week01-02-optimization-and-derivatives

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- 1 George McNinch Math 87 Spring 2025
- 2 § Week 2
- 3 Optimization & derivatives of functions
- 4 Using code to calculate derivatives

In our discussion of the oil spill problem, you may have been disappointed to have to do calculations with paper-and-pencil.

There are two possible ways around this, which I'd like to discuss briefly (with examples).

- We can use software for symbolic calculation of derivatives.
- Alternatively, we can *numerically approximate* derivatives.

This notebook will discuss these possibilities. For each method, we first treat some simple examples, and then we apply the method to the oil spill problem.

5 Symbolic calculations

First, let's investige how python can make symbolic calculations using the sympy package.

For more details about symbolic calculations in python consult the symbolic mathematics package.

5.1 A simple example

Let's find and classify the critical points for the cubic polynomial

$$G(t) = t^3 - 4t^2 - 5t - 2.$$

Let's import the sympy package, and declare tt to be a symbol:

```
[35]: import sympy as sp
sp.init_printing()

tt = sp.Symbol('t')
```

We now define the function G, and we create a corresponding symbolic version of G by evaluating the function G at the symbol tt.

[36]:
$$t^3 - 4t^2 - 5t - 2$$

Now we symbolically find the first and second derivative of G, using the function diff from the sympy package:

For example, we can see the first derivative:

- [38]: DGs
- [38]: $3t^2 8t 5$

Now we use the sympy solver to find the critical points of G - i.e the solutions of the equation DGs == 0

- [40]: list(map(lambda c: c.evalf(),crits))
- [40]: [-0.522588120943341, 3.18925478761001]

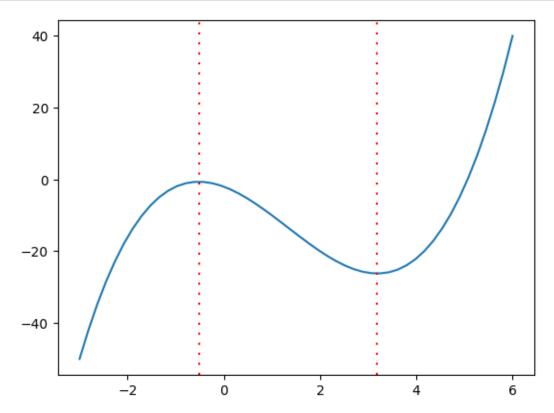
Using the fuction lambdify, we make an actual function DDG out of the symbolic expression DDGs and apply this function to each critical point:

[41]:
$$\left[-2\sqrt{31}, \ 2\sqrt{31}\right]$$

Since the value of DDG is negative at the first critical point, we see that G has a local max at $t = \frac{4}{3} - \frac{\sqrt{31}}{3}$.

Similarly, G has a local min at $t = \frac{4}{3} + \frac{\sqrt{31}}{3}$.

We confirm this with a sketch of the graph of G:



5.2 A trig example

Let $H1(t) = \sin(5t)$ and $H2(t) = \sin(5t + 3\pi/8)$. Let's classify the critical points of H1(t) and H2(t) on the interval $[-\pi, \pi]$.

This time, we use the sin function from the sympy library.

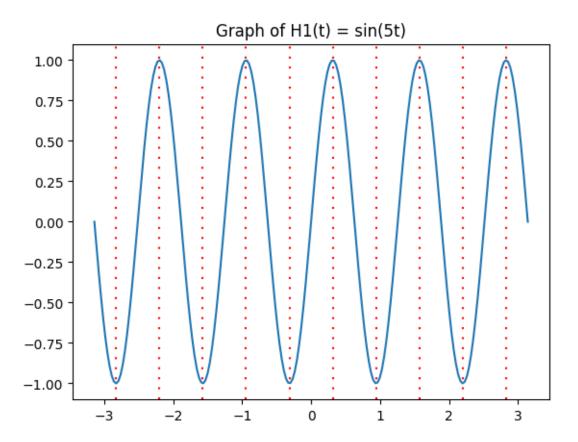
```
[43]: import sympy as sp
sp.init_printing()

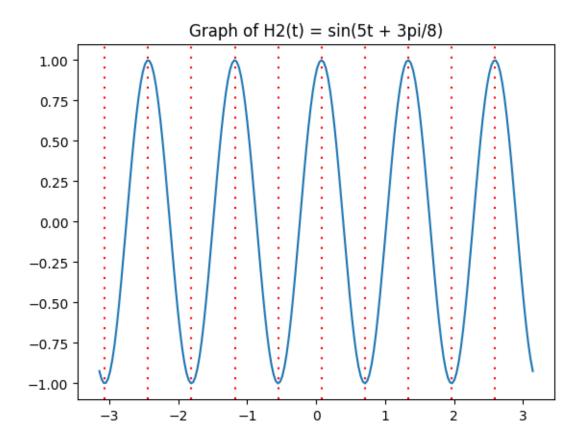
tt = sp.Symbol('t')

H1s = sp.sin(5*tt)
```

```
H2s = sp.sin(5*tt + 3*sp.S.Pi/8)
[44]: DH1s = sp.diff(H1s)
        DH1s
[44]: 5\cos{(5t)}
[45]: DH2s = sp.diff(H2s)
        DH2s
[45]:
       5\cos\left(5t + \frac{3\pi}{8}\right)
[46]: DDH1s = sp.diff(DH1s)
        DDH1s
[46]: -25\sin{(5t)}
[47]: DDH2s = sp.diff(DH2s)
        DDH2s
[47]: -25\sin\left(5t + \frac{3\pi}{8}\right)
       Now, we want to find the critical points in the interval [-\pi, \pi]. For this, we first define this interval
       and use the solveset function to find the solutions to DHs==0 on this interval:
[48]: int = sp.sets.sets.Interval(-np.pi,np.pi)
        crits1 = sp.solveset(DH1s,tt,domain=int)
        list(crits1)
-\frac{7\pi}{10}, -\frac{\pi}{2}, -\frac{3\pi}{10}, -\frac{\pi}{10}, \frac{\pi}{10}, \frac{3\pi}{10}, \frac{\pi}{2}, \frac{7\pi}{10}, \frac{9\pi}{10}
[49]: crits2 = sp.solveset(DH2s,tt,domain=int)
        crits2
\left\{-\frac{39\pi}{40}, -\frac{31\pi}{40}, -\frac{23\pi}{40}, -\frac{3\pi}{8}, -\frac{7\pi}{40}, \frac{\pi}{40}, \frac{9\pi}{40}, \frac{17\pi}{40}, \frac{5\pi}{8}, \frac{33\pi}{40}\right\}
       We now use the second derivative test to classify the critical points as a (local) min or max
[50]: def classify(DD,cp):
              if DD.subs(tt,cp)>0:
                    return "min"
              elif DD.subs(tt,cp)<0:</pre>
                    return "max"
              else: return "inconclusive"
        list(map(lambda x: (x,classify(DDH1s,x)),crits1.evalf()))
```

```
[50]: [(-2.82743338823081, 'min'),
       (-2.19911485751286, 'max'),
       (-1.57079632679490, 'min'),
       (-0.942477796076938, 'max'),
       (-0.314159265358979, 'min'),
       (0.314159265358979, 'max'),
       (0.942477796076938, 'min'),
       (1.57079632679490, 'max'),
       (2.19911485751286, 'min'),
       (2.82743338823081, 'max')]
[51]: results = list(map(lambda x: (x,classify(DDH2s,x)),crits2.evalf()))
      results
[51]: [(-3.06305283725005, 'min'),
       (-2.43473430653209, 'max'),
       (-1.80641577581413, 'min'),
       (-1.17809724509617, 'max'),
       (-0.549778714378214, 'min'),
       (0.0785398163397448, 'max'),
       (0.706858347057703, 'min'),
       (1.33517687777566, 'max'),
       (1.96349540849362, 'min'),
       (2.59181393921158, 'max')]
     Let's confirm our classification using graphs:
[52]: import matplotlib.pyplot as plt
      import numpy as np
      t1 = np.linspace(-np.pi,np.pi,200)
      def H1(t): return np.sin(5*t)
      def H2(t): return np.sin(5*t + 3*np.pi/8)
      fig, ax = plt.subplots()
      ax.set_title("Graph of H1(t) = sin(5t)")
      ax.plot(tl,H1(tl),label="H1")
      for t in crits1:
              ax.axvline(x=t, color="red", dashes=[1,4])
```





5.3 Return to the "oil spill" problem

Recall the python expressions for the main function of interest:

• \$C_{tot}(n) \$ c.cost(n)

We will make a "symbolic variable" we'll call y.

We would like to make a symbolic version the python function c.cost(n) by valuation at n=y.

Unfortunately, our definition of c.cost(n) involved a test of inequality (to decide whether the fine calculation applied). But it is not "legal" to test inequalities with the symbol y. (More precisely, such tests can't be sensibly interpreted).

For small enough n, c.cost(n) is equal to c.crew_costs(n) + c.fine_per_day * (c.time(n)-14). And this latter expression can be evaluated at the symbolic variable y.

And *sympy* permits us to symbolically differentiate the resulting expression:

In the next cell, we load the *definitions* from the oil spill notebook.

[54]: %%capture

```
%run week01-01--optimization.ipynb import *
[55]: import sympy as sp
       sp.init_printing()
       c = OilSpillCleanup()
       y = sp.Symbol('y') # symbolic variable
       def lcost(n):
            return c.crew_costs(n) + c.fine_per_day * (c.time(n) - 14)
       lcost_symb = lcost(y)
       D_lcost_symb = sp.diff(lcost_symb,y) # first derivative, for n<19</pre>
       DD_lcost_symb = sp.diff(D_lcost_symb,y) # second derivative, for n<19
       lcost_symb
[55]:
                                                160000u
       18000y
                                                                                            140000
                                                                                                          +
                               \overline{0.714285714285714y + 0.714285714285714}
                        2100000
       0.714285714285714y + 0.714285714285714
[56]: D_lcost_symb
[56]:
        -\frac{224000.0y}{\left(y+1\right)^{2}}+18000-\frac{2940000.0}{\left(y+1\right)^{2}}+\frac{160000}{0.714285714285714y+0.714285714285714}
[57]: DD_lcost_symb
[57]: \frac{448000.0y}{\left(y+1\right)^3} - \frac{448000.0}{\left(y+1\right)^2} + \frac{5880000.0}{\left(y+1\right)^3}
      Now e.g. sympy solvers are able to find the critical point for the symbolic derivative D_lcost_symb,
      as follows:
[58]: crits = sp.solve(D_lcost_symb,y)
       print(crits)
       [-13.2836838484589, 11.2836838484589]
      Notice that the value of the second derivative at the positive critical point 11.28 is positive:
[59]: DD_lcost = sp.lambdify(y,DD_lcost_symb)
       DD lcost(crits[1])>0
[59]: True
```

This the second derivative test shows that our postive critical point of 11.28 determines a *local* minimum for the cost function; this is the conclusion we came to previously.

Note that this symbolic method doesn't completely solve the problem: we still require analysis about the interval 19 < n (where the cost function isn't modeled by our symbolic function lcost_symb).

6 Numerical calculations

In another direction, rather than relying on symbolic calculations, we can use numerical methods to approximate derivatives.

Let's see what this might look like. We import the numpy package, and define some functions to extract critical points. These functions depend on the numpy function gradient which - in the case of a function of a single variable - approximates the derivative.

Let use these functions on our cubic polynomial G(t) from above. Remember that the sympy solve found the critical points to be $\frac{4}{3} \pm \frac{\sqrt{31}}{3}$.

```
[61]: def G(t): return t**3 - 4*t**2 - 5*t - 2
crit_pts_fun(G,-2,6,5E3,tol=1E-3)
```

[61]: [-0.52260000000163, 3.18919999999943]

Compare with:

```
[62]: [4/3 - np.sqrt(31)/3,4/3 + np.sqrt(31)/3]
```

[62]: [-0.522588120943341, 3.18925478761001]

But: if we change the tolerances in the argument to crit_pts_fun, we get redundant critical points, or we miss critical points.

```
[63]: crit_pts_fun(G,-2,6,5E3,tol=5E-3)
```

```
[64]: crit_pts_fun(G,-2,6,5E3,tol=1E-4)
[64]:
```

Let's return to our oil spill problem.

```
[65]: \( \%\) \( \text{capture} \) \( \text{vrun week01-01--optimization.ipynb import } \* \)
```

If we make good choices of tolerances, we can get a pretty good estimate for the critical point of the cost function:

```
[66]: c = OilSpillCleanup()

f = np.vectorize(c.cost)

res=crit_pts_fun(f,0,19,1E4,1E-1)
res
```

[66]: [11.2837]

But in some sense, this required us to already know the answer! with the wrong tolerances, it is easy to miss the critical point:

```
[67]: res=crit_pts_fun(f,0,19,1E4,1E-2) res
```

[67]:

And it is easy to get redundant reported critical points:

```
[68]: res=crit_pts_fun(f,0,19,1E4,4E-1) res
```

[68]: [11.2836, 11.2837, 11.2838]