Week 2 Optimisation for Machine Learning

Neimhin Robinson Gunning, 16321701

March 11, 2024

funcs.txt Wed Feb 21 15:03:56 2024 1

function: $3*(x-5)^4+10*(y-9)^2$ function: Max(x-5,0)+10*|y-9|

Figure 1: Two bivariate functions downloaded from https://www.scss.tcd.ie/Doug.Leith/CS7DS2/week4.php

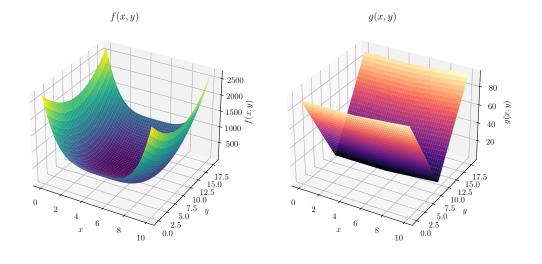


Figure 2

Let

$$f(x,y) = 3(x-5)^4 + 10(y-9)^2$$
(1)

and

$$g(x,y) = \max(x-5,0) + 10|y-9| \tag{2}$$

Using sympy we find the derivatives:

$$\nabla f = \left[\frac{df}{dx}, \frac{df}{dy}\right] = \left[12(x-5)^3, 20y - 180\right]$$

$$\nabla g = [\frac{dg}{dx}, \frac{dg}{dy}] = [\mathsf{Heaviside}(x-5), 10\mathsf{sign}(y-9)]$$

Clearly, the minimum of both f(x,y) and g(x,y) is 0 and they are both minimized by $x=5,\,y=9.$

The Polyak step size is

$$\alpha_{\text{Polyak}} = \frac{f(x) - f^*}{\nabla f(x)^T \nabla f(x)} \tag{3}$$

where x is the parameter vector, f(x) is the function to optimise, and $f^* \approx \min_x f(x)$.

Listing 1: A python function to calculate the Polyak step size on a sympy function.

```
src/polyak_step_size.py
                             Wed Feb 14 15:12:30 2024
                                                              1
    1: import numpy as np
    2:
    3:
    4: def polyak_step_size(self, sp_func, sp_x, x, f_star):
    5:
           assert len(sp_x) == len(x)
    6:
           subs = {sp_xi: xi for sp_xi, xi in zip(sp_x, x)}
    7:
           fx = sp\_func.subs(subs)
           grad = [sp_func.diff(sp_xi).subs(subs) for sp_xi in sp_x]
    8:
    9:
           grad = np.array(grad)
   10:
           denominator = sum(grad * grad)
   11:
           numerator = fx - f_star
           return numerator / denominator
   12:
```

```
1: import lib
 2: import numpy as np
 3:
 4:
 5: def iterate(self):
 6:
        x_value = self._start
 7:
        old_x_value = None
 8:
        iteration = 0
 9:
        m = np.zeros(x_value.shape, dtype=np.float64)
10:
        v = np.zeros(x_value.shape, dtype=np.float64)
11:
        converged = False
12:
        grad_value = self._gradient(x_value)
13:
14:
        def yielded():
15:
            print (x_value)
16:
            print (iteration)
17:
            return {
                 "iteration": iteration,
18:
                 "x": x_value,
19:
20:
                 "f(x)": self._function(x_value),
                 "sum": sum,
21:
                 "epsilon": self._epsilon,
22:
                 "converged": converged,
23:
24:
                 "gradient": grad_value,
                 "m": m,
25:
                 "v": v,
26:
                 "beta1": self._beta,
27:
                 "beta2": self._beta2,
"alpha": self._step_size,
28:
29:
30:
             }
31:
        yield yielded()
32:
33:
34:
        while not converged:
35:
            if self._max_iter > 0 and iteration > self._max_iter:
36:
                 break
            grad_value = self._gradient(x_value)
37:
            m = self._beta * m + (1-self._beta) *grad_value
38:
            # grad_value * grad_value gives element-wise product of np array
39:
            v = self._beta2 * v + (1-self._beta2) * (grad_value*grad_value)
40:
41:
            old_x_value = x_value
42:
            iteration += 1
43:
            m_hat = m / (1-(self._beta ** iteration))
            v_hat = np.array(v / (1-(self._beta2 ** iteration)))
44:
45:
            print('v', v, type(v))
            print('v_hat', v_hat, type(v_hat))
46:
47:
            print(np, type(np))
            v_hat_aug = v_hat**(0.5) + self._epsilon
48:
            adam\_grad = m\_hat / v\_hat\_aug
49:
            x_value = x_value - self._step_size * adam_grad
50:
51:
            converged = self._converged(x_value, old_x_value)
52:
            yield yielded()
53:
54:
55: if __name__ == "__main__":
56:
        adam = lib.GradientDescent()
57:
        adam.epsilon(0.0001)
58:
        adam.step_size(10**-2)
59:
        adam.beta(0.8)
60:
        adam.beta2(0.9)
61:
        adam.max_iter(-1)
62:
        adam.start(np.array([0, 0]))
63:
64:
        def converged(x1, x2):
65:
            d = np.max(x1-x2)
66:
            return d < 0.000001
67:
        def fn(x):
68:
            return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
69:
70:
71:
        def grad(x):
72:
            return np.array(
73:
                 [lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1])
74:
                     for var in (lib.x, lib.y)])
75:
        adam.converged(converged)
76:
        adam.function(fn)
77:
        adam.gradient(grad)
78:
        adam.set_iterate(iterate)
79:
        adam.run2csv("adam.csv")
```

Fri Feb 23 19:17:53 2024

1

src/adam.py

```
Wed Feb 07 15:48:23 2024
src/argmins_f_q.py
    1: from sympy import symbols, diff, solve
    2: import sympy as sp
   3:
   4: # Define the symbolic variables
   5: x, y = symbols('x y', real=True)
    6:
   7: # Define the functions
   8: f = 3 * (x - 5) **4 + 10 * (y - 9) **2
    9: q = sp.Max(x - 5, 0) + 10 * sp.Abs(v - 9)
   10:
   11: qrad_f = [diff(f, var) for var in (x, y)]
   12: argmin_f = solve(grad_f, (x, y))
   13: print(f"Argmin of f(x, y): {argmin_f}")
   14:
   15: qrad_q = [diff(q, var) for var in (x, y)]
   16: argmin_g = solve(grad_g, (x, y))
   17: print(f"Argmin of g(x, y): {argmin_g}")
```

```
src/b1.py
                   Thu Feb 01 14:29:35 2024
                                                          1
    1: import sympy as sp
    2: import sys
     3: import numpy as np
    4: import matplotlib.pyplot as plt
5: from matplotlib.pyplot import cm
     6: import seaborn as sns
     7: import pandas as pd
    8: from lib import GradientDescent
    9:
   10: LINEWIDTH = 0.5
   11:
        x = sp.symbols('x')
   12: y = x**4
   13: dydx = y.diff()
   14:
   15: fig, ax = plt.subplots(1, 3, figsize=(12, 8))
   16:
   17: blowup = 0.8
   18:
       # alpha * (blowup ** 3) * 4 = 1.2
   19:
   20:
   21: results = {
             "alpha":
                        [],
   22:
             "start":
                        [],
   23:
   24:
             "convergence time": [],
             "final guess": [],
   25:
   26: }
   27: iota = 0.00000000001
   28: settings = [
   29:
                       (0.1, 1),
   30:
                       (0.03, 1),
                       (0.5, 1),
   31:
   32:
                       (0.25, 1),
                       ((2*blowup)/((blowup**3)*4) + iota, blowup),
((2*blowup)/((blowup**3)*4) - iota, blowup),
   33:
   34:
   35:
                       (0.05, 0.7),
                       (0.1, 0.7)
   36:
   37:
                       (0.15, 0.7),
   38:
                       (0.1, 2),
   39:
        ]
   40: color = cm.rainbow(np.linspace(0, 1, len(settings)))
41: settings_with_color = zip(settings, color)
42: for ((step_size, start), color) in settings_with_color:
             print(step_size, start, color)
   43:
   44:
             g = GradientDescent()
   45:
             g.max_iter(100)
   46:
             g.step_size(step_size)
   47:
             g.start(start)
   48:
             g.function(lambda x1: float(y.subs(x, x1)))
   49:
             y_diff = y_diff()
   50:
             g.gradient(lambda x1: float(y_diff.subs(x, x1)))
   51:
             g.debug(True)
   52:
             def is_inf(x):
   53:
   54:
                  import math
   55:
                  if x == math.inf or x == -math.inf:
   56:
                      return True
   57:
             def converged(x1, x2):
    if is_inf(x1) or is_inf(x2):
   58:
   59:
                       return True
   60:
   61:
                  abs = np.abs(x1-x2)
   62:
                  print(abs, x1, x2)
   63:
                  return abs < 0.001</pre>
   64:
             g.converged(converged)
             iterations, estimates, y_of_x = zip(*[(x[0], x[1], x[2]) for x in g.iterate()])
   65:
   66:
             results["alpha"].append(step_size)
   67:
             results["start"].append(start)
   68:
   69:
             results["convergence time"].append(len(iterations))
   70:
             results["final guess"].append(estimates[-1])
             print('y_of_x', y_of_x)
print('iterations', iterations)
   71:
   72:
             print('estimates', estimates)
   73:
   74:
             sns.lineplot(
   75:
                  x=iterations,
   76:
                  y=np.abs(np.array(estimates)),
   77:
                  ax=ax[0],
   78:
                  linewidth=LINEWIDTH,
                  legend=False,
   79:
   80:
                  color=color,
   81:
                  label=f"$\\alpha={step_size}$,
                                                       $x={start}$")
             sns.lineplot(
   82:
   83:
                  x=iterations,
   84:
                  y=y_of_x,
   85:
                  ax=ax[1].
   86:
                  linewidth=LINEWIDTH,
   87:
                  color=color,
   88:
                  label=f"$\\alpha={step_size}$, $x={start}$")
   89:
             ax[2].step(
   90:
                  estimates,
                  y_of_x,
   91:
   92:
                  linewidth=LINEWIDTH,
   93:
                  color=color,
   94:
                  label=f"$\\alpha={step_size}$, $x={start}$")
             xs = np.arange(-2, 2, 0.01)

ys = [y.subs(x, xi) for xi in xs]
   95:
   96:
   97:
             ax[2].plot(
   98:
                  XS,
   99:
                  ys,
  100:
                  linewidth=LINEWIDTH,
```

```
src/b1.py
                 Thu Feb 01 14:29:35 2024
                                                  2
  101:
               label="$x^4$",
  102:
               color='vellow',
  103:
  104:
           ax[2].scatter(
  105:
               start,
  106:
               g._function(start),
  107:
               color=color)
  108:
  109:
       ax[1].legend(framealpha=1)
       ax[0].set_ylabel("$ \ \ x $")
 110:
       ax[0].set_xlabel("iteration")
  111:
 112: ax[0].set_yscale('log')
  113: ax[1].set_yscale('log')
  114: ax[0].set_title("(a)")
  115: ax[1].set vlabel("$v(\\hat{x})$")
  116: ax[1].set_xlabel("iteration")
  117: ax[1].set_title("(b)")
 118: ax[2].set_xlabel("$x$")
  119: ax[2].set_ylabel("$y$")
  120: ax[2].set_title("(c)")
  121: ax[0].set_ylim([10**-2, 1.5])
  122: ax[1].set_ylim([10**-6, 1.5])
       ax[2].set_ylim([-0.2, 2.2])
  123:
  124:
       ax[2].set_xlim([-2, 2])
  125:
  126:
      plt.tight_layout()
  127:
 128:
      outfile = "fig/gradient-descent-b1.pdf"
  129: if len(sys.argv) > 1:
  130:
           outfile = sys.argv[1]
 131: plt.savefig(outfile)
 132: df = pd.DataFrame(results)
 133: print (df)
       df.to_csv("fig/gradient-descent-b1.csv")
  134:
```

```
src/b-crazy.py
                      Tue Jan 16 18:21:05 2024
                                                       1
    1: import sympy as sp
    2: import sys
    3: import numpy as np
    4: import matplotlib.pyplot as plt
    5: import seaborn as sns
    6: from lib import GradientDescent
    7:
    8: LINEWIDTH = 0.7
    9: x = sp.symbols('x')
   10: y = x**4
   11: dydx = y.diff()
   12:
   13: fig, ax = plt.subplots(1, 2)
   14:
   15: for step_size in np.array([0.5]):
   16:
           for start in np.array([1.00001]):
   17:
               print(step_size, start)
   18:
               g = GradientDescent()
   19:
               g.max_iter(100)
   20:
               g.step_size(step_size)
   21:
               q.start(start)
   22:
               g.function(lambda x1: float(y.subs(x, x1)))
   23:
               y_diff = y_diff()
   24:
               g.gradient(lambda x1: float(y_diff.subs(x, x1)))
   25:
               a.debua(True)
   26:
   27:
               def converged(x1, x2):
   28:
                   abs = np.abs(x1-x2)
   29:
                   print(abs, x1, x2)
   30:
                   return abs < 0.001
   31:
               g.converged(converged)
   32:
               iterations, estimates, y_0f_x = zip(*[(x[0], x[1], x[2])) for x in g.iterate()])
   33:
               print('y_of_x', y_of_x)
   34:
               print('iterations', iterations)
   35:
               print('estimates', estimates)
   36:
               sns.lineplot(
   37:
                   x=iterations,
   38:
                   y=estimates,
   39:
                   ax=ax[0],
   40:
                   linewidth=LINEWIDTH,
   41:
                   legend=False,
   42:
                   label=f"$\\alpha={step_size}$, $x={start}$")
   43:
               sns.lineplot(
   44:
                   x=iterations,
   45:
                   y=y_of_x,
   46:
                   ax=ax[1],
   47:
                   linewidth=LINEWIDTH,
   48:
                   label=f"$\\alpha={step_size}$, $x={start}$")
   49:
   50: ax[0].set_ylabel("estimate of $\\mathrm{arg\\,min}_x x^4$")
   51: ax[0].set_xlabel("iteration")
   52: ax[1].set_ylabel("$y(\\hat{x})$")
   53: ax[1].set_xlabel("iteration")
   54: ax[0].set_ylim([-10000, 10000])
   55: ax[1].set_ylim([-100, 10000])
   56: plt.tight_layout()
   57:
   58: outfile = "fig/gradient-descent-x^4-crazy.pdf"
   59: if len(sys.argv) > 1:
   60:
           outfile = sys.argv[1]
   61: print(outfile)
   62: plt.savefig(outfile)
```

```
src/bi.py
                   Thu Feb 01 12:51:14 2024
    1: import sympy as sp
    2: import sys
    3: import numpy as np
4: import matplotlib.pyplot as plt
5: import seaborn as sns
6: import pandas as pd
    7:
       from lib import GradientDescent
    8:
    9: LINEWIDTH = 0.5
   10: x = sp.symbols('x')
11: y = x**4
12: dydx = y.diff()
   13:
   14: fig, ax = plt.subplots(1, 3, figsize=(12, 4))
   15:
   16: blowup = 0.8
   17:
   18:
       # alpha * (blowup ** 3) * 4 = 1.2
   19:
   20: results = {
   21:
             "alpha": [],
             "start": [],
   22:
             "convergence time": [],
   23:
   24:
             "final guess": [],
   25:
   26: iota = 0.00000000001
   27: for (step_size, start, color) in [
   28:
                       (0.1, 1, 'gray'),
   29:
   30:
             print(step_size, start, color)
   31:
             g = GradientDescent()
   32:
             g.max_iter(100)
   33:
             g.step_size(step_size)
   34:
             g.start(start)
   35:
             g.function(lambda x1: float(y.subs(x, x1)))
   36:
               _diff = y.diff()
   37:
             g.gradient(lambda x1: float(y_diff.subs(x, x1)))
   38:
             g.debug(True)
   39:
             def is_inf(x):
   40:
   41:
                  import math
   42:
                  if x == math.inf or x == -math.inf:
   43:
                      return True
   44:
             def converged(x1, x2):
    if is_inf(x1) or is_inf(x2):
   45:
   46:
   47:
                      return True
                  abs = np.abs(x1-x2)
   48:
                 print(abs, x1, x2)
   49:
   50:
                  return abs < 0.001</pre>
   51:
             g.converged(converged)
             iterations, estimates, y_of_x = zip(*[
    (x[0], x[1], x[2]) for x in g.iterate()])
results["alpha"].append(step_size)
   52:
   53:
   54:
             results["start"].append(start)
   55:
   56:
             results["convergence time"].append(len(iterations))
   57:
             results \hbox{\tt ["final guess"].append (estimates \hbox{\tt [-1]})}
             print('y_of_x', y_of_x)
print('iterations', iterations)
   58:
   59:
             print('estimates', estimates)
   60:
             sns.lineplot(
   61:
   62:
                 x=iterations,
   63:
                 y=np.abs(np.array(estimates)),
   64:
                  ax=ax[0],
   65:
                  linewidth=LINEWIDTH,
   66:
                  legend=False,
   67:
                  color=color,
   68:
                  label=f"$\\alpha={step_size}$, $x={start}$")
   69:
             sns.lineplot(
   70:
                  x=iterations,
   71:
                  y=y_of_x,
   72:
                  ax=ax[1],
   73:
                  linewidth=LINEWIDTH,
   74:
                  color=color,
   75:
                  label=f"$\\alpha={step_size}$, $x={start}$")
   76:
             ax[2].step(
   77:
                  estimates,
   78:
                  y_of_x
   79:
                  linewidth=LINEWIDTH,
   80:
                  color=color,
             xs = np.arange(-2, 2, 0.01)
ys = [y.subs(x ...)
   81:
                 label=f"$\\alpha={step_size}$,
                                                       $x={start}$")
   82:
   83:
                   [y.subs(x, xi) for xi in xs]
   84:
             ax[2].plot(
   85:
                 xs,
                  ys,
   86:
   87:
                  linewidth=LINEWIDTH,
                  label="$x^4$",
   88:
                  color='yellow',
   89:
   90:
   91:
             ax[2].scatter(
   92:
                  start,
                  g._function(start),
   93:
                  color=color)
   94:
   95:
   96:
        ax[0].set_ylabel("$|\hat x|$")
   97:
   98: ax[0].set_xlabel("iteration")
   99: ax[0].set_yscale('log')
  100: ax[0].set_title("(a)")
```

```
src/bi.pv
                Thu Feb 01 12:51:14 2024
  101: ax[1].set_yscale('log')
  102: ax[1].set vlabel("$v(\\hat{x})$")
  103: ax[1].set xlabel("iteration")
 104: ax[1].set_title("(b)")
 105: ax[2].set_xlabel("$x$")
  106: ax[2].set vlabel("$v$")
  107: ax[2].set title("(c)")
 108: \# ax[0].set_ylim([-7, 7])
 109: \# ax[1].set\_vlim([-1, 4])
  110: ax[2].set vlim([-0.2, 1.2])
 111: \# ax[2].set xlim([-2, 2])
 112: plt.tight_layout()
  113:
  114: outfile = "fig/gradient-descent-bi.pdf"
 115: if len(sys.argv) > 1:
  116:
           outfile = sys.argv[1]
 117: plt.savefig(outfile)
  118: df = pd.DataFrame(results)
  119: print (df)
  120: df.to_csv("fig/gradient-descent-bi.csv")
```

```
Wed Jan 24 17:19:09 2024
src/ci.py
    1: import sympy as sp
    2: import sys
    3: import numpy as np
    4: import matplotlib.pyplot as plt5: import seaborn as sns6: import pandas as pd
    7:
       from lib import GradientDescent
    8:
    9: LINEWIDTH = 0.1
   10: x = sp.symbols('x')
11: y = x**4
12: dydx = y.diff()
   13:
   14: fig, ax = plt.subplots(1, 3, figsize=(12, 4))
   15:
   16: blowup = 0.8
   17:
   18:
       # alpha * (blowup ** 3) * 4 = 1.2
   19:
   20: results = {
   21:
            "alpha":
                       [],
            "start":
   22:
                       [],
            "gamma":
   23:
                       [],
            "$f(x)$": [],
   24:
             "convergence time": [],
   25:
             "final guess": [],
   26:
   27: }
28: iota = 0.005
29: def run(gamma, color, max_iter=99, plot=True):
   27:
   30:
            g = GradientDescent()
   31:
            g.max_iter(max_iter)
   32:
            alpha = 1
            start = 1
   33:
   34:
            g.step_size(alpha)
   35:
            g.start(start)
            y = gamma * (x**2)
   36:
            g.function(lambda x1: float(y.subs(x, x1)))
   37:
            y_diff = y_diff()
   38:
   39:
            g.gradient(lambda x1: float(y_diff.subs(x, x1)))
   40:
            g.debug(True)
   41:
             def is_inf(x):
   42:
   43:
                 import math
   44:
                 if x == math.inf or x == -math.inf:
   45:
                      return True
   46:
            def converged(x1, x2):
    if is_inf(x1) or is_inf(x2):
   47:
   48:
   49:
                      return True
   50:
                 abs = np.abs(x1-x2)
   51:
                 print (abs, x1, x2)
return abs < 0.001</pre>
   52:
   53:
             g.converged(converged)
   54:
                                        y_of_x = zip(*[
             iterations, estimates, y_of_x = zip(*[(x[0], x[1], x[2]) for x in g.iterate()])
   55:
   56:
            results ["alpha"] .append (alpha)
   57:
            results["gamma"].append(gamma)
             results["$f(x)$"].append(str(y))
   58:
             results["start"].append(start)
   59:
             results["convergence time"].append(len(iterations))
   60:
            results["final guess"].append(estimates[-1])
   61:
   62:
             if plot:
   63:
                 sns.lineplot(
   64:
                      x=iterations,
   65:
                      y=estimates,
   66:
                      ax=ax[0],
   67:
                      linewidth=LINEWIDTH,
   68:
                      legend=False,
   69:
                      color=color,
   70:
                      label=f"$\\gamma={gamma}$")
   71:
                 sns.lineplot(
   72:
                      x=iterations,
   73:
                      y=y_of_x,
   74:
                      ax=ax[1],
   75:
                      linewidth=LINEWIDTH,
                      color=color,
   76:
   77:
                      label=f"$\\gamma={gamma}$")
   78:
                 ax[2].step(
   79:
                      estimates,
   80:
                      y_of_x
                      linewidth=LINEWIDTH,
   81:
                      color=color,
   82:
   83:
                      label=f"$\\gamma={gamma}$")
                 xs = np.arange(-2, 2, 0.01)
   84:
                 ys = [y.subs(x, xi) \text{ for } xi \text{ in } xs]
   85:
   86:
                 ax[2].plot(
   87:
                      xs,
   88:
                      ys,
   89:
                      linewidth=LINEWIDTH,
                      label="$\\gamma x^2$",
   90:
                      color='yellow',
   91:
   92:
                 ax[2].scatter(
   93:
                      start,
   94:
   95:
                      g._function(start),
   96:
                      color=color)
   97:
   98:
   99: for (gamma, color) in [
  100:
                      ( 0.01, 'green'),
```

```
src/ci.py
                Wed Jan 24 17:19:09 2024
                                                 2
  101:
                    ( 0.1, 'blue'),
  102:
                    ( 1 - iota, 'black'),
                    (1 + iota, 'orange'),
 103:
                    ( 1, 'red'),
  104:
                    (-0.05, 'purple'),
 105:
 106:
               1:
 107:
           run (gamma, color)
 108:
 109:
       run(-1000, 'pink', max_iter=10000, plot=False)
  110:
  111: ax[0].set_ylabel("$x$")
  112: ax[0].set_xlabel("iteration")
  113: ax[0].set title("(a)")
  114: ax[1].set_ylabel("$y(\\hat{x})$")
  115: ax[1].set xlabel("iteration")
  116: ax[1].set title("(b)")
  117: ax[2].set xlabel("$x$")
  118: ax[2].set_ylabel("$y$")
  119: ax[2].set title("(c)")
  120: ax[0].set_ylim([-7, 7])
  121: ax[1].set_ylim([-1, 4])
  122: ax[2].set_ylim([-1, 2.2])
  123: ax[2].set xlim([-2, 2])
  124: plt.tight_layout()
  125:
  126: outfile = "fig/gradient-descent-ci.pdf"
  127: if len(sys.argv) > 1:
  128:
         outfile = sys.argv[1]
 129: plt.savefig(outfile)
  130: df = pd.DataFrame(results)
  131: print (df)
  132: df.to_csv("fig/gradient-descent-ci.csv")
```

```
Tue Jan 23 16:02:37 2024
                                                          1
src/csv_to_pdf.py
    1: #!/usr/bin/env python
    2:
    3: import pandas as pd
    4: import sys
    5: import subprocess
    6: import os
    7:
    8:
    9: def csv_to_latex_pdf(input_csv, output_pdf="output.pdf"):
   10:
           # Read the CSV file into a pandas DataFrame
   11:
           df = pd.read_csv(input_csv, dtype=str)
   12:
   13:
           # Convert the DataFrame to LaTeX tabular format
   14:
           df_to_latex_pdf(df, output_pdf=output_pdf)
   15:
   16:
   17: def format_float(x):
   18:
           if isinstance(x, float):
   19:
               import math
   20:
               if x == math.inf:
                   return "$\\infty$"
   21:
   22:
               if x == -math.inf:
   23:
                   return "$-\\infty"
   24:
               if x == math.nan:
   25:
                   return "NaN"
   26:
               return ("\\num{{{0:.2g}}}".format(x))
   27:
   28:
   29: def df_to_latex_pdf(df, output_pdf="output.pdf"):
   30:
           # Create the tmp directory if it doesn't exist
   31:
           if not os.path.exists("tmp"):
   32:
               os.makedirs("tmp")
   33:
           latex_tabular = df.to_latex(float_format=format_float)
   34:
   35:
           # Wrap the tabular code in a LaTeX document
   36:
           latex_document = r"""\documentclass{article}
   37: \usepackage{booktabs}
   38: \usepackage{siunitx}
   39: \begin{document}
   40: \thispagestyle{empty}
   41:
           """ + latex_tabular + r"""\end{document}"""
   42:
   43:
           output_tex = "tmp/output.tex"
   44:
   45:
           # Save the LaTeX code to a file
   46:
           with open(output_tex, 'w') as f:
   47:
               f.write(latex_document)
   48:
   49:
           # Compile the LaTeX file using pdflatex
           subprocess.run(["pdflatex", "-jobname=tmp/output", output_tex])
   50:
           subprocess.run(["pdfcrop", "tmp/output.pdf", output_pdf])
   51:
   52:
   53:
           print(f"PDF generated as {output_pdf}")
   54:
   55:
   56: if __name__ == "__main__":
   57:
           if len(sys.argv) != 3:
   58:
               print("Usage: python script_name.py input.csv output.pdf")
   59:
               sys.exit(1)
   60:
   61:
           input_csv = sys.argv[1]
           output_pdf = sys.argv[2]
   62:
   63:
           csv_to_latex_pdf(input_csv, output_pdf)
```

```
src/exp.py
                 Mon Mar 11 14:18:56 2024
                                                   1
    1: import lib
    2: import sys
    3: import argparse
    4: import numpy as np
    5: import rms2
    6: import adam
    7: import hb
    8:
    9:
   10: def converged(x1, x2):
          d = np.max(x1-x2)
   11:
   12:
           return d < 0.001
   13:
   14:
   15: parser = argparse.ArgumentParser(
   16:
           prog="Run Gradient Descent A Step Size Algorithm")
   17:
   18: parser.add_argument('-al', '--algorithm', choices=[
           'rmsprop', 'adam', 'polyak', 'heavy_ball'], required=True)
   19:
   20:
   21: parser.add_argument('-b', '--beta', type=float)
   22: parser.add_argument('-b2', '--beta2', type=float)
   23: parser.add_argument('-a', '--alpha', type=float)
   24: parser.add_argument('filename')
   25:
   26: args = parser.parse_args()
   27:
   28: print (args.filename)
   29:
   30: gd = lib.GradientDescent()
31: if 0:
   32:
           pass
   33: elif args.algorithm == 'rmsprop':
   34:
           gd.set_iterate(rms2.iterate)
   35: elif args.algorithm == 'adam':
   36:
           gd.set_iterate(adam.iterate)
   37: elif args.algorithm == 'heavy_ball':
   38:
           gd.set_iterate(hb.iterate)
   39: else:
          print("no algorithm")
   41:
           sys.exit(1)
   42:
   43: gd.start(np.array([4, 8]))
   44: gd.converged(converged)
   45: gd.step_size(args.alpha)
   46: gd.beta(args.beta)
   47: gd.beta2(args.beta2)
   48: gd.epsilon(0.0001)
   49: qd.max_iter(-1)
   50:
   51:
   52: def fn(x):
   53:
           return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
   54:
   55:
   56: def grad(x):
   57:
           return np.array([
   58:
               lib.f.diff(var).subs(
   59:
                   lib.x, x[0]
   60:
               ).subs(
   61:
                    lib.y, x[1]
   62:
               ) for var in (lib.x, lib.y)])
   63:
   64:
   65: gd.converged(converged)
   66: gd.function(fn)
   67: gd.gradient(grad)
   68: gd.run2csv(args.filename)
```

```
src/gradient_descent_listing.py
                                       Wed Jan 31 15:38:46 2024
   1: class GradientDescent():
   2: # ...
   3:
          def iterate(self):
   4:
               import math
   5:
               x value = self._start
   6:
               old x value = None
   7:
               iteration = 0
   8:
               while True:
   9:
                   vield [iteration, float(x value), float(self. function(x value))]
  10:
                   iteration += 1
  11:
                   if self. max iter > 0 and iteration > self. max iter:
  12:
                       break
  13:
                   grad_value = self._gradient(x_value)
  14:
                   x_value -= self._step_size * grad_value # Update step
  15:
                   if old_x_value is not None and self._converged(x_value, old_x_value):
  16:
                       vield [iteration, float(x value), float(self. function(old x value))]
  17:
                       print ("converged")
  18:
                       break
   19:
                   old x value = x value
```

```
src/hb.py
                 Mon Mar 11 12:49:50 2024
                                                   1
    1: import lib
    2:
    3:
    4: def iterate(self):
    5:
           x_value = self._start
    6:
           old_x_value = None
    7:
           iteration = 0
    8:
           converged = False
    9:
           grad_value = self._gradient(x_value)
   10:
   11:
           z = 0
   12:
   13:
           def yielded():
   14:
                print (x_value)
   15:
                print (iteration)
   16:
                return {
   17:
                    "iteration": iteration,
   18:
                    "z": Z,
   19:
                    "x": x_value,
                    "f(x)": self._function(x_value),
   20:
                    "sum": sum,
   21:
   22:
                    "epsilon": self._epsilon,
   23:
                    "converged": converged,
   24:
                    "gradient": grad_value,
   25:
                }
   26:
   27:
           yield yielded() # yield initial values
   28:
   29:
           while not converged:
   30:
                iteration += 1
   31:
                if self._max_iter > 0 and iteration > self._max_iter:
   32:
                    break
   33:
                grad_value = self._gradient(x_value)
   34:
                old_x_value = x_value
   35:
                z = self._beta * z + self._step_size * grad_value
   36:
                x_value = x_value - z
   37:
                converged = self._converged(x_value, old_x_value)
   38:
                yield yielded()
   39:
   40:
   41: if __name__ == "__main__
   42:
           import numpy as np
   43:
           hb = lib.GradientDescent()
   44:
           hb.step\_size(10**-3)
   45:
           hb.beta(0.5)
   46:
           hb.max_iter(-1)
   47:
           hb.start(np.array([0, 0]))
   48:
   49:
           def converged(x1, x2):
   50:
                d = np.max(x1-x2)
   51:
                return d < 0.000001
   52:
           def fn(x):
   53:
   54:
                return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
   55:
   56:
           def grad(x):
   57:
                return np.array([
   58:
                    lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1])
   59:
                    for var in (lib.x, lib.y)])
   60:
           hb.converged (converged)
   61:
           hb.function(fn)
   62:
           hb.gradient (grad)
   63:
           hb.set_iterate(iterate)
   64:
           hb.run2csv("hb.csv")
```

```
Mon Mar 11 14:00:58 2024
                                                            1
src/heavy_ball.py
    1: import lib
    2:
    3:
    4: def iterate(self):
    5:
           x_value = self._start
    6:
           old_x_value = None
           iteration = 0
    7:
    8:
           converged = False
    9:
           grad_value = self._gradient(x_value)
   10:
   11:
           z = 0
   12:
   13:
           def yielded():
   14:
                print (x_value)
   15:
                print (iteration)
   16:
                return {
   17:
                    "iteration": iteration,
   18:
                    "z": Z,
   19:
                    "x": x_value,
                    "f(x)": self._function(x_value),
   20:
                    "sum": sum,
   21:
   22:
                    "epsilon": self._epsilon,
   23:
                    "converged": converged,
   24:
                    "gradient": grad_value,
   25:
                }
   26:
   27:
           yield yielded() # yield initial values
   28:
   29:
           while not converged:
   30:
                iteration += 1
   31:
                if self._max_iter > 0 and iteration > self._max_iter:
   32:
                    break
   33:
                grad_value = self._gradient(x_value)
   34:
                old_x_value = x_value
   35:
                z = self._beta * z + self._step_size * grad_value
   36:
                x_value = x_value - z
   37:
                converged = self._converged(x_value, old_x_value)
   38:
                yield yielded()
   39:
   40:
   41: if __name__ == "__main__
   42:
           import numpy as np
   43:
           hb = lib.GradientDescent()
   44:
           hb.step\_size(10**-3)
   45:
           hb.beta(0.5)
   46:
           hb.max_iter(-1)
   47:
           hb.start(np.array([0, 0]))
   48:
   49:
           def converged(x1, x2):
   50:
                d = np.max(x1-x2)
   51:
                return d < 0.000001
   52:
           def fn(x):
   53:
   54:
                return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
   55:
   56:
           def grad(x):
   57:
                return np.array([
   58:
                    lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1])
   59:
                    for var in (lib.x, lib.y)])
   60:
           hb.converged (converged)
   61:
           hb.function(fn)
   62:
           hb.gradient (grad)
   63:
           hb.set_iterate(iterate)
   64:
           hb.run2csv("hb.csv")
```

```
1: import sympy as sp
2: import functools
 3:
 4: x, y = sp.symbols('x y', real=True)

5: f = 3 * (x - 5) **4 + (10 * ((y - 9) **2))

6: g = sp.Max(x - 5, 0) + (10 * sp.Abs(y - 9))
 8:
 9: class GradientDescent():
10:
         def __init__(self):
              self._max_iter = 1000
11:
12:
              self._debug = False
13:
              self._converged = lambda x1, x2: False
14:
              self.\_epsilon = 0.0001
15:
              self.\_beta = 0
16:
         def step_size(self, a):
    self._step_size = a
17:
18:
19:
              return self
20:
21:
         def beta(self, b):
22:
              self.\_beta = b
23:
              return self
24:
25:
         def beta2(self, b):
26:
              self.\_beta2 = b
27:
              return self
28:
29:
         def epsilon(self, e):
30:
              self.\_epsilon = e
31:
              return self
32:
         def function(self, f):
33:
34:
              self.\_function = f
35:
              return self
36:
37:
         def gradient(self, g):
38:
              self._gradient = g
39.
              return self
40:
41:
         def max_iter(self, m):
42:
              self._max_iter = m
43:
              return self
44:
45:
         def start(self, s):
    self._start = s
46:
47:
              return self
48:
49:
         def debug(self, d):
              self.\_debug = d
50:
51:
              return self
52:
53:
         def converged(self, c):
54:
              self._converged = c
55:
              return self
56:
57:
         def set_iterate(self, f):
              self.iterate = functools.partial(f, self)
58:
59:
              return self
60:
61:
         def iterate(self):
62:
              x_value = self._start
63:
              old_x_value = None
64:
              iteration = 0
65:
              while True:
66:
                   yield [iteration, x_value, self._function(x_value)]
67:
                   iteration += 1
68:
                   if self._max_iter > 0 and iteration > self._max_iter:
69:
                       break
70:
                   grad_value = self._gradient(x_value)
71:
                   print(x_value, type(x_value))
72:
                   print (grad_value, type (grad_value))
x_value -= self._step_size * grad_value # Update step
73:
74:
                   if old_x_value is not None and self._converged(x_value, old_x_value):
75:
                       yield [iteration, float(x_value), float(self._function(old_x_value))]
76:
                       print ("converged")
77:
                       break
78:
                   old_x_value = x_value
79:
80:
         def run2csv(self, fname, summarise=True):
81:
              import pandas as pd
82:
              iterations = list(self.iterate())
              df = pd.DataFrame(iterations)
84:
              df.to_csv(fname)
85:
              if(summarise):
                   with open(fname + ".summary", "w") as f:
86:
                       print(f"iterations: {len(df)}", file=f)
print(f"start: {df['x'][0]}", file=f)
print(f"final: {df['x'][len(df) - 1]}", file=f)
87:
88:
89:
90:
91:
92: if _
                  == "
          name
                         main
     print(f.diff(x), f.diff(y))
93:
94:
        print(q.diff(x), q.diff(y))
```

src/lib.py

Mon Mar 11 14:18:37 2024

```
src/polyak_step_size.py
                                Wed Feb 14 15:12:30 2024
    1: import numpy as np
    2:
    3:
    4: def polyak_step_size(self, sp_func, sp_x, x, f_star):
    5:
           assert len(sp_x) == len(x)
    6:
           subs = \{ \text{sp xi: xi for sp xi, xi in zip}(\text{sp x, x}) \}
    7:
           fx = sp\_func.subs(subs)
    8:
           grad = [sp_func.diff(sp_xi).subs(subs) for sp_xi in sp_x]
    9:
           grad = np.array(grad)
   10:
           denominator = sum(grad * grad)
   11:
           numerator = fx - f star
   12:
           return numerator / denominator
```

```
src/rms2.py
                  Mon Mar 11 12:39:16 2024
    1: import lib
    2:
    3:
    4: def iterate(self):
    5:
           import numpy as np
    6:
           x_value = self._start
    7:
           old_x_value = None
    8:
           iteration = 0
    9:
           sum = np.zeros(x_value.shape)
   10:
           alpha_n = np.zeros(x_value.shape)
   11:
           alpha_n.fill(self._step_size)
   12:
           converged = False
  13:
           grad_value = self._gradient(x_value)
  14:
  15:
           def yielded():
  16:
               print (x_value)
  17:
               print (iteration)
   18:
               return {
   19:
                    "iteration": iteration,
   20:
                    "x": x_value,
   21:
                    "f(x)": self._function(x_value),
   22:
                    "sum": sum,
   23:
                    "epsilon": self._epsilon,
   24:
                   "converged": converged,
   25:
                   "gradient": grad_value,
   26:
                    "alpha_n": alpha_n,
   27:
   28:
   29:
           yield yielded()
   30:
   31:
           while not converged:
   32:
               iteration += 1
   33:
               if self._max_iter > 0 and iteration > self._max_iter:
   34:
   35:
               grad_value = self._gradient(x_value)
               old_x_value = x_value
   36:
   37:
               print (grad_value, type (grad_value))
   38:
               print(alpha_n, type(alpha_n))
   39:
               print(x_value, type(x_value))
   40:
               x_value = x_value - alpha_n * grad_value
               sum = self._beta * sum + (1-self._beta) * (grad_value**2)
   41:
   42:
               alpha_n = self._step_size / (sum**0.5+self._epsilon)
   43:
               converged = self._converged(x_value, old_x_value)
   44:
               yield yielded()
   45:
   46:
   47: def rms_gradient_descent():
   48:
           rms = lib.GradientDescent()
   49:
           rms.set_iterate(iterate)
   50:
           return rms
   51:
   52:
   53: if __name__ == "__main__":
   54:
           import numpy as np
   55:
           rms = lib.GradientDescent()
   56:
           rms.epsilon(0.0001)
   57:
           rms.step_size(10**-2)
   58:
           rms.beta(0.1)
   59:
           rms.max_iter(-1)
   60:
           rms.start(np.array([0, 0]))
   61:
   62:
           def converged(x1, x2):
               d = np.max(x1-x2)
   63:
               return d < 0.000001
   64:
   65:
   66:
           def fn(x):
               return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
   67:
   68:
   69:
           def grad(x):
               return np.array([lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1]) for var in (lib.x, lib.y)])
   70:
   71:
           rms.converged(converged)
   72:
           rms.function(fn)
   73:
           rms.gradient(grad)
   74:
           rms.set_iterate(iterate)
   75:
           rms.run2csv("rms2.csv")
```

```
Wed Feb 14 16:31:00 2024
src/rms_prop.py
    1: class RMSPropGradientDescent():
    2:
           def __init__(self):
    3:
                self._max_iter = 1000
    4:
                self._debug = False
    5:
                self._converged = lambda x1, x2: False
                self.\_sum = 0
    6:
    7:
                self.\_epsilon = 0.0001
    8:
    9:
            def step_size(self, a):
   10:
                self._step_size = a
   11:
                return self
   12:
   13:
            def epsilon(self, e):
   14:
                self._epsilon = e
   15:
                return self
            def beta(self, b):
   17:
   18:
                self.\_beta = b
   19:
                return self
   20:
   21:
            def function(self, f):
                self.\_function = f
   22:
   23:
                return self
   24:
   25:
            def gradient(self, g):
   26:
                self._gradient = g
   27:
                return self
   28:
   29:
            def max_iter(self, m):
                self._max_iter = m
   30:
   31:
                return self
   32:
   33:
            def start(self, s):
    self._start = s
   34:
   35:
                return self
   36:
   37:
            def debug(self, d):
   38:
                self.\_debug = d
   39:
                return self
   40:
            def converged(self, c):
   41:
   42:
                self._converged = c
   43:
                return self
   44:
            def run2csv(self, fname):
    import pandas as pd
   45:
   46:
   47:
                iterations = list(self.iterate())
   48:
                df = pd.DataFrame(iterations)
   49:
                df.to_csv(fname)
   50:
   51:
            def iterate(self):
                import math
   52:
   53:
                import numpy as np
   54:
                x_value = self._start
   55:
                old_x_value = None
   56:
                iteration = 0
   57:
                sum = np.zeros(x_value.shape)
   58:
                alpha_n = np.zeros(x_value.shape)
   59:
                alpha_n.fill(self._step_size)
   60:
                converged = False
                grad_value = self._gradient(x_value)
   61:
   62:
   63:
                def yielded():
                     print (x_value)
   65:
                     print (iteration)
   66:
                     return {
                          "iteration": iteration,
   67:
   68:
                         "x": x_value,
   69:
                          "f(x)": self._function(x_value),
                          "sum": sum,
   70:
   71:
                         "epsilon": self._epsilon,
                         "converged": converged,
   72:
   73:
                         "gradient": grad_value,
   74:
                          "alpha_n": alpha_n,
   75:
                     }
   76:
   77:
                yield yielded()
   78:
                while not converged:
   79:
   80:
                    iteration += 1
                     if self._max_iter > 0 and iteration > self._max_iter:
   81:
   82:
                         break
   83:
                     grad_value = self._gradient(x_value)
   84:
                     old_x_value = x_value
                     print (grad_value, type (grad_value))
   85:
                     print(alpha_n, type(alpha_n))
   86:
   87:
                     print(x_value, type(x_value))
                     x_value = x_value - alpha_n * grad_value
   88:
                     sum = self._beta * sum + (1-self._beta) * (grad_value**2)
alpha_n = self._step_size / (sum**0.5+self._epsilon)
   89:
   90:
                     converged = self._converged(x_value, old_x_value)
   91:
   92:
                     yield yielded()
   93:
   94:
                    _== "_
   95:
             name
                           _main_
           import numpy as np
   96:
            import lib
   97:
   98:
            rms = RMSPropGradientDescent()
   99:
            rms.epsilon(0.0001)
           rms.step size(10**-2)
  100:
```

```
src/rms_prop.py
                       Wed Feb 14 16:31:00 2024
 101:
           rms.beta(0.1)
 102:
           rms.max iter(-1)
 103:
           rms.start(np.array([0, 0]))
 104:
           def converged(x1, x2):
 105:
 106:
               d = np.max(x1-x2)
 107:
               return d < 0.000001
 108:
 109:
           def fn(x):
               return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
 110:
 111:
 112:
           def grad(x):
 113:
               return np.array([lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1]) for var in (lib.x, lib.y)])
 114:
           rms.converged(converged)
 115:
           rms.function(fn)
 116:
           rms.gradient(grad)
 117:
           rms.run2csv("rms.csv")
```

```
src/rmsprop.py
                      Mon Mar 11 14:00:47 2024
    1: import lib
    2:
    3:
    4: def iterate(self):
    5:
           import numpy as np
    6:
           x_value = self._start
    7:
           old_x_value = None
    8:
           iteration = 0
    9:
           sum = np.zeros(x_value.shape)
   10:
           alpha_n = np.zeros(x_value.shape)
   11:
           alpha_n.fill(self._step_size)
   12:
           converged = False
  13:
           grad_value = self._gradient(x_value)
  14:
  15:
           def yielded():
  16:
               print (x_value)
  17:
               print (iteration)
   18:
               return {
   19:
                    "iteration": iteration,
   20:
                    "x": x_value,
   21:
                    "f(x)": self._function(x_value),
   22:
                    "sum": sum,
   23:
                    "epsilon": self._epsilon,
   24:
                   "converged": converged,
   25:
                   "gradient": grad_value,
   26:
                    "alpha_n": alpha_n,
   27:
   28:
   29:
           yield yielded()
   30:
   31:
           while not converged:
   32:
               iteration += 1
   33:
               if self._max_iter > 0 and iteration > self._max_iter:
   34:
   35:
               grad_value = self._gradient(x_value)
               old_x_value = x_value
   36:
   37:
               print (grad_value, type (grad_value))
   38:
               print(alpha_n, type(alpha_n))
   39:
               print(x_value, type(x_value))
   40:
               x_value = x_value - alpha_n * grad_value
               sum = self._beta * sum + (1-self._beta) * (grad_value**2)
   41:
   42:
               alpha_n = self._step_size / (sum**0.5+self._epsilon)
   43:
               converged = self._converged(x_value, old_x_value)
   44:
               yield yielded()
   45:
   46:
   47: def rms_gradient_descent():
   48:
           rms = lib.GradientDescent()
   49:
           rms.set_iterate(iterate)
   50:
           return rms
   51:
   52:
   53: if __name__ == "__main__":
   54:
           import numpy as np
   55:
           rms = lib.GradientDescent()
   56:
           rms.epsilon(0.0001)
   57:
           rms.step_size(10**-2)
   58:
           rms.beta(0.1)
   59:
           rms.max_iter(-1)
   60:
           rms.start(np.array([0, 0]))
   61:
   62:
           def converged(x1, x2):
               d = np.max(x1-x2)
   63:
               return d < 0.000001
   64:
   65:
   66:
           def fn(x):
               return lib.f.subs(lib.x, x[0]).subs(lib.y, x[1])
   67:
   68:
   69:
           def grad(x):
               return np.array([lib.f.diff(var).subs(lib.x, x[0]).subs(lib.y, x[1]) for var in (lib.x, lib.y)])
   70:
   71:
           rms.converged(converged)
   72:
           rms.function(fn)
   73:
           rms.gradient(grad)
   74:
           rms.set_iterate(iterate)
   75:
           rms.run2csv("rms2.csv")
```

```
src/sympy1.py
                     Tue Jan 09 12:48:37 2024
    1: import sympy as sp
    2:
    3: x = sp.symbols('x')
    4: print(x)
    5: f = x ** 4
    6: print(f)
    7: print(f.diff())
    8: print(f.subs(x, x**2))
    9: print (f.conjugate())
   10: print(f)
   11: print (f.subs())
```

```
Wed Feb 07 11:52:44 2024
                                                        1
src/vis_f_g.py
    1: import matplotlib.pyplot as plt
    2: import numpy as np
    3: import sys
    4:
    5:
    6: def f(x, y):
           return 3 * (x - 5)**4 + 10 * (y - 9)**2
    7:
    8:
    9:
   10: def g(x, y):
   11:
           return np.maximum (x - 5, 0) + 10 * np.abs (y - 9)
   12:
   13:
   14: def main (outfile):
           x = np.linspace(0, 10, 400)
   15:
   16:
           y = np.linspace(0, 18, 400)
   17:
           X, Y = np.meshgrid(x, y)
   18:
           Z_f = f(X, Y)
   19:
           Z_q = q(X, Y)
   20:
   21:
           fig = plt.figure(figsize=(12, 6))
   22:
           ax = fig.add_subplot(1, 2, 1, projection='3d')
   23:
   24:
           ax.plot_surface(X, Y, Z_f, cmap='viridis')
           ax.set_title('$f(x, y)$')
   25:
           ax.set_xlabel('$x$')
   26:
   27:
           ax.set_ylabel('$y$')
   28:
           ax.set_zlabel('$f(x, y)$')
   29:
           ax = fig.add_subplot(1, 2, 2, projection='3d')
   30:
           ax.plot_surface(X, Y, Z_g, cmap='magma')
   31:
   32:
           ax.set_title('\$q(x, y)\$')
   33:
           ax.set_xlabel('$x$')
   34:
           ax.set_ylabel('$y$')
   35:
           ax.set_zlabel('$q(x, y)$')
   36:
   37:
           plt.savefig(outfile)
   38:
           plt.show()
   39:
   40:
   41: if __name__ == "__main__":
   42:
           if len(sys.argv) != 2:
   43:
               print("Usage: python script.py <output_file>")
   44:
               sys.exit(1)
   45:
   46:
           outfile = sys.argv[1]
   47:
           main(outfile)
   48:
```