.427011010, -22.01262040, 6.536434989, -1.248082478, 0.157159012,
        -0.012990941, 0.000678657, -2.03269E-05, 2.66065E-07
    ])
    base = np.zeros((len(x) if isarray else 1, 14))
    for i in range(1, 14):
```

```
base[:,i] += x ** i
result = base.dot(coefs)
return result if isarray else np.sum(result)
```

```
In [18]: x = np.linspace(0, 9, 100)
plt.plot(x, func(x))
```

Out[18]: [<matplotlib.lines.Line2D at 0x19dd4949fd0>]



```
In [19]: def golden_section(func, start, end, reference, tol):
             if end - start < tol:</pre>
                  return {'x':reference, 'y':func(reference)}
             else:
                  if reference - start < end - reference:</pre>
                      new reference = end - (end - reference) * 0.618
                      if func(new_reference) > func(reference):
                          return golden_section(func, start, new_reference, reference, tol)
                      else:
                          return golden_section(func, reference, end, new_reference, tol)
                  else:
                      new_reference = start + (reference - start) * 0.618
                      if func(new_reference) > func(reference):
                          return golden_section(func, new_reference, end, reference, tol)
                      else:
                          return golden_section(func, start, reference, new_reference, tol)
```

```
In [20]: golden_section(func, 0, 9, 9*0.618, 1e-5)
```

Out[20]: {'x': 4.9642569571739665, 'y': -11.400276695145294}

In []: