NotebookSolutions

September 1, 2024

```python
import numpy as np
import matplotlib.pyplot as plt
import plotly.graph_objects as go
```
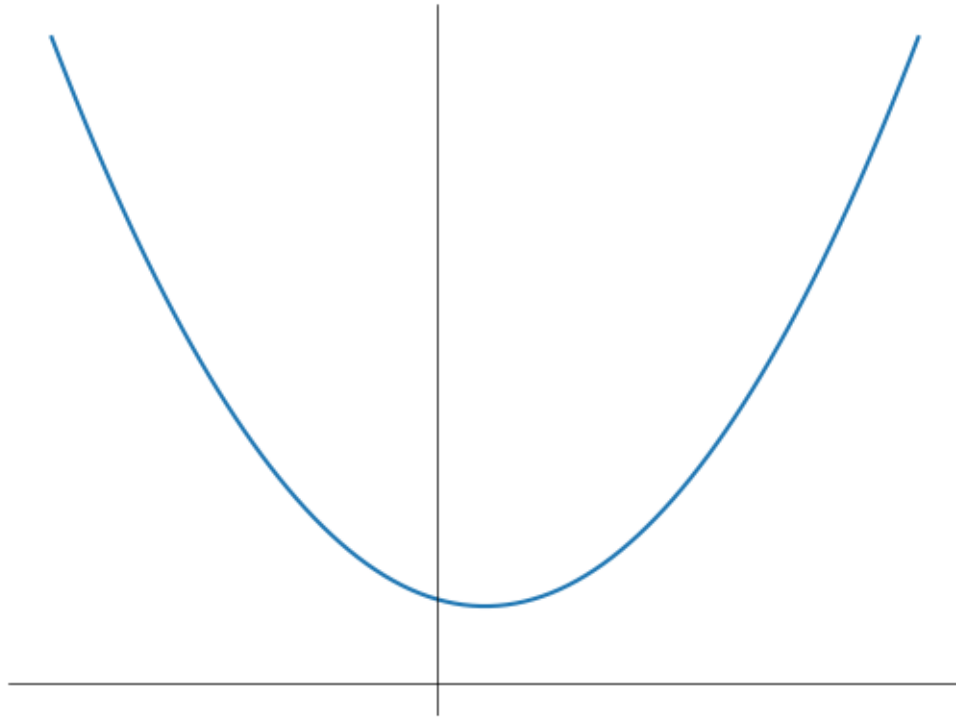
1 Finding minimum value of a function

1.1 One dimensional function

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

```python
def f(x):
    return x**2 - x + 3
```

Simple plot of the function. Note that if the fucntion had many (> 2 parameters, then plotting would not be possible).

```python
xs = np.linspace(-4, 5, 100)
ys = f(xs)
plt.plot(xs, ys)
plt.axis('off')
plt.axhline(0, color='black', lw=0.5)
plt.axvline(0, color='black', lw=0.5)
plt.show()
```

1.1.1 Method 1: Grid search

```
[ ]: x_vals = [-1.75, -0.75, -0.25, 0.25, 0.75, 1.25, 1.75, 2.25, 2.75, 3.25]
     for x in x_vals:
         print(f'f({x}) = {f(x)}')
```

```
f(-1.75) = 7.8125
f(-0.75) = 4.3125
f(-0.25) = 3.3125
f(0.25) = 2.8125
f(0.75) = 2.8125
f(1.25) = 3.3125
f(1.75) = 4.3125
f(2.25) = 5.8125
f(2.75) = 7.8125
f(3.25) = 10.3125
```

More visual version:

```
[ ]: x_vals = [-1.75, -0.75, -0.25, 0.25, 0.75, 1.25, 1.75, 2.25, 2.75, 3.25]
     for x in x_vals:
         plt.scatter(x, f(x), color='red')
         plt.plot([x, x], [f(x), 0], color='black', lw=0.5, linestyle='--')
     plt.plot(xs, ys)
```

```
plt.axis('off')
plt.axhline(0, color='black', lw=0.5)
plt.axvline(0, color='black', lw=0.5)
plt.show()
```
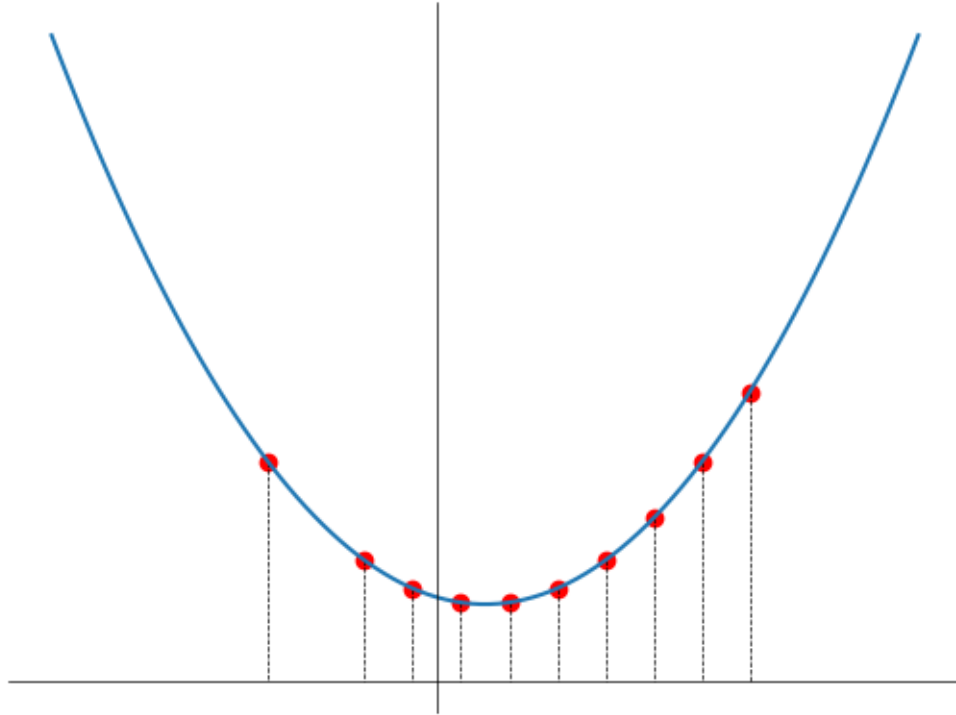

Minimum value of $f(x)$ found is 2.8125 at $x = 0.25$ and $x = 0.75$.

1.1.2 Method 2: Dichotomy

```
a = -5
b = 5
for i in range(6):
    print(f"a: f({a}) = {f(a)} \t b: f({b}) = {f(b)}", end='\t\t')
    if f(a)>f(b):
        a = (a+b)/2
        print(f'set a = {a}')
    else:
        b = (a+b)/2
        print(f'set b = {b}')

x = ((a+b)/2)
print(f"best guess: x = {x}")
```

```
a: f(-5) = 33    b: f(5) = 23            set a = 0.0
```

3

```
a: f(0.0) = 3.0           b: f(5) = 23           set b = 2.5
a: f(0.0) = 3.0           b: f(2.5) = 6.75            set b = 1.25
a: f(0.0) = 3.0           b: f(1.25) = 3.3125         set b = 0.625
a: f(0.0) = 3.0           b: f(0.625) = 2.765625      set a = 0.3125
a: f(0.3125) = 2.78515625     b: f(0.625) = 2.765625        set a = 0.46875
best guess: x = 0.546875
```

More visual version

```python
a = -5
b = 5
plt.plot([a,b], [1, 1], color='green')
plt.scatter([a,b], [1, 1], color='green')
for i in range(6):
    if f(a)>f(b):
        a = (a+b)/2
    else:
        b = (a+b)/2
    plt.plot([a,b], [-i, -i], color='green')
    plt.scatter([a,b], [-i, -i], color='green')
x = ((a+b)/2)
plt.scatter([x], [-6], color='black')
plt.plot(xs, ys)
plt.axis('off')
plt.axhline(0, color='black', lw=0.5)
plt.axvline(0, color='black', lw=0.5)
plt.show()
```
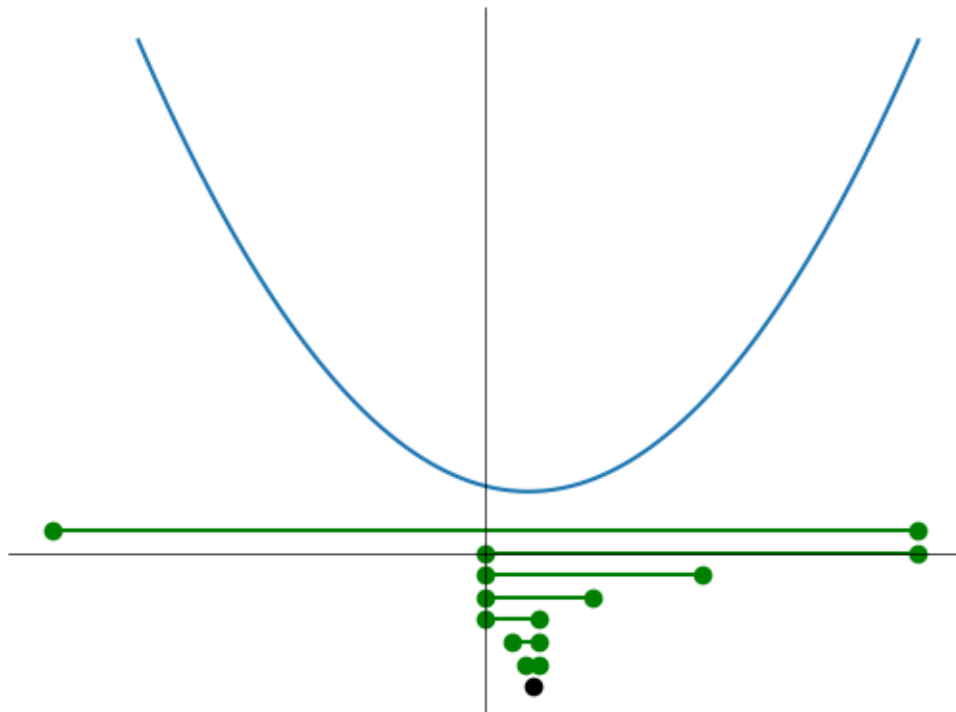
1.1.3 Method 3: Gradient descent

We first calculate the derivative $f'(x) = 2x - 1$

```
[ ]: def df(x):
         return 2*x-1
```

```
[ ]: lr = 0.8
     x = -1
     l = [x]
     for _ in range(7):
         print(f"f({x:.2f}) = {f(x):.2f}  \t f'({x:.2f}) = {df(x):.2f}")
         x = x - lr * df(x)
         l.append(x)
     print(f'Final guess: x = {x:.2f}')

     xs = np.linspace(min(l)-0.5, max(l+[2])+0.5, 100)
     ys = f(xs)
```

```
f(-1.00) = 5.00          f'(-1.00) = -3.00
f(1.40) = 3.56           f'(1.40) = 1.80
f(-0.04) = 3.04          f'(-0.04) = -1.08
f(0.82) = 2.85           f'(0.82) = 0.65
f(0.31) = 2.79           f'(0.31) = -0.39
f(0.62) = 2.76           f'(0.62) = 0.23
f(0.43) = 2.75           f'(0.43) = -0.14
Final guess: x = 0.54
```

Let's try other values for learning rate

```
[ ]: for lr in [0.3, 0.01, 1, 2]:
         print(f'\t learning rate: {lr}')
         x = -1
         l = [x]
         for _ in range(7):
             print(f"f({x:.2f}) = {f(x):.2f}  \t f'({x:.2f}) = {df(x):.2f}")
             x = x - lr * df(x)
             l.append(x)
         print(f'Final guess: x = {x:.2f} \n\n\n')

         xs = np.linspace(min(l)-0.5, max(l+[2])+0.5, 100)
         ys = f(xs)
```

```
         learning rate: 0.3
f(-1.00) = 5.00          f'(-1.00) = -3.00
f(-0.10) = 3.11          f'(-0.10) = -1.20
f(0.26) = 2.81           f'(0.26) = -0.48
```

```
f(0.40) = 2.76              f'(0.40) = -0.19
f(0.46) = 2.75              f'(0.46) = -0.08
f(0.48) = 2.75              f'(0.48) = -0.03
f(0.49) = 2.75              f'(0.49) = -0.01
Final guess: x = 0.50




        learning rate: 0.01
f(-1.00) = 5.00             f'(-1.00) = -3.00
f(-0.97) = 4.91             f'(-0.97) = -2.94
f(-0.94) = 4.83             f'(-0.94) = -2.88
f(-0.91) = 4.74             f'(-0.91) = -2.82
f(-0.88) = 4.66             f'(-0.88) = -2.77
f(-0.86) = 4.59             f'(-0.86) = -2.71
f(-0.83) = 4.52             f'(-0.83) = -2.66
Final guess: x = -0.80




        learning rate: 1
f(-1.00) = 5.00             f'(-1.00) = -3.00
f(2.00) = 5.00              f'(2.00) = 3.00
f(-1.00) = 5.00             f'(-1.00) = -3.00
f(2.00) = 5.00              f'(2.00) = 3.00
f(-1.00) = 5.00             f'(-1.00) = -3.00
f(2.00) = 5.00              f'(2.00) = 3.00
f(-1.00) = 5.00             f'(-1.00) = -3.00
Final guess: x = 2.00




        learning rate: 2
f(-1.00) = 5.00             f'(-1.00) = -3.00
f(5.00) = 23.00             f'(5.00) = 9.00
f(-13.00) = 185.00          f'(-13.00) = -27.00
f(41.00) = 1643.00          f'(41.00) = 81.00
f(-121.00) = 14765.00       f'(-121.00) = -243.00
f(365.00) = 132863.00       f'(365.00) = 729.00
f(-1093.00) = 1195745.00          f'(-1093.00) = -2187.00
Final guess: x = 3281.00
```
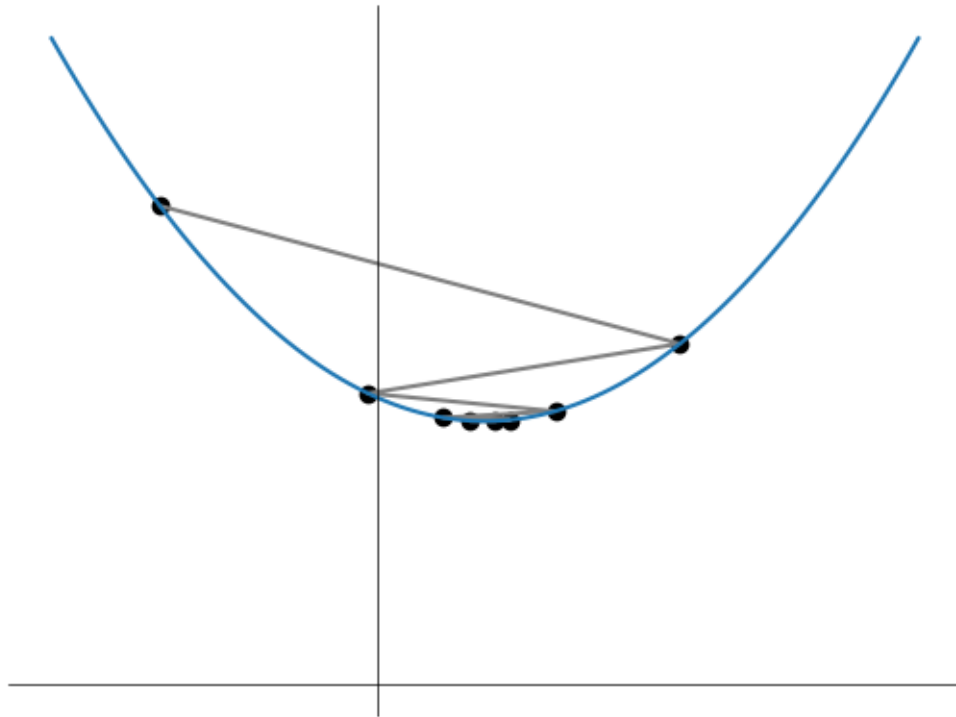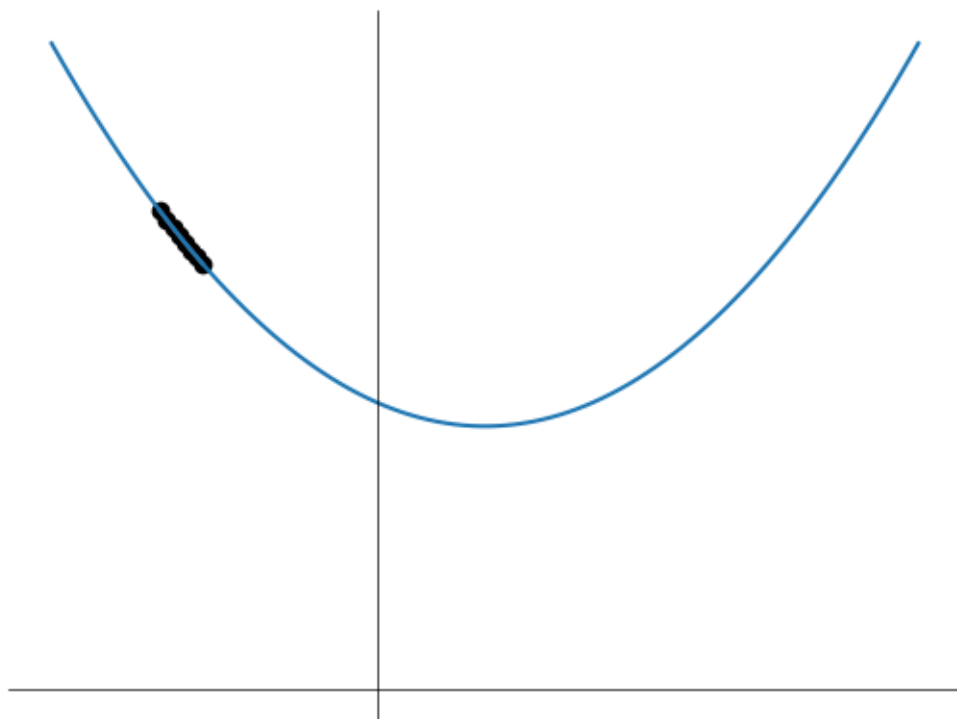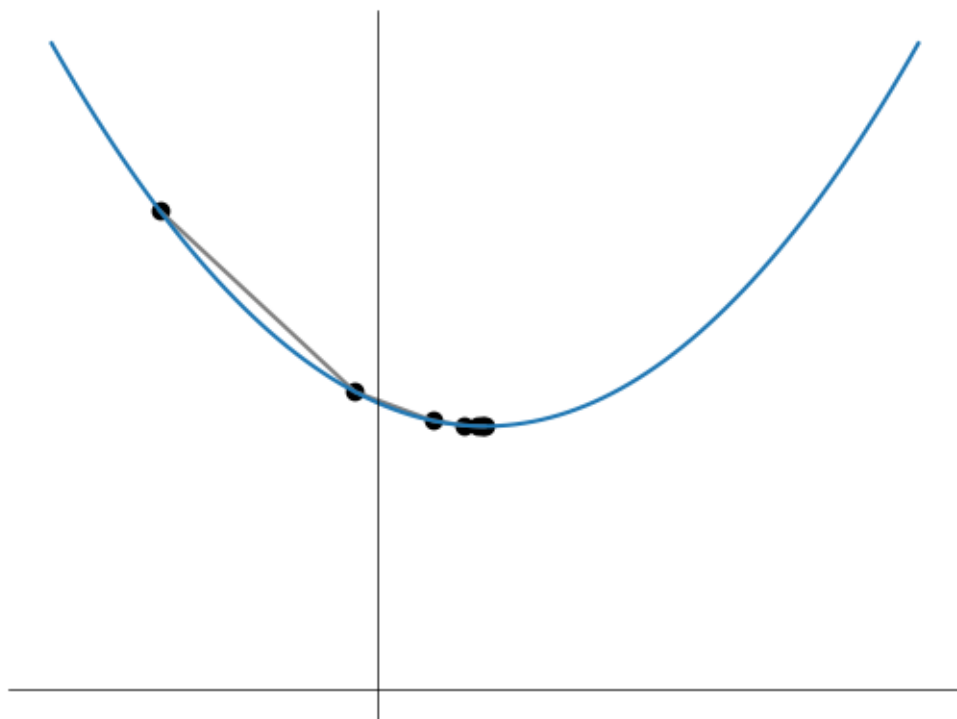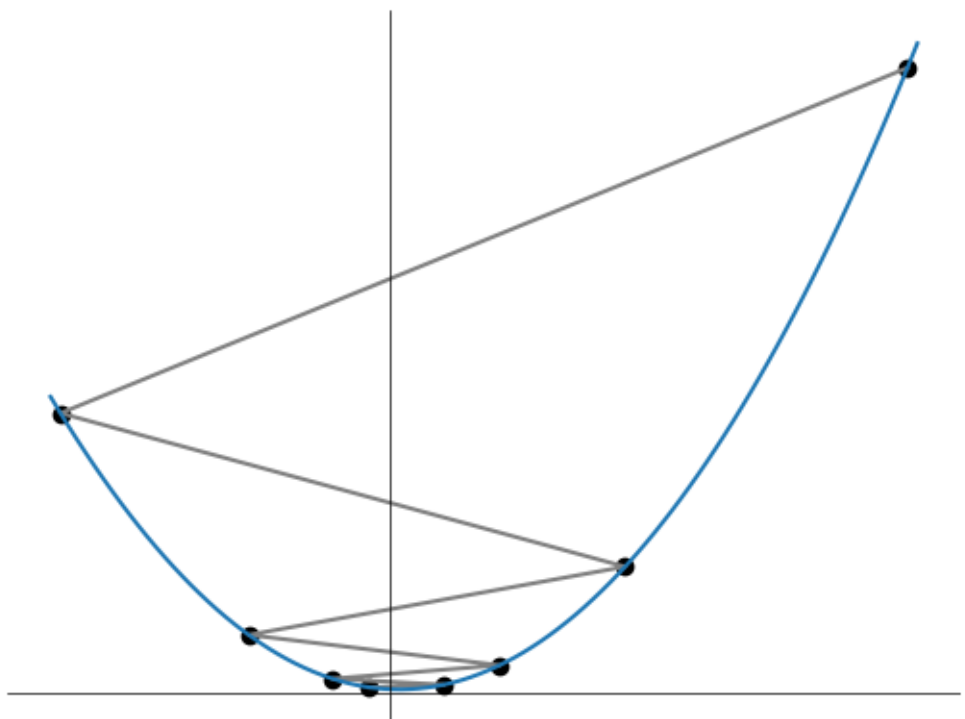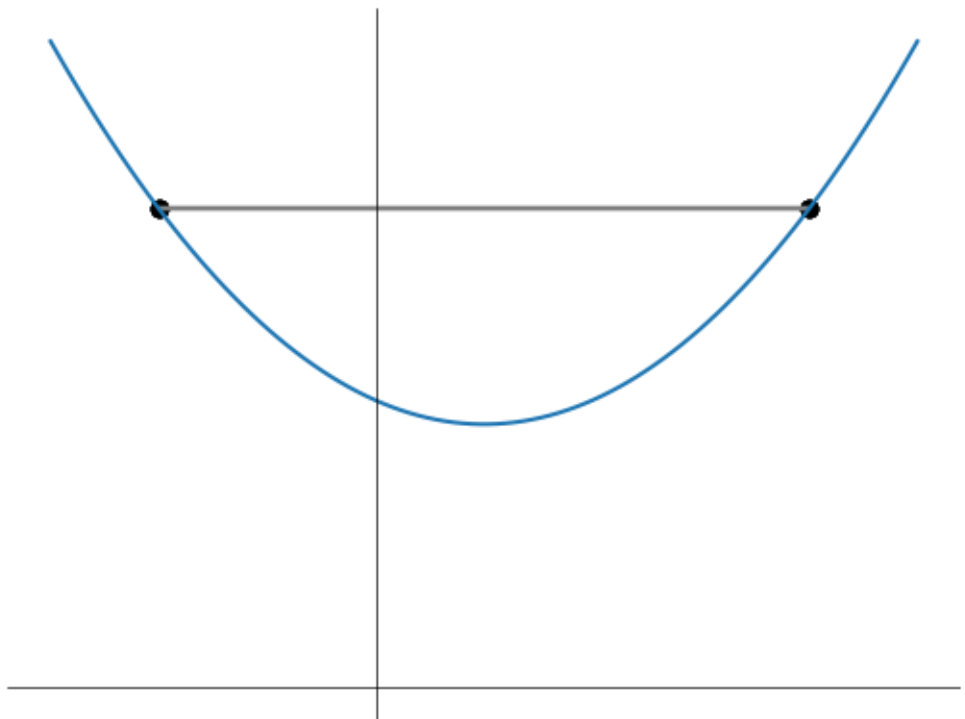
Visually:

```python
for lr in [0.8, 0.3, 0.01, 1, 1.25]:
    x = -1
    l = [x]
    for _ in range(7):
        x = x - lr * df(x)
        l.append(x)

    plt.plot(l, [f(x) for x in l], color='grey')
    plt.scatter(l, [f(x) for x in l], color='black')
    xs = np.linspace(min(l)-0.5, max(l+[2])+0.5, 100)
    ys = f(xs)
    plt.plot(xs, ys)
    plt.axis('off')
    plt.axhline(0, color='black', lw=0.5)
    plt.axvline(0, color='black', lw=0.5)
    plt.show()
```

1.2 Two dimensional function

$f(x, y) = (x + y - 1)^2 + \frac{1}{5}(x - y)^2$

```python
def f(x, y):
    return (x+y-1)**2 + 0.2*(x-y)**2
```

Plotting the function as a 2D surface. Plotting log of the function helps to see the minimum more clearly.

```python
# interactive
x = np.linspace(-1, 2, 100)
y = np.linspace(-1, 2, 100)
X, Y = np.meshgrid(x, y)
Z = f(X, Y)
Zlog = np.log(Z)
go.Figure(data=[go.Surface(z=Z)])
```

```python
# not interactive
x = np.linspace(-1, 2, 100)
y = np.linspace(-1, 2, 100)
X, Y = np.meshgrid(x, y)
Z = f(X, Y)
Zlog = np.log(Z)

# plot a heatmap of the function
plt.figure(figsize=(10,5))
plt.subplot(1,2,1)
plt.imshow(Z, extent=(-1, 2, -1, 2))
plt.colorbar()
plt.title('$f(x,y)$')
plt.xlabel('x')
plt.ylabel('y')
plt.subplot(1,2,2)
plt.imshow(Zlog, extent=(-1, 2, -1, 2))
plt.colorbar()
plt.title('$log(f(x,y))$')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```
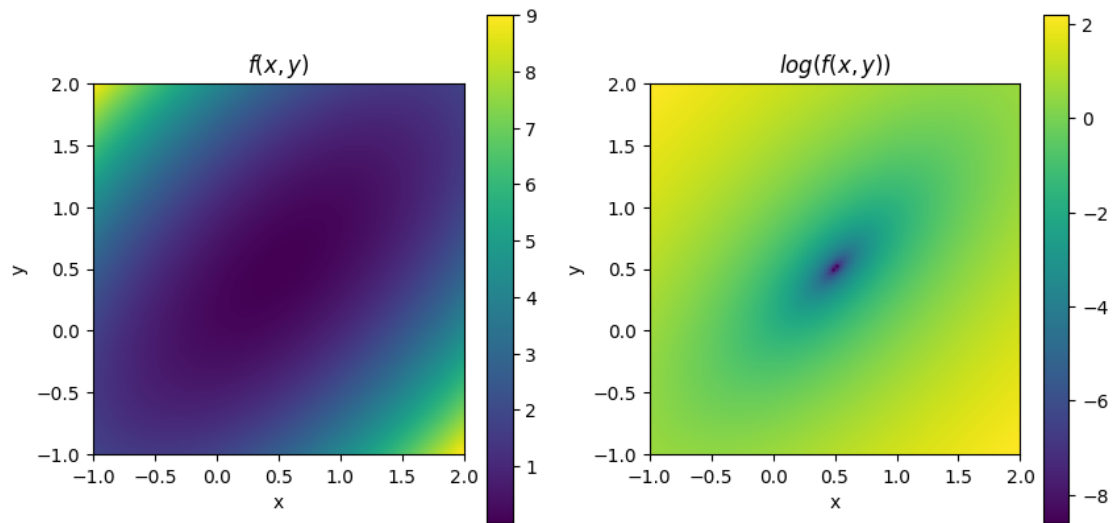
1.2.1 Method 1: Grid search

```
[ ]: for x in np.arange(-1, 2.5, 0.5):
         for y in np.arange(-1, 2.5, 0.5):
             print(f'f({x}, {y}) = {f(x, y)}')
```

```
f(-1.0, -1.0) = 9.0
f(-1.0, -0.5) = 6.3
f(-1.0, 0.0) = 4.2
f(-1.0, 0.5) = 2.7
f(-1.0, 1.0) = 1.8
f(-1.0, 1.5) = 1.5
f(-1.0, 2.0) = 1.8
f(-0.5, -1.0) = 6.3
f(-0.5, -0.5) = 4.0
f(-0.5, 0.0) = 2.3
f(-0.5, 0.5) = 1.2
f(-0.5, 1.0) = 0.7
f(-0.5, 1.5) = 0.8
f(-0.5, 2.0) = 1.5
f(0.0, -1.0) = 4.2
f(0.0, -0.5) = 2.3
f(0.0, 0.0) = 1.0
f(0.0, 0.5) = 0.3
f(0.0, 1.0) = 0.2
f(0.0, 1.5) = 0.7
f(0.0, 2.0) = 1.8
f(0.5, -1.0) = 2.7
f(0.5, -0.5) = 1.2
f(0.5, 0.0) = 0.3
```

```
f(0.5, 0.5) = 0.0
f(0.5, 1.0) = 0.3
f(0.5, 1.5) = 1.2
f(0.5, 2.0) = 2.7
f(1.0, -1.0) = 1.8
f(1.0, -0.5) = 0.7
f(1.0, 0.0) = 0.2
f(1.0, 0.5) = 0.3
f(1.0, 1.0) = 1.0
f(1.0, 1.5) = 2.3
f(1.0, 2.0) = 4.2
f(1.5, -1.0) = 1.5
f(1.5, -0.5) = 0.8
f(1.5, 0.0) = 0.7
f(1.5, 0.5) = 1.2
f(1.5, 1.0) = 2.3
f(1.5, 1.5) = 4.0
f(1.5, 2.0) = 6.3
f(2.0, -1.0) = 1.8
f(2.0, -0.5) = 1.5
f(2.0, 0.0) = 1.8
f(2.0, 0.5) = 2.7
f(2.0, 1.0) = 4.2
f(2.0, 1.5) = 6.3
f(2.0, 2.0) = 9.0
```

Note that it becomes computationally expensive to search for the minimum in a 2D grid. For higher dimensions, this method is not feasible.

More visually:

```python
# plot a heatmap of the function
plt.figure(figsize=(10,5))
plt.subplot(1,2,1)
plt.imshow(Z, extent=(-1, 2, -1, 2))
for x in np.arange(-1, 2.5, 0.5):
    for y in np.arange(-1, 2.5, 0.5):
        plt.scatter(x, y, color='red')
plt.colorbar()
plt.title('$f(x,y)$')
plt.xlabel('x')
plt.ylabel('y')
plt.subplot(1,2,2)
plt.imshow(Zlog, extent=(-1, 2, -1, 2))
for x in np.arange(-1, 2.5, 0.5):
    for y in np.arange(-1, 2.5, 0.5):
        plt.scatter(x, y, color='red')
plt.colorbar()
```

```
plt.title('$log(f(x,y))$')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```
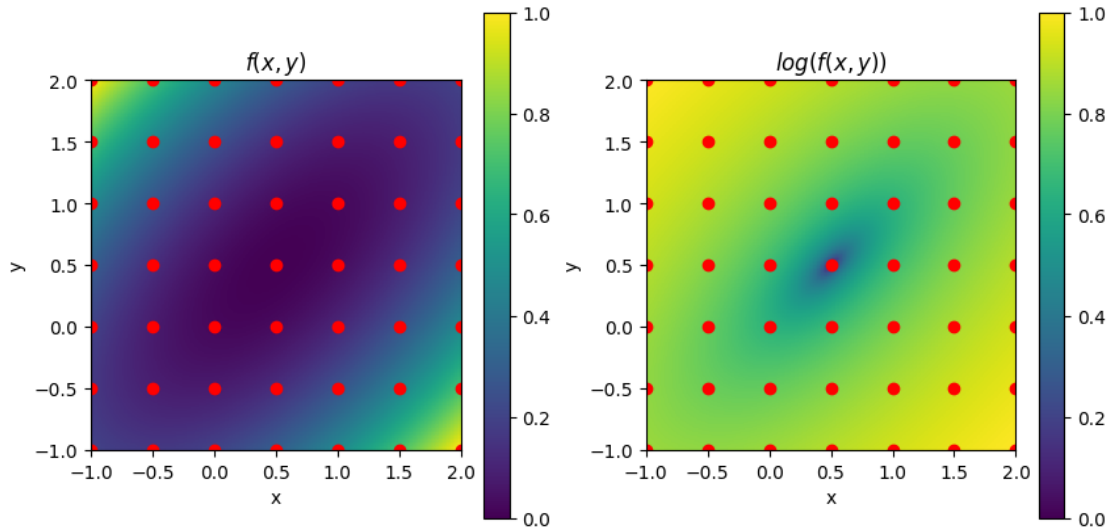

1.2.2   Method 2: Dichotomy

```
[ ]: a, b = -10, 10
c, d = -10, 10
for _ in range(10):
    f1 = f(a, c)
    f2 = f(a, d)
    f3 = f(b, c)
    f4 = f(b, d)
    if f1<=f2 and f1<=f3 and f1<=f4:
        b = (a+b)/2
        d = (c+d)/2
    if f2<=f1 and f2<=f3 and f2<=f4:
        b = (a+b)/2
        c = (c+d)/2
    if f3<=f2 and f3<=f1 and f3<=f4:
        a = (a+b)/2
        d = (c+d)/2
    if f4<=f2 and f4<=f3 and f4<=f1:
        a = (a+b)/2
        c = (c+d)/2
    print(f'f({(a+b)/2:.2f}, {(c+d)/2:.2f}) = {f((a+b)/2, (c+d)/2):.4f} \t {a:.
    ↪2f} < x < {b:.2f} \t {c:.2f} < y < {d:.2f} \t ')
```

```
print(f'Best guess: x = {(a+b)/2:.2f}, y = {(c+d)/2:.2f}')
```

```
f(-2.50, 2.50) = 6.0000          -5.00 < x < 0.00          0.00 < y < 5.00
f(-1.25, 1.25) = 2.2500          -2.50 < x < 0.00          0.00 < y < 2.50
f(-0.62, 0.62) = 1.3125          -1.25 < x < 0.00          0.00 < y < 1.25
f(-0.31, 0.94) = 0.4531          -0.62 < x < 0.00          0.62 < y < 1.25
f(-0.16, 0.78) = 0.3164          -0.31 < x < 0.00          0.62 < y < 0.94
f(-0.08, 0.86) = 0.2236          -0.16 < x < 0.00          0.78 < y < 0.94
f(-0.04, 0.82) = 0.1956          -0.08 < x < 0.00          0.78 < y < 0.86
f(-0.02, 0.84) = 0.1800          -0.04 < x < 0.00          0.82 < y < 0.86
f(-0.01, 0.83) = 0.1734          -0.02 < x < 0.00          0.82 < y < 0.84
f(-0.00, 0.83) = 0.1699          -0.01 < x < 0.00          0.83 < y < 0.84
Best guess: x = -0.00, y = 0.83
```

More visual version

```python
a, b = -5, 5
c, d = -5, 5

fig = plt.figure(figsize=(15,5))
x = np.linspace(a,b, 100)
y = np.linspace(c,d, 100)
X, Y = np.meshgrid(x, y)
Z = f(X, Y)
Zlog = np.log(Z)
plt.subplot(1,3,1)
plt.imshow(Z, extent=(a, b, c, d))
plt.title('$f(x,y)$')
plt.xlabel('x')
plt.ylabel('y')
plt.subplot(1,3,2)
plt.imshow(Zlog, extent=(a, b, c, d))
plt.title('$log(f(x,y))$')
plt.xlabel('x')
plt.ylabel('y')

ax = plt.subplot(1,3,3)
rectangles = []
for _ in range(10):
    rectangle = plt.Rectangle((a, c), b-a, d-c, facecolor='green', alpha=0.1)
    ax.add_patch(rectangle)
    f1 = f(a, c)
    f2 = f(a, d)
    f3 = f(b, c)
    f4 = f(b, d)
    if f1<=f2 and f1<=f3 and f1<=f4:
        b = (a+b)/2
```

```
        d = (c+d)/2
    if f2<=f1 and f2<=f3 and f2<=f4:
        b = (a+b)/2
        c = (c+d)/2
    if f3<=f2 and f3<=f1 and f3<=f4:
        a = (a+b)/2
        d = (c+d)/2
    if f4<=f2 and f4<=f3 and f4<=f1:
        a = (a+b)/2
        c = (c+d)/2
plt.plot((a+b)/2, (c+d)/2, '+', color='black')
plt.axis('equal')
plt.show()
```
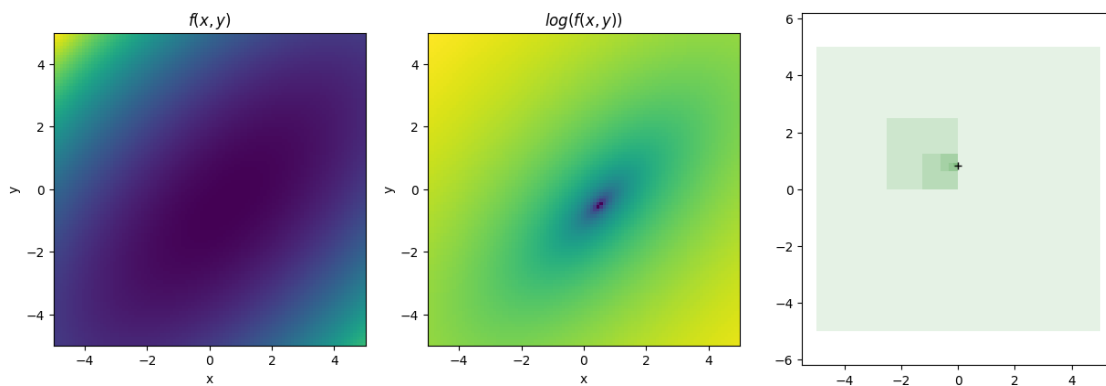

1.2.3   Method 3: Gradient descent

We start by calculating the partial derivatives of the function with respect to x and y.

$\frac{\partial f}{\partial x}(x, y) = 2(x + y - 1) + \frac{2}{5}(x - y)$

$\frac{\partial f}{\partial y}(x, y) = 2(x + y - 1) - \frac{2}{5}(x - y)$

```
[ ]: def dfx(x, y):
         return 2*(x+y-1) + 0.4*(x-y)
     def dfy(x, y):
         return 2*(x+y-1) - 0.4*(x-y)
```

```
[ ]: lr = 0.6
     x = 2.5
     y = 3
     lx = [x]
     ly = [y]
     for _ in range(7):
         x = x - lr * dfx(x,y)
```

```
        y = y - lr * dfy(x,y)
        lx.append(x)
        ly.append(y)
        print(f'f(x,y) = {f(x,y):.2f} \t (x,y) = ({x:.2f}, {y:.2f})')
```

```
f(x,y) = 7.20      (x,y) = (-2.78, 2.55)
f(x,y) = 0.85      (x,y) = (-0.02, 0.10)
f(x,y) = 0.25      (x,y) = (1.11, 0.09)
f(x,y) = 0.04      (x,y) = (0.63, 0.56)
f(x,y) = 0.01      (x,y) = (0.39, 0.58)
f(x,y) = 0.00      (x,y) = (0.47, 0.49)
f(x,y) = 0.00      (x,y) = (0.52, 0.48)
```

```
[ ]: lr = 0.6
     for lr in [0.3, 0.1, 0.01, 1.25]:
         print(f'learning rate: {lr}')
         x = 2.5
         y = 3
         lx = [x]
         ly = [y]
         for _ in range(7):
             x = x - lr * dfx(x,y)
             y = y - lr * dfy(x,y)
             lx.append(x)
             ly.append(y)
             print(f'f(x,y) = {f(x,y):.2f} \t (x,y) = ({x:.2f}, {y:.2f})')
         print('\n\n\n')
```

```
learning rate: 0.3
f(x,y) = 0.68      (x,y) = (-0.14, 1.51)
f(x,y) = 0.32      (x,y) = (-0.16, 1.10)
f(x,y) = 0.16      (x,y) = (0.03, 0.90)
f(x,y) = 0.07      (x,y) = (0.18, 0.77)
f(x,y) = 0.03      (x,y) = (0.28, 0.68)
f(x,y) = 0.01      (x,y) = (0.35, 0.62)
f(x,y) = 0.01      (x,y) = (0.40, 0.58)
```

```
learning rate: 0.1
f(x,y) = 8.14      (x,y) = (1.62, 2.22)
f(x,y) = 3.29      (x,y) = (1.08, 1.72)
f(x,y) = 1.36      (x,y) = (0.74, 1.39)
f(x,y) = 0.58      (x,y) = (0.54, 1.17)
f(x,y) = 0.27      (x,y) = (0.43, 1.02)
f(x,y) = 0.14      (x,y) = (0.36, 0.92)
f(x,y) = 0.08      (x,y) = (0.33, 0.84)
```

```
learning rate: 0.01
f(x,y) = 18.72    (x,y) = (2.41, 2.91)
f(x,y) = 17.27    (x,y) = (2.33, 2.82)
f(x,y) = 15.93    (x,y) = (2.25, 2.74)
f(x,y) = 14.69    (x,y) = (2.17, 2.66)
f(x,y) = 13.55    (x,y) = (2.09, 2.58)
f(x,y) = 12.50    (x,y) = (2.02, 2.51)
f(x,y) = 11.53    (x,y) = (1.95, 2.44)
```

```
learning rate: 1.25
f(x,y) = 112.80              (x,y) = (-8.50, 13.50)
f(x,y) = 324.80             (x,y) = (-7.50, -9.50)
f(x,y) = 1804.80            (x,y) = (36.50, -51.50)
f(x,y) = 5196.80           (x,y) = (32.50, 40.50)
f(x,y) = 28876.80           (x,y) = (-143.50, 208.50)
f(x,y) = 83148.80           (x,y) = (-127.50, -159.50)
f(x,y) = 462028.80          (x,y) = (576.50, -831.50)
```

A more visual version of the gradient descent method

```python
for lr in [0.6, 0.3, 0.1, 0.01, 1.25]:
    x = 2.5
    y = 3
    lx = [x]
    ly = [y]
    for _ in range(7):
        x = x - lr * dfx(x,y)
        y = y - lr * dfy(x,y)
        lx.append(x)
        ly.append(y)

    # plot a heatmap of the function with the line search
    x = np.linspace(-3, 4, 100)
    y = np.linspace(-3, 4, 100)
    X, Y = np.meshgrid(x, y)
    Z = f(X, Y)
    Zlog = np.log(Z)
```
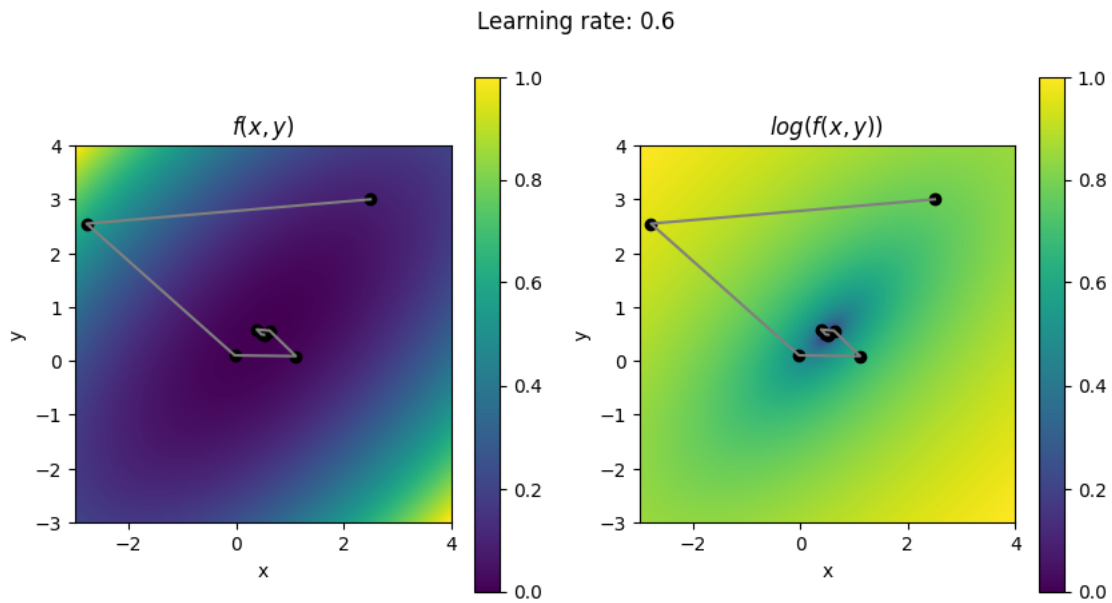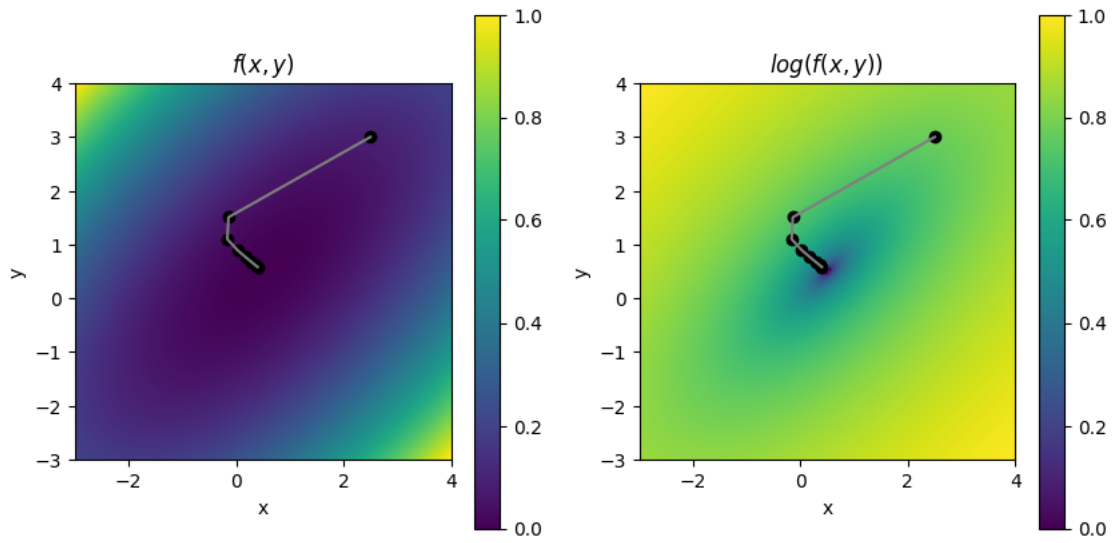
```
plt.figure(figsize=(10,5))
plt.subplot(1,2,1)
plt.imshow(Z, extent=(-3, 4, -3, 4))
plt.plot(lx, ly, color='grey')
plt.scatter(lx, ly, color='black')
plt.colorbar()
plt.title('$f(x,y)$')
plt.xlabel('x')
plt.ylabel('y')
plt.subplot(1,2,2)
plt.imshow(Zlog, extent=(-3, 4, -3, 4))
plt.plot(lx, ly, color='grey')
plt.scatter(lx, ly, color='black')
plt.colorbar()
plt.title('$log(f(x,y))$')
plt.xlabel('x')
plt.ylabel('y')
plt.suptitle(f'Learning rate: {lr}')
plt.show()
```
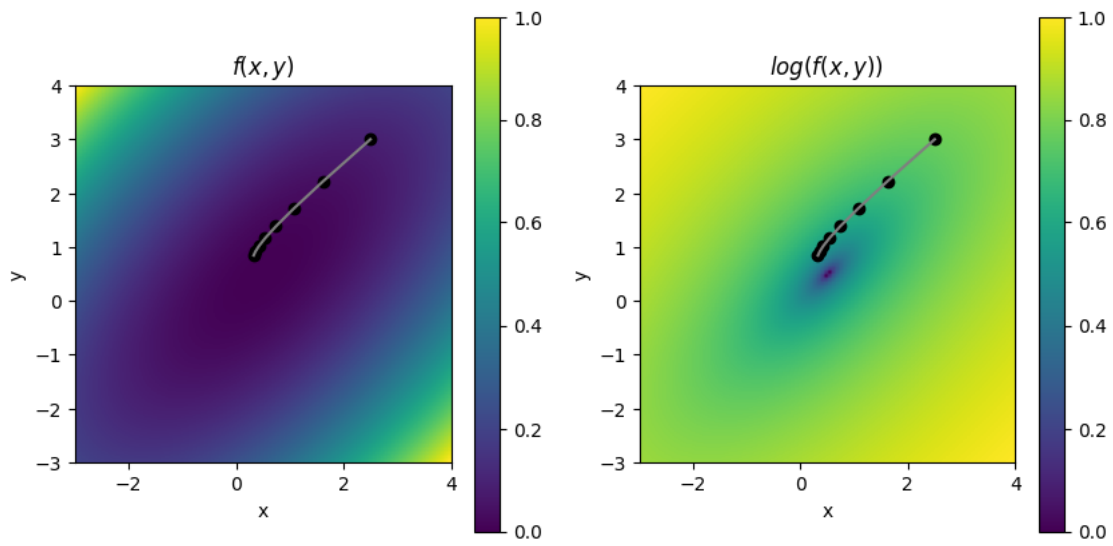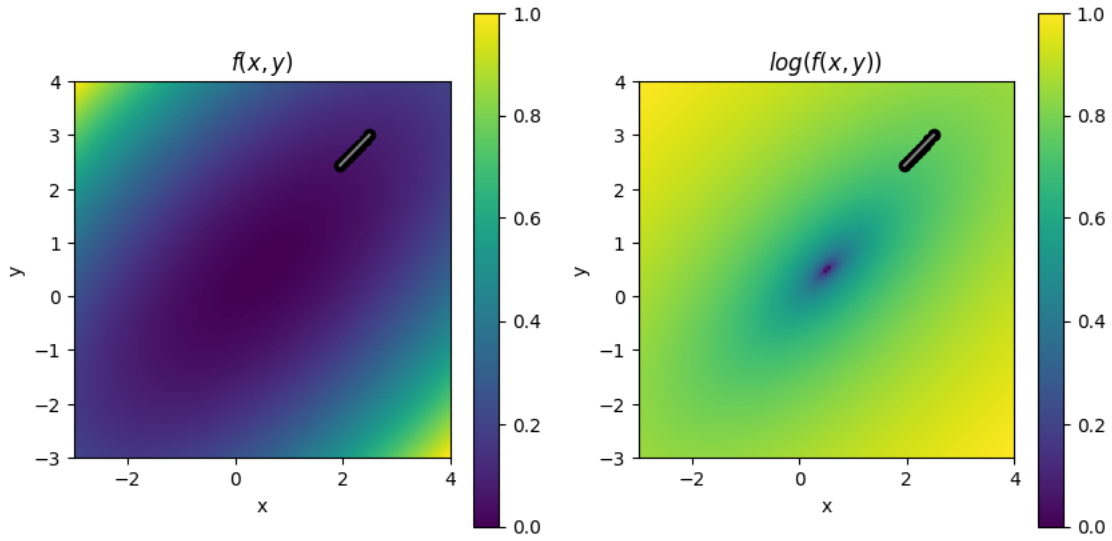
Learning rate: 0.3

$f(x, y)$

$log(f(x, y))$

Learning rate: 0.1

$f(x, y)$

$log(f(x, y))$

Learning rate: 0.01

$f(x, y)$ $log(f(x, y))$

Learning rate: 1.25

$f(x, y)$ $log(f(x, y))$